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ANSWER™ is a General Purpose CFD package based on the Navier-Stokes Equations. It has been used to analyze problems as diverse as low pressure film deposition, cooling of electronic components, automobile fluid dynamics, ventilation of tunnels, HVAC design optimization, analysis of process tanks, design of ramjets and aircraft engines, and missile launch tube simulations, lubrication of bearings, and performance of high Mach number missiles.

PORFLOW™ software tool simulates flow in porous and or fractured media based on Darcy Equation. It has been used to analyze problems as diverse as salinity intrusion into fresh water aquifers and remediation of hazardous waste sites. It has been used to evaluate pumping of an aquifer over a period of days, remediation of waste sites over a period of years, corrosion of waste canisters over tens of years, and transport of contaminants from nuclear waste over a time span of hundreds of thousands of years.

TIDAL™ is based on the Shallow Water Equations and has been used to analyze a wide range of problems including impact of Tsunamis and hurricanes, pollution management of coastal waters, design of marinas, optimization of water treatment outfall locations, transport of oil spills and impact of offshore oil terminals on coastal ecosystem.

ACRi Software Tools have evolved with the user’s needs to provide a flexible format that is bound neither to a specific algorithm, nor to a particular methodology. Rather, these provide a framework that facilitates experimentation. The user can change numerical schemes, solution method, matrix inversion algorithms, or any of the physical or mathematical features. Two features deserve special mention: generality of applications, and ease of use provided by the conversational FREEFORM™ command language. These have enabled ACRi Software Tools to emerge as leading software in their field of application.

ACRi Software Tools are distinguished by the diversity of users. These include commercial, research and educational organizations in over 20 countries. Among our users are AECL (Canada), Aerospatiale (France), Allison Gas Turbine, ANDRA (France), ASCI, S.A. (Spain), BAe-Sema (U.K.), Battelle Pacific Northwest Laboratory, C.N.I.M. (France), Department of Education (Mexico), Fluor Daniel, GERPY (FRANCE), General Electric Company, Idaho National Engineering Laboratory, James M. Montgomery, Lam Research Corporation, Lockheed Martin, Marquardt Company, National Aeronautical and Space Administration, Oak Ridge National Laboratory, Renault (France), Rockwell, Savannah River Laboratory, SCK-CEN (Belgium)SNECMA (France), Southwest Research Institute, University of California, US Air Force, US Army, US Navy, U.S. Department of Energy, U.S. Nuclear Regulatory Commission, U.S. Geological Survey, Watkins-Johnson, Westinghouse Corporation, WS Atkins (UK), and a number of other commercial organizations.

Hundreds of publications and project reports on the applications, benchmarking, and verification of ACRi Software Tools are currently available. ACRi Software Tools has been extensively peer-reviewed and these details are available both on the internet and as well as from our website.

ACRi Software Tools rely on the numerical solution of complex mathematical equations. Some familiarity with the strengths and weaknesses of mathematical and numerical algorithms is highly recommended. Every attempt has been made to provide the necessary information for satisfactory use of ACRi Software Tools in this manual. As is the case for any software of this type, it is not possible to anticipate all questions and users’ requirements. In addition to this manual, we also provide training and support in the use of the software. For additional questions and inquiries, please contact:

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Akshai Runchal
Bel Air, California
ACKNOWLEDGEMENTS

The ACRi Software Tools would not have been possible without the support and active contributions of a number of individuals. As can be expected for any scientific application software designed to meet the evolving needs of its users over an extended period of time, many individuals have contributed to its growth. Users have actively participated in the development process by testing the software and contributing suggestions for its improvement.

The contributions of numerous users of the software from all over the world are gratefully acknowledged. Their faith in the value of this software, suggestions for improvements in the user interface and, critique of the user document have proved invaluable. They contributed to the software in numerous ways and enhanced the value of the software immeasurably.
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<thead>
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<th>MEANING</th>
<th>UNITS</th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>GENERIC</td>
</tr>
<tr>
<td>a</td>
<td>A constant or exponent</td>
<td>various</td>
</tr>
<tr>
<td>a&lt;sub&gt;ir&lt;/sub&gt;</td>
<td>Absorptivity coefficient</td>
<td>L&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>b</td>
<td>A constant or exponent</td>
<td>various</td>
</tr>
<tr>
<td>c</td>
<td>A constant or exponent</td>
<td>various</td>
</tr>
<tr>
<td>c</td>
<td>Speed of sound</td>
<td>L t&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>C&lt;sub&gt;D&lt;/sub&gt;</td>
<td>Drag coefficient</td>
<td>-----</td>
</tr>
<tr>
<td>C&lt;sub&gt;P&lt;/sub&gt;</td>
<td>Specific heat</td>
<td>L&lt;sup&gt;2&lt;/sup&gt; t&lt;sup&gt;2&lt;/sup&gt; T&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>E</td>
<td>Black body radiation energy</td>
<td>M t&lt;sup&gt;3&lt;/sup&gt;</td>
</tr>
<tr>
<td>f</td>
<td>A frequency</td>
<td>t&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>F</td>
<td>General transport variable</td>
<td>various</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational acceleration</td>
<td>L t&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>h</td>
<td>Enthalpy</td>
<td>L&lt;sup&gt;2&lt;/sup&gt; t&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>h&lt;sup&gt;s&lt;/sup&gt;</td>
<td>Enthalpy of formation of a species</td>
<td>L&lt;sup&gt;2&lt;/sup&gt; t&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>h&lt;sub&gt;s&lt;/sub&gt;</td>
<td>Stagnation enthalpy</td>
<td>L&lt;sup&gt;2&lt;/sup&gt; t&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>H&lt;sub&gt;R&lt;/sub&gt;</td>
<td>Heat of reaction</td>
<td>L&lt;sup&gt;2&lt;/sup&gt; t&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>I</td>
<td>Radiation intensity</td>
<td>M t&lt;sup&gt;3&lt;/sup&gt;</td>
</tr>
<tr>
<td>k</td>
<td>Kinetic energy of turbulence</td>
<td>L&lt;sup&gt;2&lt;/sup&gt; t&lt;sup&gt;2&lt;/sup&gt;</td>
</tr>
<tr>
<td>m</td>
<td>Rate of injection of fluid per unit volume</td>
<td>M L&lt;sup&gt;-3&lt;/sup&gt; t&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>m</td>
<td>Mass fraction of a species</td>
<td>-----</td>
</tr>
<tr>
<td>M</td>
<td>Molecular weight</td>
<td>M mol&lt;sup&gt;-1&lt;/sup&gt;</td>
</tr>
<tr>
<td>N</td>
<td>Coordinate normal to a boundary</td>
<td>L</td>
</tr>
<tr>
<td>N&lt;sub&gt;sn&lt;/sub&gt;</td>
<td>Density of soot nuclei</td>
<td>L&lt;sup&gt;3&lt;/sup&gt;</td>
</tr>
<tr>
<td>N&lt;sub&gt;s&lt;/sub&gt;</td>
<td>Concentration of soot particles</td>
<td>M L&lt;sup&gt;-3&lt;/sup&gt;</td>
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<td>P</td>
<td>Thermodynamic pressure</td>
<td>M L&lt;sup&gt;-1&lt;/sup&gt; t&lt;sup&gt;-2&lt;/sup&gt;</td>
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<tr>
<td>P&lt;sub&gt;R&lt;/sub&gt;</td>
<td>Reference value of Thermodynamic pressure</td>
<td>M L&lt;sup&gt;-1&lt;/sup&gt; t&lt;sup&gt;-2&lt;/sup&gt;</td>
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<tr>
<td>P&lt;sub&gt;k&lt;/sub&gt;</td>
<td>Rate of production of turbulent energy</td>
<td>M L&lt;sup&gt;-1&lt;/sup&gt; t&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>r</td>
<td>Radius of curvature</td>
<td>L</td>
</tr>
<tr>
<td>R</td>
<td>Radiation flux</td>
<td>M t&lt;sup&gt;3&lt;/sup&gt;</td>
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<tr>
<td>Symbol</td>
<td>MEANING</td>
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<tr>
<td>--------</td>
<td>---------</td>
<td>-------</td>
</tr>
<tr>
<td>R</td>
<td>Gas constant</td>
<td>L² t² T⁻¹</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
<td>-----</td>
</tr>
<tr>
<td>Rₚ</td>
<td>Universal gas constant</td>
<td>L² t² T⁻¹</td>
</tr>
<tr>
<td>s</td>
<td>Reaction or decay rate of a property</td>
<td>M L⁻³ t⁻¹</td>
</tr>
<tr>
<td>sₚ</td>
<td>Scattering coefficient</td>
<td>L⁻¹</td>
</tr>
<tr>
<td>S</td>
<td>Source of a fluid property</td>
<td>various</td>
</tr>
<tr>
<td>t</td>
<td>Time</td>
<td>t</td>
</tr>
<tr>
<td>T</td>
<td>Thermodynamic Temperature</td>
<td>T</td>
</tr>
<tr>
<td>Tₛ</td>
<td>Convert temperature to absolute units</td>
<td>T</td>
</tr>
<tr>
<td>Tₖ</td>
<td>Critical temperature of the fluid</td>
<td>T</td>
</tr>
<tr>
<td>uu</td>
<td>Autocorrelation of U</td>
<td>L² t²</td>
</tr>
<tr>
<td>U</td>
<td>Fluid velocity in x-direction</td>
<td>L t⁻¹</td>
</tr>
<tr>
<td>vv</td>
<td>Autocorrelation of V</td>
<td>L² t²</td>
</tr>
<tr>
<td>V</td>
<td>Fluid velocity in y-direction</td>
<td>L t⁻¹</td>
</tr>
<tr>
<td>Vᵢ</td>
<td>Velocity in iᵗʰ direction</td>
<td>L t⁻¹</td>
</tr>
<tr>
<td>ww</td>
<td>Autocorrelation of W</td>
<td>L² t²</td>
</tr>
<tr>
<td>W</td>
<td>Fluid velocity in z-direction</td>
<td>L t⁻¹</td>
</tr>
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<td>x-coordinate</td>
<td>L</td>
</tr>
<tr>
<td>y</td>
<td>y-coordinate</td>
<td>L</td>
</tr>
<tr>
<td>z</td>
<td>z-coordinate</td>
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## GREEK SYMBOLS

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<tr>
<td></td>
<td></td>
<td>GENERIC</td>
</tr>
<tr>
<td>α</td>
<td>A coefficient</td>
<td>various</td>
</tr>
<tr>
<td>β</td>
<td>A coefficient</td>
<td>various</td>
</tr>
<tr>
<td>γ</td>
<td>Ratio of specific heats</td>
<td>-----</td>
</tr>
<tr>
<td>Γ</td>
<td>Diffusion coefficient</td>
<td>M L⁻¹ t⁻¹</td>
</tr>
<tr>
<td>ε</td>
<td>Rate of dissipation of turbulence energy</td>
<td>L² t⁻³</td>
</tr>
<tr>
<td>ε</td>
<td>A small quantity</td>
<td>-----</td>
</tr>
<tr>
<td>θ</td>
<td>Angular coordinate</td>
<td>radian</td>
</tr>
<tr>
<td>κ</td>
<td>Von Karman Constant</td>
<td>-----</td>
</tr>
<tr>
<td>λ</td>
<td>Decay rate constant</td>
<td>t⁻¹</td>
</tr>
<tr>
<td>μ</td>
<td>Fluid viscosity</td>
<td>M L⁻¹ t⁻¹</td>
</tr>
<tr>
<td>ρ</td>
<td>Fluid density</td>
<td>M L⁻³</td>
</tr>
<tr>
<td>σ</td>
<td>Prandtl or Schmidt number</td>
<td>-----</td>
</tr>
<tr>
<td>σ</td>
<td>Stefan-Boltzman constant</td>
<td>M t⁻³ T⁻⁴</td>
</tr>
<tr>
<td>τ</td>
<td>Shear stress</td>
<td>M L⁻¹ t⁻²</td>
</tr>
<tr>
<td>Φ</td>
<td>Density-related variable</td>
<td>M L⁻³</td>
</tr>
<tr>
<td>Φₑ</td>
<td>Equivalence ratio</td>
<td>-----</td>
</tr>
<tr>
<td>χ</td>
<td>Fuel fraction in fine or ambient scale of flow</td>
<td>-----</td>
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### SUBSCRIPTS

<table>
<thead>
<tr>
<th>SYMBOL</th>
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<tbody>
<tr>
<td>e</td>
<td>Effective value of a fluid property</td>
</tr>
<tr>
<td>Φ</td>
<td>Fluid property F</td>
</tr>
<tr>
<td>i</td>
<td>The i\textsuperscript{th} coordinate direction or i\textsuperscript{th} phase</td>
</tr>
<tr>
<td>inj</td>
<td>Injected fluid</td>
</tr>
<tr>
<td>j</td>
<td>The j\textsuperscript{th} coordinate direction or j\textsuperscript{th} phase</td>
</tr>
<tr>
<td>k</td>
<td>The k\textsuperscript{th} coordinate direction or k\textsuperscript{th} phase</td>
</tr>
<tr>
<td>t</td>
<td>Turbulent state of fluid</td>
</tr>
<tr>
<td>t</td>
<td>The time coordinate</td>
</tr>
<tr>
<td>w</td>
<td>The wall</td>
</tr>
<tr>
<td>x</td>
<td>The x direction</td>
</tr>
<tr>
<td>y</td>
<td>The y or r direction</td>
</tr>
<tr>
<td>z</td>
<td>The z or θ direction</td>
</tr>
</tbody>
</table>

### SUPERSCRIPTS

<table>
<thead>
<tr>
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<th>PERTAINING TO</th>
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<tbody>
<tr>
<td>Φ</td>
<td>Pertaining to property Φ</td>
</tr>
<tr>
<td>j</td>
<td>Pertaining to the j\textsuperscript{th} coordinate direction or j\textsuperscript{th} phase</td>
</tr>
<tr>
<td>t</td>
<td>Pertaining to the time coordinate</td>
</tr>
<tr>
<td>*</td>
<td>Approximate or reference value of a variable</td>
</tr>
<tr>
<td>'</td>
<td>Variation in the value of a variable</td>
</tr>
<tr>
<td>n</td>
<td>Pertaining to the n\textsuperscript{th} fluid or the n\textsuperscript{th} chemical species</td>
</tr>
<tr>
<td>k</td>
<td>Pertaining to the k\textsuperscript{th} time step</td>
</tr>
</tbody>
</table>
ACRi FREEFORM™ command language, developed by Analytic & Computational Research, Inc. (ACRi), provides a simple and easy to use user interface for complex software packages through a set of conversational, English-like commands. These commands are free of any requirements of format or hierarchy except those naturally arising from the nature of the input. These provide for interactive input or emulate the interactive input in batch mode. Since the input commands are in conversational English-like language, FREEFORM™ provides a very powerful tool to perform Quality Assurance (QA) and ensure that the input correctly reflects the intended problem specification.

All ACRi Software Tools including ANSWER™ PORFLOW™ and TIDAL™ employ the FREEFORM™ command language. In addition the CFDStudio™ provides a flexible, simple to use, versatile pre-and post processor Graphical User Interface (GUI). The CFDStudio™ allows the user to build grids painlessly and display the computed results in a variety of graphical images. The software is written in a mix of FORTRAN, C, C++, JAVA and HTML languages and is essentially independent of any specific platform.
1.1 FREEFORM™ INPUT RECORDS

The FREEFORM™ Input is specified through three types of records: KEYWORD, CONTINUATION and COMMENT records. These are described below.

1.1.1 Keyword Record

**Function**

To specify the numeric and character data.

**Structure**

- A keyword record must begin with a keyword.
- Only one keyword per record is allowed.
- Modifiers and numerical fields may follow the keyword.
- Comment, separator, or terminator fields must separate all the keyword, the modifiers and the numerical fields from each other.
- Any character or numeric data on a keyword record after the first occurrence of a terminator are ignored.

1.1.2 Continuation Record

**Function**

To continue numeric and character input started by a previous keyword record.

**Structure**

- A continuation record must begin with either a separator or a numeric character as the first character of the record. It must not begin with an alphabetic ('A' through 'Z' or 'a' through 'z') character as the first character of a record.
- A continuation record may only occur after a keyword record for that group.
- A continuation record must consist only of a combination of modifiers and numerical fields separated from each other by separators.
- Any character or numeric data on a continuation record after the first occurrence of a terminator is ignored.
- Any number of continuation records may follow a keyword record.

1.1.3 Comment Record

**Function**

To enhance the clarity and readability of the input.

**Structure**

- A comment record must begin with a back-slash (/), asterisk (*), dollar ($) or exclamation (!) character in the first column of a record. Any combination of characters may follow the first character.
- A comment record is not processed. No numerical or character data are extracted; the record is merely written to the output file.
- A comment record cannot be extended by a continuation record.
- A comment record can be inserted anywhere in the input.
1.2 ELEMENTS OF INPUT RECORD

One or more of the following seven basic components comprise an input record: KEYWORD, MODIFIER, NUMERIC, SEPARATOR, TERMINATOR, COMMENT and PROMPT fields. These are described below.

1.2.1 Keyword

Function The keyword identifies the input group.

Structure

- The keyword may consist of any characters except separator (Section 1.2.4) or terminator (Section 1.2.5) characters. However, the first character of a keyword must be alphabetic ('A' through 'Z' or 'a' through 'z'). To this extent, the concept of a keyword is similar to that of a variable name in FORTRAN.

- The keyword may be in upper or lower case.

- A keyword must begin in the first column of a record unless a command with INDENT keyword occurred before the current keyword. In this case, leading blanks may precede the keyword. The INDENT option is deactivated if a command with INDENT OFF is encountered.

- The keyword is terminated with the first occurrence of a valid separator or terminator character.

- The keyword may consist of 1 to 256 characters. In general, if there are more than four characters, only the first four are considered meaningful and machine-identifiable. However specific exemptions may exist where more than 4 characters are meaningful and these are identified as needed.

EXAMPLES

ABCD, A123, A&B+, A&B. are all valid examples of a keyword. The keyword specifications of ABCD, abcd, ABCDEFGH, AbCd123, ABCDxxxxxxx (where x stands for any character) are all equivalent because only the first four characters are significant and the input is case-insensitive.

1ABC, 567, (abc, 'abc, .abc are all invalid keywords since the 1st character in all of these is not alphabetic.

Note that a specification of ABC) or ABC’, ABC$, although valid, is equivalent to that of ABC because the last character in all of these examples is either a separator (Section 1.2.4) or a terminator (Section 1.2.5).
1.2.2 Modifier

Any character information on an input record following a keyword, except that embedded in a numeric or comment field (see Sections 1.2.3 and 1.2.6), is treated as modifier(s).

Function To specify character data that helps in interpretation of the rest of the input data

Structure

♦ A modifier in any input group, if present, must follow the keyword.

♦ The modifier is identical to the keyword in its structure. It may consist of any characters, except separator and terminator characters, of which the first character must be alphabetic.

♦ A modifier must not start in the first column of a record. It can be from 1 to 32 characters in length; in general, if there are more than four characters, only the first four are considered meaningful and machine-identifiable. However, specific exemptions may exist where more than 4 characters are meaningful and these are identified as needed.

♦ The modifier must be separated from the keyword, other modifiers and numeric data by a valid separator, terminator or comment field.

EXAMPLES

The structure of a modifier is identical to that of a keyword except that it must not start in the first column of a record. Examples are given in Section 1.2.1
1.2.3 Numeric Field

Any numeric characters on a keyword or continuation record following a keyword, except those embedded in a keyword, modifier or comment field (see Sections 1.2.1, 1.2.2 and 1.2.6), are treated as numeric data.

Function

A numeric field contains numeric data for input variables.

Structure

- A numeric field is a continuous string of characters that must begin with the numeric character set. In this context, the numeric character set consists of the numerals (0-9), the decimal point (.), and the plus (+) and minus (-) operators.
- A numeric field must consist only of the numeric character set defined above, the asterisk (*), and the exponent in lower (e, d) or upper (E, D) case. It must not contain any other character.
- The plus (+) or minus (-) sign, if present, must immediately precede the numerical value without any intervening blank or other characters.
- The asterisk (*) or the exponent (E, D, e or d), if present, must be embedded; the numeric field must not begin or end with one of these characters.
- A numeric field must be separated from the keyword, modifiers and other numeric fields by a valid separator, terminator or comment field.
- Numeric field may be located anywhere on a keyword or continuation record.
- The numeric values may be specified in any of the following formats:
  - Integer, (e.g., 999),
  - Real (e.g., 999.0, 999.),
  - Exponent (e.g., 9.99E2, 1.2349E1, 9.99D+01 or 1.2345d-01)
- Successive, repetitive, identical numeric values may be specified by the asterisk (*) option. Thus, (30., 30., 30.) may be represented as (3*30. or 3*3.0E+1); embedded separators or non-numeric characters must not appear in such specification.

Examples

The input character strings, 1, 0.1234, .567, +123., -1.0005, 1.2e00, 1.35E0, and 3*1.2 are all valid examples of a numerical field. Input specifications of 123, 123., 1.23e02, +0.123E+3, 1.23D2, 1*123, 1*1.23E02 are all equivalent.

The strings 1ABC, 11X11, 1+2, 11.., 1+1.E1 are all invalid numeric specifications. In the first three, non-numeric characters follow a leading numeric character, and in the last three, a valid numeric character occurs in an invalid, embedded location.

Note that a specification of 1.2)2. or 1.2=2, although valid, will be equivalent to a specification of two numeric fields, 1.2 and 2 because of the embedded separator (Section 1.2.4) in both cases. A specification of 1.2$2 is equivalent to a specification of 1.2 because the 2 following the $ will be ignored (Section 1.2.5).
1.2.4 Separator Field

Function
To separate the keyword, the modifiers and the numeric fields of an input record.

Structure
- Any string of characters on an input record, which consists only of the characters from the separator character set, is treated as a separator field. The set of separator characters may vary from one installation to another. The common recognized separator characters for all ACRi™ Software are:

Table 1.2.4.1: Valid Separator Characters In FREEFORM™ Language

<table>
<thead>
<tr>
<th>Number</th>
<th>Character</th>
<th>Description</th>
<th>ASCII Sequence #</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>'</td>
<td>Space or Blank</td>
<td>32</td>
</tr>
<tr>
<td>2</td>
<td>(</td>
<td>Left parenthesis</td>
<td>40</td>
</tr>
<tr>
<td>3</td>
<td>)</td>
<td>Right parenthesis</td>
<td>41</td>
</tr>
<tr>
<td>4</td>
<td>,</td>
<td>Comma</td>
<td>44</td>
</tr>
<tr>
<td>5</td>
<td>:</td>
<td>Colon</td>
<td>58</td>
</tr>
<tr>
<td>6</td>
<td>;</td>
<td>Semicolon</td>
<td>59</td>
</tr>
<tr>
<td>7</td>
<td>=</td>
<td>Equal sign</td>
<td>61</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
<td>Vertical Line</td>
</tr>
<tr>
<td>9</td>
<td>Tab</td>
<td>Horizontal Tab Character</td>
<td>9</td>
</tr>
</tbody>
</table>

EXAMPLES
The sequence of characters ';;:: ');, ======. =', and : are all valid separator fields. However, (a) or (1) are not valid separator fields. In the first case, the character "a" will be processed by FREEFORM™ as a modifier; in the second, the character "1" will be processed as a numeric field.
1.2.5  Terminator Character

Function  To terminate all input on a keyword or continuation record and to provide a vehicle for the user to insert comments on these records.

Structure

♦ The dollar ($) and exclamation mark (!) characters are the only valid terminators.
♦ The terminator terminates the input for the keyword or continuation record on which it occurs; input associated with that particular keyword may continue on a continuation record which follows.
♦ The terminator may appear anywhere in a record.
♦ Any characters following the terminator on that input record are not processed but are treated as user comments and are merely written to the output file.

EXAMPLES

The character sequences:

```
XYZ $comments now
! any comments here
123.456 l789.123
```

are all examples of sequences with embedded terminators. In the first sequence, XYZ will be treated as valid character data (either keyword or modifier, depending on its starting position on the input record) whereas the characters following $ will be ignored. In the second example, the complete sequence will be treated as comments. In the third example, the numerical field 789.123 will be ignored, whereas 123.456 will be treated as numeric data.
1.2.6 Comment Field

Function

To provide a vehicle for the user to insert comments in input to enhance the clarity and readability of the input.

Structure

- A comment field may be in the form of an embedded comment or a comment record.
- An embedded comment field is one which occurs on a keyword or continuation record. It must begin with a terminator ($ or !) character. Any combination of characters may follow the terminator. The comment field is terminated at the end of the 256th character in that record (Section 1.2.5).
- A comment field on a comment record may consist of any combination of characters. In this case, the comment field begins with the back slash (/), asterisk (*), or a terminator ($ or !) character as the first character and terminates with the 256th character.

EXAMPLES

In the input record:

```
ARRAY = 1., 2., 3., 4., 5.                      $ EXAMPLE 1
```

the character string "$ EXAMPLE 1" is an example of the embedded comment on a keyword record. Input processing stops with the $ character; all characters on that record following, and including, the $ character are ignored.

As examples of comment records, the character strings:

```
/ARRAY = 1., 2., 3., 4., 5.                      $ EXAMPLE 1
* ARRAY = 1., 2., 3., 4., 5.                     - another EXAMPLE
!****/// AR RAY = 1., 2., 3., 4., 5.           $ another example
```

will all be treated as comment records and no processing will be done because one of the comment record identifier characters appears as the first character of the input record.
1.2.7  Prompt Character

Function  To allow for interactive or runtime input of a partial or entire input record.

Structure

- The user may insert a '?' in place of either an entire input record or numerical or character string in the input itself. The command interpreter will pause and prompt the user for input at this stage.
- The input obtained by the prompt may be comprised of one or more of the elements of an input record described in Sections 1.2.1 through 1.2.6.
- Any input specified by the prompt is inserted in the input command string starting with the location of the question mark symbol.
- All input in the original command string following the prompt in that record will be disregarded.
- The input for the prompt may consist of 1 to 256 characters depending on where the question mark symbol is located. The prompt will pause and display a message telling the user the maximum number of characters allowed.
- It is possible to avoid the message, referred to above, from being displayed by placing two question mark symbols in succession (eg. '??'). The command interpreter will still pause and wait for input, however it will not display a message.

EXAMPLES

In the input record:

    SOLVe ?  ! Prompt user for input

the character string '?' has the effect of pausing the command interpreter during run-time and displaying a message that asks the user for up to 74 characters of input, since the '?' appears in the 7th location of the input record. The comment '! Prompt user for input' will be overwritten by the input provided by the user at run-time or will be replaced by blank characters if the user input is less than 74 characters long.

Alternatively the user may choose to write:

    SOLVe ??  ! Prompt user for input without a message

This input record has the same effect as above except no message is displayed.
(This page left intentionally blank.)
ACRi™ Software Tools consist of flexible and user-oriented software packages. The software employs CFDStudio™ GUI for user interface. This GUI provides a very powerful, convenient and versatile pre- and post-processor. Underlying the user interface is the FREEFORM™ command language to provide an adaptable, simple to use and format-free commands to communicate with the software. The structure and syntax of the command language are fully described in Chapter 1. The FREEFORM™ command language is a "keyword"-oriented language. A complete discussion of the input and output options, and the keyword commands is given in chapter 7. The user controls the input and much of the operation of the program. Hence, the solution process can be modified during progression of the calculations by convenient user-specified options. The output is largely controlled by the user, both in terms of its extent and its frequency. This chapter provides an introduction to the important input and output features of ACRi™ Software Tools.
2.1 OVERVIEW OF KEYWORD COMMAND LANGUAGE

The user input is divided into several groups. Each group is identified by a "keyword" command and may consist of one or more input records. Each input record must be no more than 256 characters long. Each input-record group, in addition to the keyword that identifies the group, may contain "numeric data", "modifiers" and "comments". Separator, terminator or comment fields must separate the keyword, numeric data and modifiers from each other. Comments may be embedded within input records to enhance the clarity and readability of the input. A detailed description of the FREEFORM™ command language is given in Chapter 1.

The commands that constitute the I/O interface are listed in Table 2.1.1. These commands, and the modifiers and numeric data that are associated with them, are described in alphabetical order in Chapter 3. Except for the geometry and grid of a problem, all other commands may be used repeatedly to accommodate problem requirements that change with time.
## TABLE 6.1.1: KEYWORDS OF ACRI™ SOFTWARE TOOLS AND THEIR FUNCTIONS

<table>
<thead>
<tr>
<th>NO.</th>
<th>KEYWORD</th>
<th>INPUT FUNCTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ACRI</td>
<td>Select the ACRI Software Tool for Simulations</td>
</tr>
<tr>
<td>2</td>
<td>ADAPTIVE</td>
<td>Refine the specified grid by to Adapt to the computational solution</td>
</tr>
<tr>
<td>3</td>
<td>ADIABATIC</td>
<td>Specify adiabatic external walls</td>
</tr>
<tr>
<td>4</td>
<td>ALLOCATE</td>
<td>Allocate table space for storage of user input</td>
</tr>
<tr>
<td>5</td>
<td>ARRHENIUS</td>
<td>Specify the Arrhenius reaction rate constants</td>
</tr>
<tr>
<td>6</td>
<td>BANNER</td>
<td>Print user &amp; program identification to output file</td>
</tr>
<tr>
<td>7</td>
<td>BLOCKAGE</td>
<td>Specify blockage or solid objects in flow field</td>
</tr>
<tr>
<td>8</td>
<td>BOUNDARY</td>
<td>Override built-in boundary conditions</td>
</tr>
<tr>
<td>9</td>
<td>BRINK</td>
<td>Include Brinkman-Forchheimer terms in governing equations</td>
</tr>
<tr>
<td>10</td>
<td>CAPILLARY</td>
<td>Effect of temperature and chemical species on capillary pressure</td>
</tr>
<tr>
<td>11</td>
<td>CLOSE</td>
<td>Close specified output device immediately</td>
</tr>
<tr>
<td>12</td>
<td>COMPRESSIBLE</td>
<td>Select compressible flow option</td>
</tr>
<tr>
<td>13</td>
<td>CONDUCTIVITY</td>
<td>Specify conduction or diffusion constants, coefficients and options</td>
</tr>
<tr>
<td>14</td>
<td>CONNECTIVITY</td>
<td>To specify element and vertex connectivity for unstructured grid</td>
</tr>
<tr>
<td>15</td>
<td>CONVERGENCE</td>
<td>Specify convergence criterion</td>
</tr>
<tr>
<td>16</td>
<td>COORDINATE</td>
<td>Specify grid coordinates</td>
</tr>
<tr>
<td>17</td>
<td>CORIOLIS</td>
<td>Specify Coriolis force constant</td>
</tr>
<tr>
<td>18</td>
<td>CORRELATION</td>
<td>Computation of correlations between variables and locations</td>
</tr>
<tr>
<td>19</td>
<td>CPU</td>
<td>Specify number of Central Processing Units for parallel processing</td>
</tr>
<tr>
<td>20</td>
<td>DATUM</td>
<td>Specify reference datum level for hydraulic head</td>
</tr>
<tr>
<td>21</td>
<td>DEBUG</td>
<td>Specify debug options</td>
</tr>
<tr>
<td>22</td>
<td>DECY</td>
<td>Specify decay constants for chemical species</td>
</tr>
<tr>
<td>23</td>
<td>DEFINE</td>
<td>Specify value of a symbolic variable</td>
</tr>
<tr>
<td>24</td>
<td>DENSITY</td>
<td>Select fluid mass density options</td>
</tr>
<tr>
<td>25</td>
<td>DIAGNOSTIC</td>
<td>Diagnostic output options</td>
</tr>
<tr>
<td>26</td>
<td>DIFFUSION</td>
<td>Specify conduction or diffusion constants, coefficients and options</td>
</tr>
<tr>
<td>27</td>
<td>DISABLE</td>
<td>Disable certain built-in default options</td>
</tr>
<tr>
<td>28</td>
<td>DISTRIBUTION</td>
<td>Specify distribution coefficient and options</td>
</tr>
<tr>
<td>29</td>
<td>EBU</td>
<td>Select Eddy-break-up limiting options for chemical reactions</td>
</tr>
<tr>
<td>30</td>
<td>ELSE</td>
<td>Define the “ELSE” part of the IF-ELSE-ENDIF construct</td>
</tr>
<tr>
<td>31</td>
<td>END</td>
<td>End of a problem</td>
</tr>
<tr>
<td>32</td>
<td>ENDIF</td>
<td>Terminate the IF-ELSE-ENDIF construct</td>
</tr>
<tr>
<td>33</td>
<td>FILE</td>
<td>Open or close selected I/O device</td>
</tr>
<tr>
<td>34</td>
<td>FIX</td>
<td>Fixed pressure, temperature or concentration nodes</td>
</tr>
<tr>
<td>35</td>
<td>FLOW</td>
<td>Specify mass flux entering at boundary</td>
</tr>
<tr>
<td>36</td>
<td>FLUID</td>
<td>Specify thermal and transport properties of the fluid</td>
</tr>
<tr>
<td>37</td>
<td>FLUX</td>
<td>Compute flux of fluid, heat or chemical species crossing a sub-domain</td>
</tr>
<tr>
<td>38</td>
<td>FRICTION</td>
<td>Specify bottom and wind stress friction coefficients</td>
</tr>
<tr>
<td>39</td>
<td>FUEL</td>
<td>Specify fuel composition and heat of combustion</td>
</tr>
<tr>
<td>40</td>
<td>GAS</td>
<td>Specify gas constant and parameters</td>
</tr>
</tbody>
</table>

... Table 6.1.1 continued
<table>
<thead>
<tr>
<th>NO.</th>
<th>KEYWORD</th>
<th>INPUT FUNCTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>41</td>
<td>GEOMETRY</td>
<td>Specify or modify problem geometry</td>
</tr>
<tr>
<td>42</td>
<td>GAS</td>
<td>Specify gas constant and parameters</td>
</tr>
<tr>
<td>43</td>
<td>GEOMETRY</td>
<td>Specify or modify problem geometry</td>
</tr>
<tr>
<td>44</td>
<td>GRAVITY</td>
<td>Specify constants of gravitational acceleration</td>
</tr>
<tr>
<td>45</td>
<td>GRID</td>
<td>Number of grid nodes in the x, y and z directions</td>
</tr>
<tr>
<td>46</td>
<td>HISTORY</td>
<td>Provide time history output at selected nodes</td>
</tr>
<tr>
<td>47</td>
<td>HYDRAULIC</td>
<td>Hydraulic properties of porous matrix</td>
</tr>
<tr>
<td>48</td>
<td>IF</td>
<td>To initiate the IF-ELSE-ENDIF construct</td>
</tr>
<tr>
<td>49</td>
<td>INCLUDE</td>
<td>To include a file at run time in the input data stream</td>
</tr>
<tr>
<td>50</td>
<td>INDENT</td>
<td>To allow command input to be indented</td>
</tr>
<tr>
<td>51</td>
<td>INITIAL</td>
<td>Initial conditions for state variables</td>
</tr>
<tr>
<td>52</td>
<td>INJECTION</td>
<td>Specification for injection of Liquid Films and Sprays</td>
</tr>
<tr>
<td>53</td>
<td>INLET</td>
<td>To specify an inflow boundary for the domain of computation</td>
</tr>
<tr>
<td>54</td>
<td>INTEGRATION</td>
<td>Index for selection of integration profile</td>
</tr>
<tr>
<td>55</td>
<td>LAMINAR</td>
<td>Specify laminar flow</td>
</tr>
<tr>
<td>56</td>
<td>LAND</td>
<td>Define Land Boundary</td>
</tr>
<tr>
<td>57</td>
<td>LATENT</td>
<td>Specify latent heat of fluid</td>
</tr>
<tr>
<td>58</td>
<td>LIMIT</td>
<td>Set upper and lower limits for dependent variables</td>
</tr>
<tr>
<td>59</td>
<td>LOCATE</td>
<td>Specify location of sub-regions or boundaries</td>
</tr>
<tr>
<td>60</td>
<td>MATERIAL</td>
<td>Specify material types and properties</td>
</tr>
<tr>
<td>61</td>
<td>MATRIX</td>
<td>Specify Options for solution of matrix of equations</td>
</tr>
<tr>
<td>62</td>
<td>META</td>
<td>Specify a meta command file to generate multiple simulations</td>
</tr>
<tr>
<td>63</td>
<td>MOVE</td>
<td>Specify moving surface within flow domain</td>
</tr>
<tr>
<td>64</td>
<td>MULTIPHASE</td>
<td>Specify multi-phase or multi-fluid hydraulic characterisitics</td>
</tr>
<tr>
<td>65</td>
<td>NOZZLE</td>
<td>Specify liquid fuel nozzle injection parameters</td>
</tr>
<tr>
<td>66</td>
<td>OPEN</td>
<td>Specify an open boundary through which fluid may enter or leave</td>
</tr>
<tr>
<td>67</td>
<td>OPTION</td>
<td>Modify built-in default options</td>
</tr>
<tr>
<td>68</td>
<td>OUTLET</td>
<td>Specify an outflow boundary for the domain of computation</td>
</tr>
<tr>
<td>69</td>
<td>OUTPUT</td>
<td>Frequency and extent of tabular output</td>
</tr>
<tr>
<td>70</td>
<td>OXIDIZER</td>
<td>Oxygen to nitrogen ratio in the oxidizer stream</td>
</tr>
<tr>
<td>71</td>
<td>PAUSE</td>
<td>Cause a temporary pause in processing</td>
</tr>
<tr>
<td>72</td>
<td>PAUSE</td>
<td>Cause a temporary pause in processing</td>
</tr>
<tr>
<td>73</td>
<td>PERMEABILITY</td>
<td>Specify permeability of the porous medium</td>
</tr>
<tr>
<td>74</td>
<td>PHASE</td>
<td>Specify phase change mode and constants</td>
</tr>
<tr>
<td>75</td>
<td>POROSITY</td>
<td>Specify material porosity for porous matrix</td>
</tr>
<tr>
<td>76</td>
<td>PRANDTL</td>
<td>Specify Prandtl numbers</td>
</tr>
<tr>
<td>77</td>
<td>PRECIPITATE</td>
<td>Specify precipitation reaction from fluid to solid phase</td>
</tr>
<tr>
<td>78</td>
<td>PRINT</td>
<td>Print flow rate, sources and statistical measures of variables</td>
</tr>
<tr>
<td>79</td>
<td>PROBLEM</td>
<td>Specify general nature and type of problem</td>
</tr>
<tr>
<td>80</td>
<td>PROPERTY</td>
<td>Option for mode of property specification</td>
</tr>
</tbody>
</table>

**Table 6.1.1 continued**

**TABLE 6.1.1: KEYWORDS OF ANSWER™ AND THEIR FUNCTIONS(continued)**

<table>
<thead>
<tr>
<th>NO.</th>
<th>KEYWORD</th>
<th>INPUT FUNCTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>81</td>
<td>QUIT</td>
<td>Terminate solution process</td>
</tr>
<tr>
<td>82</td>
<td>RADIATION</td>
<td>Activate thermal radiation calculation</td>
</tr>
<tr>
<td>No.</td>
<td>Option</td>
<td>Description</td>
</tr>
<tr>
<td>-----</td>
<td>-------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>83</td>
<td>REACTION</td>
<td>Specify reaction rate constants</td>
</tr>
<tr>
<td>84</td>
<td>READ</td>
<td>Read initial conditions from archive file</td>
</tr>
<tr>
<td>85</td>
<td>REFERENCE</td>
<td>Reference values for key variables</td>
</tr>
<tr>
<td>86</td>
<td>REGENERATION</td>
<td>Specify regeneration rate for chemical decay chain</td>
</tr>
<tr>
<td>87</td>
<td>RELAX</td>
<td>Relaxation factors for governing variables</td>
</tr>
<tr>
<td>88</td>
<td>RENAME</td>
<td>Allows renaming of output variables listed in Table 6.8.1</td>
</tr>
<tr>
<td>89</td>
<td>RETARDATION</td>
<td>Specify retardation coefficient for a transport variable</td>
</tr>
<tr>
<td>90</td>
<td>SAVE</td>
<td>Frequency of output to archive file</td>
</tr>
<tr>
<td>91</td>
<td>SCALE</td>
<td>Internal scaling of specified input</td>
</tr>
<tr>
<td>92</td>
<td>SCHMIDT</td>
<td>Specify Schmidt numbers</td>
</tr>
<tr>
<td>93</td>
<td>SCREEN</td>
<td>Echo some of the diagnostic output to screen</td>
</tr>
<tr>
<td>94</td>
<td>SELECT</td>
<td>Specify location of sub-regions or boundaries</td>
</tr>
<tr>
<td>95</td>
<td>SET</td>
<td>Set value of a variable as a function of space and time</td>
</tr>
<tr>
<td>96</td>
<td>SOLID</td>
<td>Specify conjugate heat transfer and properties</td>
</tr>
<tr>
<td>97</td>
<td>SOLVE</td>
<td>Start of solution of equations</td>
</tr>
<tr>
<td>98</td>
<td>SOOT</td>
<td>Activate soot computations and specify constants</td>
</tr>
<tr>
<td>99</td>
<td>SOURCE</td>
<td>Specify source, injection or withdrawal terms</td>
</tr>
<tr>
<td>100</td>
<td>SPECIFIC HEAT</td>
<td>Select specific heat options and constants for the fluid</td>
</tr>
<tr>
<td>101</td>
<td>STACK</td>
<td>To specify stack transformation operations</td>
</tr>
<tr>
<td>102</td>
<td>STATISTICS</td>
<td>Obtain output of statistical parameters of variables</td>
</tr>
<tr>
<td>103</td>
<td>STORAGE</td>
<td>Specify storage coefficient for a governing transport equation</td>
</tr>
<tr>
<td>104</td>
<td>SWIRL</td>
<td>To specify characteristics of swirl imposed on flow</td>
</tr>
<tr>
<td>105</td>
<td>SYMMETRY</td>
<td>To identify an external boundary as a symmetry plane or axis</td>
</tr>
<tr>
<td>106</td>
<td>THERMAL</td>
<td>Thermal properties of solid or porous matrix</td>
</tr>
<tr>
<td>107</td>
<td>TIDE</td>
<td>Specify history of tide at a boundary</td>
</tr>
<tr>
<td>108</td>
<td>TIME</td>
<td>Set initial time for simulations</td>
</tr>
<tr>
<td>109</td>
<td>TITLE</td>
<td>Problem title specification</td>
</tr>
<tr>
<td>110</td>
<td>TORTUOSITY</td>
<td>Specify tortuosity of the porous matrix</td>
</tr>
<tr>
<td>111</td>
<td>TRACK</td>
<td>Compute Particle tracks and corresponding elapsed time in flow field</td>
</tr>
<tr>
<td>112</td>
<td>TRANSFER</td>
<td>Transfer mass and property variables within the computational domain</td>
</tr>
<tr>
<td>113</td>
<td>TRANSPORT</td>
<td>Transport properties of porous matrix</td>
</tr>
<tr>
<td>114</td>
<td>TURBULENT</td>
<td>Select turbulent model and specify constants</td>
</tr>
<tr>
<td>115</td>
<td>USER</td>
<td>User identification for input and output files</td>
</tr>
<tr>
<td>116</td>
<td>VELOCITY</td>
<td>Select method of computation of Darcy velocity</td>
</tr>
<tr>
<td>117</td>
<td>VISCOSITY</td>
<td>Select fluid viscosity options</td>
</tr>
<tr>
<td>118</td>
<td>WALL</td>
<td>Specify internal walls within domain of interest</td>
</tr>
<tr>
<td>119</td>
<td>WRITE</td>
<td>Generate output of variables</td>
</tr>
<tr>
<td>120</td>
<td>ZONE</td>
<td>Specify host media zones</td>
</tr>
</tbody>
</table>
2.2 ORDER OF INPUT COMMANDS

The FREEFORM™ command language allows an order-free input format except for the constraints imposed by common sense. For example, the command that initiates the solution of the equations must follow complete specification of the geometry and physics of the problem. Similarly, the command that signifies the end of calculations must be the last input record for a given problem. Table 2.2.1 lists the relationship of the keyword commands to various functional aspects of problem specification. Although it is not necessary, it may be convenient to follow this functional order. The SOLVE\(^1\) command initiates solution of the governing equations and must; therefore, follow complete specification of the problem. The END command terminates the execution of a solution and, therefore, must be the last command of an input sequence for a problem.

Certain other constraints may be inherent to the nature of a specific problem. For example, any input in terms of sub-regions (e.g., the SOURCE command) must obviously follow the subregion specification (LOCATE command). Similarly, if the subregion is specified in terms of grid coordinates, then the LOCATE command must come after the COORDINATE commands that specify the grid coordinates.

<table>
<thead>
<tr>
<th>ORDER</th>
<th>FUNCTION</th>
<th>RELATED KEYWORD COMMAND</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Identification</td>
<td>BANNER, TITLE, USER</td>
</tr>
<tr>
<td>2</td>
<td>Grid specification</td>
<td>ADAPTIVE, CONNECTIVITY, COORDINATE, GEOMETRY, GRID, SCALE</td>
</tr>
<tr>
<td>3</td>
<td>Problem definition</td>
<td>ACRI, BLOCKAGE, BOREHOLE, BRINK, CAPILLARY, DATUM, FRACTURE, GRAVITY, INCLUDE, INJECTION, INLET, LAND, LOCATE, MATERIAL, MOVING, NOZZLE, OPEN, OPTION, OUTLET, PHASE, PROBLEM, RENAME, SELECT, SYMMETRY, WALL, ZONE</td>
</tr>
<tr>
<td>4</td>
<td>Initial and boundary conditions</td>
<td>ADIABATIC, BOUNDARY, FIX, FLOW, FRICTION, INITIAL, INLET, OPEN, OUTLET, PERIODIC, READ, SET, SWIRL, SYMMETRY, TIDE, TIME</td>
</tr>
<tr>
<td>5</td>
<td>Fluid and Host Matrix Properties and constants</td>
<td>CONDUCTION, DENSITY, DIFFUSION, DISTRIBUTION, FLUID, FUEL, HYDRAULIC, GAS, LATENT, MULTIPHASE, OXIDIZER, PERMEABILITY, POROSITY, PRANDTL, PROPERTY, REFERENCE, RETARDATION, SCHMIDT, SPECIFIC, STORAGE, THERMAL, TORTUOSITY, TRANSPORT, VISCOSITY</td>
</tr>
<tr>
<td>6</td>
<td>Nature of Flow</td>
<td>COMPRESSIBLE, LAMINAR, RADIATION, REACTION, SOLID, SOOT, TURBULENT</td>
</tr>
<tr>
<td>7</td>
<td>Source and sink specifications</td>
<td>AHRRENIEUS, CORIOLIS, EBU, DECAY, PRECIPITATE, REACTION, REGENERATION, SOURCE</td>
</tr>
<tr>
<td>8</td>
<td>Solution options</td>
<td>DISABLE, INTEGRATION, LIMIT, MATRIX, RELAX</td>
</tr>
<tr>
<td>9</td>
<td>Output control</td>
<td>CLOSE, CORRELATION, DEBUG, DIAGNOSTIC, FLUX, HISTORY, PRINT, OUTPUT, SAVE, SCREEN, STACK, STATISTICS, TRACK, VELOCITY, WRITE</td>
</tr>
<tr>
<td>10</td>
<td>Operational control</td>
<td>ALLOCATE, CONVERGENCE, DEFINE, ELSE, END, ENDF, FILE, IF, INDENT, META, PAUSE, QUIT, SOLVE</td>
</tr>
</tbody>
</table>

\(^1\) The keywords are denoted by bold uppercase letters.
2.3 SPECIFICATION OF GRID AND PROBLEM DIMENSIONALITY

The computations may be in three-dimensional (3D) or two-dimensional (2D) mode. One or the other mode is selected by the GRID command. In the 3D mode, the Cartesian geometry is specified in terms of the (x, y, z) and the cylindrical geometry in terms of (x, r, θ) or (x, y, z) coordinates. In the 2D mode, the geometry is specified in terms of (x, y) for cartesian and (x, r) or (x, y) cylindrical geometry.

Each grid consists of a number of elements. A node is nominally placed in each element. By default this node is located at the geometric center of the element. However it can be located anywhere in the element. Each element and the node contained within it is denoted by a number which varies from 1 to NELEM irrespective of the dimensionality of the problem. In addition a boundary node (equivalent to a linear or planar element in Finite Element Terminology) is automatically inserted at each exterior boundary segment of the computational domain. These boundary nodes greatly facilitate the imposition of complex boundary conditions. The boundary nodes are number sequentially from NELEM+1 to NMAX. In this case, the total number of nodes, NMAX, is the sum of number of elements and the number of exterior boundary segments. The sequence in which the element and boundary nodes are numbered depends on the nature of the grid. If the grid is unstructured, then the nodes are numbered exactly in the same order in which the elements are specified on the geometry input. The boundary nodes are also numbered in the order in which the element with exterior boundary is encountered. For a structured grid the element are numbered, in order, along the x, y and then z direction grid lines respectively. These are followed by the boundary nodes which are defined in order of the boundaries along the x, y and z planes.

For the structured grids, a grid index is defined for each grid node. This index varies from (1,1,1) to (IMAX, JMAX, KMAX) for the 3D and from (1,1) to (IMAX, JMAX) for the 2D geometry. IMAX, JMAX and KMAX are, respectively, the maximum number of grid lines in the x, y (or r) and z (or θ) directions. For 2D computations, KMAX is automatically set to 1. One-dimensional computations are performed in a pseudo-2D mode where the gradients of all variables in the y direction are set to zero. The total number of nodes, including the boundaries is NMAX where NMAX= IMAX * JMAX in 2D and NMAX=IMAX * JMAX * KMAX in 3D.

IMPORTANT NOTE: For TIDAL™ Software the velocity field is computed only in the 2D mode since only the velocity components are depth-averaged. The thermal and mass transport equations can be solved in the 3D mode but in this case, the appropriate velocity components must be specified.
2.4 INPUT AND OUTPUT FILE UNITS

ACRi™ SOFTWARE TOOLS employ a number of I/O file units. The function and default file names for these units are defined in Table 2.4.1. The default file type is FORMATTED for all these files. The user is given an opportunity to attach these units to alternate files (or devices) and change the file type for some of these. The files attached to units 15 and 16, being the standard input and output devices, may be redirected only by the operating system commands. The user may change file names for most of these files. Please see the corresponding user commands for the available options. Further operations can be performed on any of the I/O units by the FILE and CLOSE commands. The term “auto” for unit number means that the unit number is automatically selected from among the available units.

A number of temporary units may be opened in response to user commands. Many of these are named with the file extension "TMP" unless the user explicitly specifies a file name on the command.
<table>
<thead>
<tr>
<th>UNIT #</th>
<th>DEFAULT FILE NAME</th>
<th>FUNCTION OF THE FILE</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>Console</td>
<td>Read user input commands from standard input device.</td>
</tr>
<tr>
<td>16</td>
<td>xxx.out</td>
<td>Write to Standard Output Device. The string xxx in this file name is replaced by the file name (without extension) of the input command file specified by the user.</td>
</tr>
<tr>
<td>81</td>
<td>ACRINIT.ACR</td>
<td>ACRi Initialization file</td>
</tr>
<tr>
<td>82</td>
<td>ACRIMSG.ACR</td>
<td>ACRi file for diagnostic and error messages, and formats</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_DEBUG.TMP</td>
<td>User specific diagnostic and debug output (DEBUG).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_DIAGNOSTIC.TMP</td>
<td>Internally generated file with step-by-step diagnostics of convergence history for each variable for which a transport equation is solved (DIAGNOSTIC).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_HISTOR.TMP</td>
<td>Time-history data file (HISTORY).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_HISTOR_XYZ.TMP</td>
<td>Time-history at specified locations (HISTORY COORDINATE).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_SOURCE.TMP</td>
<td>Time-history of source of variables (HISTORY SOURCE).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_STORAGE.TMP</td>
<td>Time-history of storage of variables (HISTORY STORAGE).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_MATR_REDBLACK.TMP</td>
<td>Red/Black matrix split information (MATR_REDBLACK).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_NOZZLE.TMP</td>
<td>Nozzle spray trajectory information (NOZZLE TRAJECTORY).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_PRINT_FORCE.TMP</td>
<td>Time-history of forces or moments on a surface (PRINT FORCE).</td>
</tr>
<tr>
<td>11</td>
<td>xxx.SAV***</td>
<td>Write data file for restart, archiving and post-processing (SAVE).</td>
</tr>
<tr>
<td>12</td>
<td>xxx__GRID_TABLE.SAV***</td>
<td>Write archive data file in tabular form (SAVE TABLE).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_STATS.TMP</td>
<td>Statistics information pertaining to variables (STATISTICS).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_TRACK.TMP***</td>
<td>Particle Track information for the flow field (TRACK).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_XYZ_CORNERS.TMP</td>
<td>Corner coordinates for each element (WRITE CORNERS).</td>
</tr>
<tr>
<td>Auto</td>
<td>xxx__GRID_VERTX_MAP.TMP</td>
<td>Vertex Mapping information automatically generated if needed.</td>
</tr>
</tbody>
</table>

*** The string xxx is replaced by the name of the file (without extension) that is connected to the Standard Output Device (Unit 16).
2.5 UNITS OF PHYSICAL QUANTITIES

Any consistent set of units may be employed for input. However, all built-in default values for dimensional physical properties (such as the density of water) are in SI units. If other than SI units are used, then these properties must be specified in appropriate units as part of the input data.
2.6 DIAGNOSTIC OUTPUT SPECIFICATION

Four keyword commands control the diagnostic output. These are the DEBUG, DIAGNOSTIC, FLUX, and OUTPUT commands. The DEBUG command provides a printout of numerical error parameters, which are useful in evaluating the accuracy of numerical solution. The DIAGNOSTIC command provides a means to monitor the time-history of the dependent variables at a particular node and the residuals of the governing equations from one iterative step to the next. The FLUX command provides output of convective and diffusive flux terms, and the residuals and errors in mass and energy balance in the numerical solution of the equations. The OUTPUT command allows the field variables to be written in a tabular format to the standard output device (unit 16).
2.7 DEPENDENT VARIABLES OF ACRi™ SOFTWARE TOOLS

ACRi™ SOFTWARE TOOLS provide for the numerical solution of an arbitrary number of coupled transport equations. The user may elect to solve any subset of these equations. Table 2.7.1 lists the variables of the governing equations in the order in which they are solved.

<table>
<thead>
<tr>
<th>ACRi™ Software</th>
<th>Software Symbol</th>
<th>Mathematical Symbol</th>
<th>Description of the Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANSWER™ TIDAL™</td>
<td>U</td>
<td>U</td>
<td>Velocity component in x-direction</td>
</tr>
<tr>
<td>ANSWER™ TIDAL™</td>
<td>V</td>
<td>V</td>
<td>Velocity component in y or r-direction</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>W</td>
<td>W</td>
<td>Velocity component in z or θ-direction</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>PP</td>
<td>Φ</td>
<td>Density and Pressure correction variable</td>
</tr>
<tr>
<td>ALL</td>
<td>HT</td>
<td>h or h_s</td>
<td>Enthalpy or Stagnation enthalpy (See Note below)</td>
</tr>
<tr>
<td>ALL</td>
<td>T</td>
<td>T</td>
<td>Temperature</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>K</td>
<td>K</td>
<td>Kinetic energy of turbulence</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>E</td>
<td>ε</td>
<td>Dissipation of turbulence energy (See Note below)</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>FF</td>
<td>mₐ</td>
<td>Mass fraction of total carbon</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>FH</td>
<td>mₙ</td>
<td>Mass fraction of total hydrogen</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>FO</td>
<td>m₀</td>
<td>Mass fraction of total oxygen</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>FU</td>
<td>mₜ₉ₘₘₘ</td>
<td>Mass fraction of fuel species</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>CH</td>
<td>mₜ₉ₘₘₘ₂</td>
<td>Mass fraction of H₂-stripped fuel</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>CO</td>
<td>mₜ₉ₘₘ₁</td>
<td>Mass fraction of carbon monoxide</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>H₂</td>
<td>mₜ₉ₘₘ₂</td>
<td>Mass fraction of hydrogen</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>RA</td>
<td>(Rₚ+Rₚₚ+Rₚ₂)/₅</td>
<td>Net incoming thermal radiation flux.</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>SN</td>
<td>Sₙₐ</td>
<td>Concentration of soot nuclei</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>S1</td>
<td>S₁</td>
<td>Concentration of small soot particles</td>
</tr>
<tr>
<td>ANSWER™</td>
<td>S2</td>
<td>S₂</td>
<td>Concentration of large soot particles</td>
</tr>
<tr>
<td>PORFLOW™</td>
<td>P</td>
<td>P¹</td>
<td>Pressure head for 1st (primary) fluid phase</td>
</tr>
<tr>
<td>PORFLOW™</td>
<td>P2</td>
<td>P²</td>
<td>Pressure head for 2nd fluid phase</td>
</tr>
<tr>
<td>PORFLOW™</td>
<td>P3</td>
<td>P³</td>
<td>Pressure head for 3rd fluid phase</td>
</tr>
<tr>
<td>TIDAL™</td>
<td>ETA</td>
<td>η</td>
<td>Fluid elevation above datum</td>
</tr>
<tr>
<td>PORFLOW™ &amp; TIDAL™</td>
<td>C, C₂, C₃, C₄</td>
<td>C⁵</td>
<td>Mass concentration of 1st through 4th species in fluid</td>
</tr>
<tr>
<td>ALL</td>
<td>User defined</td>
<td>none</td>
<td>Variables defined by the user with the ALLOCATE command or one of the above variables renamed by the user with the RENAME command.</td>
</tr>
</tbody>
</table>

NOTE: Many of the input commands refer to the features of the transport equation rather than the variable itself. For these commands the specification of the symbol "T" is taken to be equivalent to that for the enthalpy variable, "H" and that of "L" for the dissipation energy, "E". This for example, is the case for the SOLVE command that refers to the solution of the equation or the SOURCE command that refers to the source for the equation. This is not true for commands, such as the SET command, that specify the value of the variable itself.
2.8 TABULAR OUTPUT OF FIELD VARIABLES

The user may obtain tabular output of a number of dependent, independent and supplementary variables. These include the phase space variables listed in Table 2.7.1 plus a number of supplementary variables. Tables 2.8.1-3 and 2.8.4 list these variables. ACRi Software Tools define 5 types of variables:

**Node based Variable**: This type of variable is defined at every node of the domain. One value is defined for each element and additionally one value at each boundary location. For a 2D 12 by 10 structured grid (IMAX, JMAX on GRID command) there will be a total of 120 nodes. This grid will consist of 80 elements (IMAX-2 times JMAX-2) and 40 boundary nodes. For an unstructured grid the number of total nodes will be the number of elements specified on the GRID command plus one node for each external element surface. An external surface is defined as one that is connected only to one element and therefore is not an interface between two elements. All phase space variables listed in Table 2.7.1 fall under this category.

**Element based Variable**: One value is defined for each element. For 12 by 10 structured grid, there will be 80 (10 by 8) values. For an unstructured grid the number of values will be equal to the number of elements specified on the GRID command.

**Corner or vertex based Variable**: One value is defined at every vertex of the computational domain. For a 12 by 10 structured grid there will be a total of 99 vertices or corners (IMAX-1 times JMAX-1). For an unstructured grid the vertex coordinate file (CONNECTIVITY command) determines the number of vertices.

**Face or Surface based Variable**: One value is defined at every element surface. The total number of faces a function of the grid dimensionality and the manner of arrangement of elements. It is internally computed from the grid specification and connectivity.

**List based Variable**: This type of variables is in the form of a freeform list the length of which is dictated by software and/or user specific needs.

A number of FREEFORM™ commands are provided to obtain output for these variables in different formats. The primary output of the variables can be obtained by the OUTPUT, SAVE and WRITE commands.

**Output for Node Based Variable**: Table 2.8.1-3 list the node-based variables for which output can be obtained. These are termed "standard" output variables. The output can be written to the Standard Output device (Unit 16) or to a user specified file. The extent and frequency of this output is controlled by the OUTPUT and SAVE commands.

**Output for Supplementary Variables**: Table 2.8.4 lists some supplementary variables for which output can be obtained. The output for these can be directed to the Standard Output Device or a user-specified file. This output is controlled by the WRITE command.

**Output for Derived Flow Variables**: Output for some special variables that are derived from the flow field may be obtained on demand. These variables include, the gradients of the velocity field, the vorticity, stresses, strains, and some special variables. Please see the OUTPUT and SAVE commands for a detailed description of this output.

**Output for Coefficients and Components of Transport Equation**: Output for different coefficients and components of each transport equations can be obtained during the solution process. Please see the OUTPUT and SAVE commands for a detailed description of this output.
## TABLE 2.8.1: STANDARD VARIABLES OF ANSWER™ SOFTWARE TOOL

<table>
<thead>
<tr>
<th>Software Symbol</th>
<th>Mathematical Symbol</th>
<th>Description of the Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>U</td>
<td>Velocity component in x-direction</td>
</tr>
<tr>
<td>V</td>
<td>V</td>
<td>Velocity component in y or r-direction</td>
</tr>
<tr>
<td>W</td>
<td>W</td>
<td>Velocity component in z or θ-direction</td>
</tr>
<tr>
<td>P</td>
<td>P</td>
<td>Fluid pressure</td>
</tr>
<tr>
<td>HT</td>
<td>h or hh</td>
<td>Enthalpy or Stagnation enthalpy</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>Fluid Temperature</td>
</tr>
<tr>
<td>K</td>
<td>k</td>
<td>Kinetic energy of turbulence</td>
</tr>
<tr>
<td>E</td>
<td>ε</td>
<td>Dissipation of turbulence energy</td>
</tr>
<tr>
<td>L</td>
<td>r</td>
<td>Length scale of turbulence</td>
</tr>
<tr>
<td>FF</td>
<td>mC</td>
<td>Mass fraction of total carbon</td>
</tr>
<tr>
<td>FH</td>
<td>mH</td>
<td>Mass fraction of total hydrogen</td>
</tr>
<tr>
<td>FO</td>
<td>mO</td>
<td>Mass fraction of total oxygen</td>
</tr>
<tr>
<td>FU</td>
<td>mCtoken</td>
<td>Mass fraction of fuel species</td>
</tr>
<tr>
<td>CH</td>
<td>mChim</td>
<td>Mass fraction of H₂-stripped fuel</td>
</tr>
<tr>
<td>CO</td>
<td>mCO</td>
<td>Mass fraction of carbon monoxide</td>
</tr>
<tr>
<td>H2</td>
<td>mH2</td>
<td>Mass fraction of hydrogen</td>
</tr>
<tr>
<td>O2</td>
<td>mO2</td>
<td>Mass fraction of oxygen</td>
</tr>
<tr>
<td>H2O</td>
<td>mH2O</td>
<td>Mass fraction of water</td>
</tr>
<tr>
<td>CO2</td>
<td>mCO2</td>
<td>Mass fraction of carbon dioxide</td>
</tr>
<tr>
<td>NO</td>
<td>mNO</td>
<td>Mass fraction of Nitrogen Oxides</td>
</tr>
<tr>
<td>NO2</td>
<td>mNO2</td>
<td>Mass fraction of Nitrogen Di-oxides</td>
</tr>
<tr>
<td>FG</td>
<td>G</td>
<td>The property g for the fuel fluctuation equation</td>
</tr>
<tr>
<td>FM</td>
<td>f_m</td>
<td>The mean-mixture fraction for for the fuel fluctuation equation</td>
</tr>
<tr>
<td>PV</td>
<td>v_p</td>
<td>The mixture variance for the fuel fluctuation equation</td>
</tr>
<tr>
<td>SN</td>
<td>S_n</td>
<td>Concentration of soot nuclei</td>
</tr>
<tr>
<td>LF</td>
<td>L_f</td>
<td>Liquid mass fraction from the nozzle injections</td>
</tr>
<tr>
<td>AD</td>
<td>A_d</td>
<td>Average droplet diameter for nozzle injections</td>
</tr>
<tr>
<td>S1</td>
<td>S_1</td>
<td>Concentration of small soot particles</td>
</tr>
<tr>
<td>S2</td>
<td>S_2</td>
<td>Concentration of large soot particles</td>
</tr>
<tr>
<td>RA</td>
<td>(R_x+R_y+R_z)/3</td>
<td>Net incoming thermal radiation flux.</td>
</tr>
<tr>
<td>RGAS</td>
<td>R</td>
<td>The specific gas constant for the gaseous mixture</td>
</tr>
<tr>
<td>MU</td>
<td>μ</td>
<td>Effective viscosity of fluid</td>
</tr>
<tr>
<td>RHO</td>
<td>ρ</td>
<td>Mass density of fluid</td>
</tr>
<tr>
<td>POR</td>
<td>θ_e</td>
<td>Effective porosity of a grid element</td>
</tr>
<tr>
<td>PHYD</td>
<td></td>
<td>Hydraulic head of the fluid</td>
</tr>
<tr>
<td>EBYK</td>
<td>ω/k</td>
<td>Turbulence time constant</td>
</tr>
<tr>
<td>CP</td>
<td>c_p</td>
<td>Specific Heat of fluid mixture</td>
</tr>
<tr>
<td>SPEED</td>
<td>V</td>
<td>Modulus of Velocity = Sqrt(u²+v²+w²)</td>
</tr>
<tr>
<td>EDYN</td>
<td>0.5 V²</td>
<td>Dynamic energy of fluid</td>
</tr>
<tr>
<td>PDYN</td>
<td>0.5 ρ V²</td>
<td>Dynamic pressure of fluid</td>
</tr>
<tr>
<td>PTOTAL</td>
<td>P+0.5 V²</td>
<td>Total pressure of fluid</td>
</tr>
<tr>
<td>MACH</td>
<td>c/a</td>
<td>Mach Number for the fluid = V/sqrt(γ-1)CpT</td>
</tr>
<tr>
<td>VOL</td>
<td>X</td>
<td>Volume of the Element</td>
</tr>
<tr>
<td>X, Y, Z</td>
<td>x, y, z</td>
<td>X, Y and Z Coordinates of the Node Location</td>
</tr>
<tr>
<td>User-Specific</td>
<td>---</td>
<td>User-specific variables defined in the acrNAMES.ACR file</td>
</tr>
</tbody>
</table>

Dynamically Allocated --- Dynamically allocated variables with ALLOCATE or RENAME commands
### TABLE 2.8.2: STANDARD VARIABLES OF PORFLOW™ SOFTWARE TOOL

<table>
<thead>
<tr>
<th>Software Symbol</th>
<th>Mathematical Symbol</th>
<th>Description of the Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>U</td>
<td>Velocity component in x-direction</td>
</tr>
<tr>
<td>V</td>
<td>V</td>
<td>Velocity component in y or r-direction</td>
</tr>
<tr>
<td>W</td>
<td>W</td>
<td>Velocity component in z or θ-direction</td>
</tr>
<tr>
<td>P</td>
<td>P</td>
<td>Fluid pressure</td>
</tr>
<tr>
<td>HT</td>
<td>h or hₚ</td>
<td>Enthalpy or Stagnation enthalpy</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>Fluid Temperature</td>
</tr>
<tr>
<td>POR</td>
<td>Θₑ</td>
<td>Effective porosity of a grid element</td>
</tr>
<tr>
<td>PORT</td>
<td>Θₜ</td>
<td>Total porosity of a grid element</td>
</tr>
<tr>
<td>PORD</td>
<td>Θ₀</td>
<td>Diffusional porosity of a grid element</td>
</tr>
<tr>
<td>PHYD</td>
<td></td>
<td>Hydraulic head of the fluid</td>
</tr>
<tr>
<td>CP</td>
<td></td>
<td>Specific Heat of fluid mixture</td>
</tr>
<tr>
<td>SPEED</td>
<td></td>
<td>Modulus of Velocity = sqrt(u²+v²+w²)</td>
</tr>
<tr>
<td>EDYN</td>
<td>0.5 V²</td>
<td>Dynamic energy of fluid</td>
</tr>
<tr>
<td>PDYN</td>
<td>0.5 ρ V²</td>
<td>Dynamic pressure of fluid</td>
</tr>
<tr>
<td>PTOTAL</td>
<td>P+0.5 V²</td>
<td>Total pressure of fluid</td>
</tr>
<tr>
<td>MACH</td>
<td>c/a</td>
<td>Mach Number for the fluid = V/sqrt[(γ-1)CpT]</td>
</tr>
<tr>
<td>C, C₂, C₃, C₄</td>
<td>C²</td>
<td>Mass concentration of 1st through 4th species in fluid</td>
</tr>
<tr>
<td>S, S₂, S₃</td>
<td>S², S³, S⁴</td>
<td>Saturation fraction for the 1st, 2nd and 3rd fluid phase</td>
</tr>
<tr>
<td>RHO, RHO₂,</td>
<td>R², R²</td>
<td>Normalized Density of the 1st and 2nd fluid phase</td>
</tr>
<tr>
<td>RHOG</td>
<td>R²</td>
<td>Normalized Density of the 3rd (gas) fluid phase</td>
</tr>
<tr>
<td>RHOS</td>
<td>ρₛ</td>
<td>Mass density of solid matrix</td>
</tr>
<tr>
<td>H, H₂, H₃</td>
<td>H², H³</td>
<td>Total hydraulic head for the 1st, 2nd and 3rd fluid phase</td>
</tr>
<tr>
<td>MOIS</td>
<td>Φₑ</td>
<td>Effective moisture in the first fluid phase</td>
</tr>
<tr>
<td>MU</td>
<td>pµ</td>
<td>Viscosity ratio for the primary Fluid</td>
</tr>
<tr>
<td>QX, QY, QZ</td>
<td>X, Y and Z components of element-average Darcy Velocity</td>
<td></td>
</tr>
<tr>
<td>VOL</td>
<td>δV</td>
<td>Volume of the Element</td>
</tr>
<tr>
<td>X, Y, Z</td>
<td>x, y, z</td>
<td>X, Y and Z Coordinates of the Node Location</td>
</tr>
<tr>
<td>User defined</td>
<td>---</td>
<td>User-defined variables with ALLOCATE or RENAME commands</td>
</tr>
</tbody>
</table>
### TABLE 2.8.3: STANDARD VARIABLES OF TIDAL™ SOFTWARE TOOL

<table>
<thead>
<tr>
<th>Software Symbol</th>
<th>Mathematical Symbol</th>
<th>Description of the Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>U</td>
<td>Velocity component in x-direction</td>
</tr>
<tr>
<td>V</td>
<td>V</td>
<td>Velocity component in y or r-direction</td>
</tr>
<tr>
<td>W</td>
<td>W</td>
<td>Velocity component in z or θ-direction</td>
</tr>
<tr>
<td>HT</td>
<td>h or hs</td>
<td>Enthalpy or Stagnation enthalpy</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>Fluid Temperature</td>
</tr>
<tr>
<td>RHO</td>
<td>ρ</td>
<td>Mass density of fluid</td>
</tr>
<tr>
<td>CP</td>
<td>Cp</td>
<td>Specific Heat of fluid mixture</td>
</tr>
<tr>
<td>SPEED</td>
<td>V</td>
<td>Modulus of Velocity = Sqrt(u^2 + v^2 + w^2)</td>
</tr>
<tr>
<td>EDYN</td>
<td>0.5 V^2</td>
<td>Dynamic energy of fluid</td>
</tr>
<tr>
<td>PDYN</td>
<td>0.5 ρ V^2</td>
<td>Dynamic pressure of fluid</td>
</tr>
<tr>
<td>PTOTAL</td>
<td>P + 0.5 V^2</td>
<td>Total pressure of fluid</td>
</tr>
<tr>
<td>C, C2, C3, C4</td>
<td>C</td>
<td>Mass concentration of 1st through 4th species in fluid</td>
</tr>
<tr>
<td>ETA</td>
<td>η</td>
<td>Fluid elevation above datum</td>
</tr>
<tr>
<td>H</td>
<td>H</td>
<td>Total fluid depth = h + η</td>
</tr>
<tr>
<td>DEPT</td>
<td>h</td>
<td>Bathymetric depth below datum</td>
</tr>
<tr>
<td>PA</td>
<td>P₀</td>
<td>Atmospheric pressure</td>
</tr>
<tr>
<td>WIND</td>
<td>w</td>
<td>Wind speed</td>
</tr>
<tr>
<td>ANGL</td>
<td>Θ</td>
<td>Angle that the wind vector makes with the positive direction of x</td>
</tr>
<tr>
<td>VOL</td>
<td>δV</td>
<td>Volume of the Element</td>
</tr>
<tr>
<td>X, Y, Z</td>
<td>x, y, z</td>
<td>X, Y and Z Coordinates of the Node Location</td>
</tr>
<tr>
<td>User defined</td>
<td>---</td>
<td>User-defined variables with ALLOCATE or RENAME commands</td>
</tr>
</tbody>
</table>
## TABLE 2.8.4: SUPPLEMENTARY VARIABLES OF ACRI™ SOFTWARE TOOLS

<table>
<thead>
<tr>
<th>Software Symbol</th>
<th>Variable Basis</th>
<th>Variable Type</th>
<th>Description of the Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>XC, YC, ZC</td>
<td>Vertex</td>
<td>Real</td>
<td>x, y and z coordinates for element vertices</td>
</tr>
<tr>
<td>VOLF</td>
<td>Face</td>
<td>Real</td>
<td>Volume associated with an element interface. This consists of the sum of the part volumes of the two adjoining elements. For example, in Figure 4.1.5, for the “e” face, it consists of the part volumes of the two elements contained between P and E.</td>
</tr>
<tr>
<td>VOLR</td>
<td>Face</td>
<td>Real</td>
<td>Non-dimensional fraction of face volume associated with the “-ve” side of the interface to VOLF. The “-ve” side is defined with reference to the area vector at the face. This definition of direction is arbitrary and depends on the manner in which the elements are processed.</td>
</tr>
<tr>
<td>AFX, AFY, AFZ</td>
<td>Face</td>
<td>Real</td>
<td>The x, y and z components of the area vector for an element face.</td>
</tr>
<tr>
<td>FC</td>
<td>Face</td>
<td>Real</td>
<td>Convective mass flux across an element interface.</td>
</tr>
<tr>
<td>FD</td>
<td>Face</td>
<td>Real</td>
<td>Coefficient for diffusive flux across an interface. For an orthogonal grid, the diffusive flux is defined as the product of this coefficient and the difference of the variables values between the two nodes associated with the interface (such as P and E for the “e” face in Figure 4.1.5).</td>
</tr>
<tr>
<td>NCRN</td>
<td>Vertex</td>
<td>Integer</td>
<td>Element to vertex connectivity</td>
</tr>
<tr>
<td>NBRS</td>
<td>List</td>
<td>Integer</td>
<td>Element to node connectivity. For each element, the list contains the node numbers to which the element is connected. The number of members for each element is equal to the number of surfaces for the element.</td>
</tr>
<tr>
<td>NFACE</td>
<td>List</td>
<td>Integer</td>
<td>Element to surface number connectivity. For each element, the list contains the surface numbers that comprise the element boundary.</td>
</tr>
<tr>
<td>LINK</td>
<td>List</td>
<td>Integer</td>
<td>Face to node number mapping matrix. The list is arranged by surface number. For each surface the list contains 4 members: the two nodes on the “-ve” and “+ve” sides of the surface, and the surface numbers for two neighborhood surfaces unconnected to the surface.</td>
</tr>
<tr>
<td>MTYP</td>
<td>Node</td>
<td>Integer</td>
<td>Material Type index</td>
</tr>
</tbody>
</table>
2.9 ARCHIVAL AND POST-PROCESSING OUTPUT

Files containing archival and post-processing outputs may be obtained in three distinct modes. These files are generated by the SAVE command in the SAVE BLOCK, SAVE TABLE and SAVE RESTART modes. The output from these may be used to restart a problem or for post-processing functions such as to produce contour, raster, surface or vector plots on a console screen, printer or plotter. The files can be generated at any required frequency.

Whenever output from these commands is written to a file, diagnostic messages appear on the Standard Output Device that identifies the information being transferred to the file. The file is self-documenting. In addition to the values of the field variables, it contains the file identification data, the user identification, the problem title, the time and date of creation, the basic grid information, and the names of variables stored on the archive file.

The SAVE BLOCK command provides flexibility in the selection of variables, the output frequency and the nature of data records (formatted or unformatted). In the SAVE BLOCK mode, the variables are listed individually and separately for whole of the domain of computation in a block format. The values of the grid coordinates and field variables (see Tables 2.8.1 to 2.8.3) follow the basic problem and data identification. An alphanumeric record precedes each variable field and lists the name of the variable, the time and step number of archival, the data type and the number of values. The archive information is written in either unformatted or formatted records, depending on user specification. Please see the SAVE command for further details.

In the SAVE TABLE mode of the command generates output that is arranged by rows and columns for the whole or part of the domain of computation. The basic problem and data identification fields are followed by variables listed in a tabular manner for each node individually. Only formatted data records are allowed. Each row of data pertains to a single element and each column contains the value of a variable for that element. The file can be used for archiving or post-processing purposes. Please see the SAVE command for further details.

The SAVE RESTART mode is strictly meant for restart of a given problem and is generated only in UNFORMATTED mode at the specified frequency.
2.10 RESTART OUTPUT

A special file for restart of a problem can be generated by the SAVE command with the RESTART modifier. This file is in an unformatted format and is machine specific. This file can only be read with the READ command with a RESTART modifier. If the simulations are restarted from this file, then the problem specification must be identical to that for the original simulation.
2.11 MODIFICATION OF INPUT DATA DURING SIMULATIONS

The simulation of a problem is initiated by the SOLVE command. The total span of simulations, however, may be divided into segments, and a SOLVE command used for each segment. Any time-dependent or sequential aspects of the input or output requirements may be changed between the calculation segments. For any problem, all specification relating to the geometry is considered independent of time; the rest of the problem specification, including operational control and output requirements, can all change during the course of simulations.

An example of a two-segment calculation sequence is given in Table 2.11.1. In this example, the output requirements for both the archive file and the tabular output are changed after 5 time units of simulation.
### TABLE 2.11.1: ILLUSTRATION OF A 2-SEGMENT SIMULATION SEQUENCE

<table>
<thead>
<tr>
<th>Grid</th>
<th>Coordinate X: Range = 100, grid spacing increment ratio = 1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coordinate Y: Range = 40, grid spacing increment ratio = 1.1</td>
<td></td>
</tr>
</tbody>
</table>

**Title Example of a Two Segment Calculation with Output Changes**

```
GRID 11 BY 12
COORDinate X: RANGE = 100, grid spacing increment ratio = 1.1
COORDinate Y: RANGE = 40, grid spacing increment ratio = 1.1
/
INLET at X- boundary
OUTLET at X+ boundary
/
SET U = 1. everywhere
SET T = 500 everywhere       !! except at inlet as modified below
INITial T = 300 from (1,1) to (1,11)      !! INLET
/
OUTPUT for P (pressure) at this stage   !! Print initial values of P
/
////////////////////////////////////////////////////////////////////
Comment. Start of first segment of calculations
SOLVE for 10 secs in time step of 0.1 sec
/
OUTPUT for variables P and T
SAVE variables U, V, P
/
////////////////////////////////////////////////////////////////////
Comment. Start of second segment of calculations
SOLVE for 10 secs in time step of 0.5 sec
/
OUTPUT for variables U, V, W, P and T
SAVE variables U, V, W, P and T
/
END
```
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CHAPTER 3
KEYWORD COMMAND NOTATION

This chapter describes the notation used for the keyword commands that comprise the user interface for all ACRi Software Tools including ANSWER™, PORFLOW™, and TIDAL™ software package. This interface is based on the ACRi format-free command language FREEFORM™. Knowledge of the structure and syntax of this language is essential for understanding the descriptions of keyword commands in this chapter. The command language is fully described in Chapter 1 of this document. Descriptive notation for the keyword commands is explained in this chapter.
3.1 KEYWORD COMMAND NOTATION

The notation for input commands is described below. A detailed description of the user input follows. The FREEFORM™ command language used for this input is described in Chapter 1.

**BOLD** Uppercase characters in bold typeface denote The FREEFORM™ *keyword commands*. The user may specify the keyword character string in upper or lower case. Bold typeface is used in this manual for emphasis only; it must not be used as part of user input.

**CAPS** Upper case characters in normal or bold typeface denote *modifiers* of FREEFORM™ that are *significant* for interpretation of user input. The user may specify the character string in upper or lower case.

**char** Lower-case characters denote information in commands which is *not significant* for interpreting user input but improves the clarity or readability of the input. The character strings shown may or may not be specified by the user, or other character strings may replace them.

| Vertical bar indicates a choice; only one of the items separated by the bar (and enclosed in braces or square brackets) may be specified. |

{ } Braces indicate that the enclosed item (or one of the enclosed items separated from others by vertical bars) is required and must be specified.

[ ] Square brackets indicate that the enclosed item is optional.

.... Ellipses (in horizontal or vertical format) indicate that other, similar items may follow those shown.

**Nn** The n<sup>th</sup> numeric field in an input command denoted by a keyword.

**fname** The name of a file or device; see Section 3.3.

**subrgn** The sub region for the applicable input; see Section 3.4.

**idsub** A unique identity for a sub region of the domain of computation; see Section 3.4.

**func** An analytic or tabular function for input of a numerical quantity; see Section 4.1.

**phase** Fluid phase to which the input applies; see Section 3.6.

**Vfrq** Frequency of output; see Section 3.7.
3.2 INTERACTIVE OR RUN TIME INPUT

The FREEFORM™ command language allows interactive or run time data input for any keyword command. Occurrence of a question mark (?) in the input is a prompt for interactive input by the user. The user may therefore insert a ‘?’ for a numerical or character string in the input. When a ‘?’ is read, the command interpreter pauses and prompts the user for interactive input. Any input so specified is then appended to the original input command string, starting with the location of the question-mark symbol. Additional information about this input feature is given in Chapter 1. The FREEFORM™ command interpreter is based on a 256-character input string for each input record (see Appendix B). Therefore, the number of characters that can be inserted after the question mark depends on the location of the question mark.
3.3  FILE NAME SPECIFICATION

Many input commands allow part or all of the input data to be read from a user-specified file (or device) or output to be directed to an output file. The name of the file, which is denoted by 'fname' in this manual, is specified as a character expression that must be enclosed in single or double quotes. The file or device name may be up to 256 characters long, consisting of any characters accepted by the operating system as a valid I/O file name. In the input mode, the data is read from the file in a format-free mode according to the rules of FORTRAN 90.

Some operating systems do not distinguish between the lower and upper case file names. On such systems, for example, a file named 'tmp.fil' is equivalent to a file named 'TMP.FIL' (or some other combination of upper and lower case characters). On such systems, an error may occur if file names are specified that are identical except for the case. In general, it is recommended that the user should consistently use either upper or lower case characters for file names.

By default, a file is assumed to be in "FORMATTED" mode. Some commands also allow an "UNFORMATTED" mode of input or output. If allowed, the "UNFORMATTED" modifier on the command selects this mode.

If a file name is specified on a command, then the file is immediately opened and is available for I/O operations.

In the output mode, a unique file name must be associated with each type of command that generates an output file. The user may assign a name by explicit specification on a command. Once assigned, the new file name becomes the default name until changed by a subsequent command of the same type. If the file name is different than a previously specified name, then the old file associated with that command is closed and the subsequent output is written to a new file with the specified name. If no file name is specified, then a default name is assigned to each output file (see Section 2.4).
3.4 SUB REGION IDENTIFICATION ON AN INPUT COMMAND

Some input commands may specify values for a sub region of the domain. For these commands, the desired sub region must be previously specified by a LOCATE or SELECT command (in this document “LOCATE” is used to identify both these commands). Multiple modes of LOCATE command are available to accommodate a diversity of input and output requirements. Each LOCATE command identifies a subregion with a unique identifier specified as ID=idsub, where ‘ID’ in the command must immediately precede the idsub identifier. The idsub identifier may consist of any combination of up to 32 unique alphanumeric characters without any embedded spaces or graphic characters. The valid characters are the same as those for a modifier (see Section 1.2.2). This ID=idsub identifier is then used subsequently on a keyword command to selectively provide input for that subregion.

A LOCATE command for a subregion may also be specified without a unique identifier, then this subregion may be identified on a subsequent command by specifying LOCATE or SELECT as a modifier till the occurrence of the _next LOCATE command. For some commands, a unique subregion identity may be required for proper implementation of the input features; this is discussed in the description of each command.

If a subregion specification is omitted by the user, but is required by the keyword command, then the input is assumed to be for the total domain of interest, which is relevant for that command. The choices available for the “subrgn” modifier are summarized in Table 3.4.1.

<table>
<thead>
<tr>
<th>subrgn</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>SELE</td>
<td>The input applies to the most recently defined subregion of the LOCATE or SELECT command. Same as LOCATE modifier.</td>
</tr>
<tr>
<td>LOCA</td>
<td>The input applies to the most recently defined subregion of the LOCATE or SELECT command. Same as SELECT modifier.</td>
</tr>
<tr>
<td>ID=idsub</td>
<td>The input applies to the subregion that was assigned the identity ‘idsub’ in a previous LOCATE or SELECT command.</td>
</tr>
</tbody>
</table>

_The LOCATE commands are of two types: (1) those that specify a sub-region within the computational domain and (2) those that specify exclusively a boundary of the domain._

If a LOCATE command specifies only a boundary, then only the nodes falling at the boundary are included in the subregion.

However, if a LOCATE command specifies an interior subregion, then _by default both the interior field nodes as well as any exterior boundary nodes that are immediately adjacent to the region are included in the definition_. If a FIELD modifier is present on a LOCATE command, then the exterior boundary nodes are omitted.

Two additional modifiers are available with the subregion identification on an input command (say a SET command) to further select a subset of the region specified by the LOCATE command. These are the FIELD and the “dir” modifiers. If a FIELD modifier is specified alongside an ID=idsub modifier on an input command (say a SET command), then the command applies only to the field nodes and not to the exterior boundary nodes included in the subrgn. For example, if this modifier is present on a SET command, then the values are set at all nodes in the interior of the subregion but not at the boundary. The FIELD modifier is ignored if the LOCATE command was specified for a structured grid with the grid index coordinates. In that case the values are set as defined by the (I,J,K) grid indices. For structured grids, it is also possible to specify a dir modifier along with the ID=idsub specification on an input command. In this case, only the nodes at the subregion boundary where the outward normal matches the specified dir modifier are selected. See the Section 3.5 below for available choices for the dir specification.

_The only exception to the above is an input command that specifies a node-by-node input for a subdomain (see, Sections 4.5 and 4.6) for a subregion defined by a LOCATE command that specifies a rectangular window based on (I,J,K) grid indices. In this case, the nodes selected are exactly as specified by the (I,J,K) grid indices. For this node-by-node function a FIELD modifier either on the corresponding LOCATE command or on the input command is ignored. See Sections 4.5 and 4.6 for further details._
3.5 BOUNDARY IDENTIFICATION

Some of the commands refer to input for the boundaries of the problem. These boundaries may be the external boundaries, which enclose the domain of computation, or these may be internal boundaries that are located within the domain of computation. For these commands the boundary orientation is identified either explicitly on the command by a direction modifier or it is specified as an integral part of the sub-domain specification by the LOCATE command with a PAIRED list of element and surface numbers.

The identification of the boundary orientation by a direction modifier (dir) is illustrated in Table 3.5.1. The modifier consists of a character followed by a sign that represents the direction of the outward normal at the boundary. It should be noted that this direction is a nominal direction with respect to the local orientation of the grid element (ξ, η, ζ) for a curvilinear grid). This orientation may or may not be related to the global framework in which the (x, y, z) coordinates of the element vertices are specified. The local orientation for an element is uniquely determined by the manner in which its vertices are numbered. The notation is illustrated in Figure 3.5.1 for both 2D and 3D elements. The vertices are numbered in an anti-clockwise manner in the xy-plane. Briefly, the local x (ξ) vector points from vertex 1 to vertex 2, the local y (η) vector from vertex 1 to vertex 4 and, for 3D elements, the local z (ζ) vector from vertex 1 to vertex 5. For a structured grid the local and global framework are consistent with each other. However, for an unstructured grid, the local framework may change from element to element since the vertex numbering may be completely arbitrary. In such a case a more general description is used which consists of the specification of a paired list of element and surface numbers (see LOCATE command with PAIR modifier). As illustrated in Figure 3.5.1, the surface numbers for 2D elements vary from 1 to 4 and those for 3D elements from 1 to 6.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-</td>
<td>The outward normal is in the negative direction of the local x or ξ coordinate. It is equivalent to the specification of surface number 1 of Figure 3.51.</td>
</tr>
<tr>
<td>X+</td>
<td>The outward normal is in the positive direction of the local x or ξ coordinate. It is equivalent to the specification of surface number 2 of Figure 3.51.</td>
</tr>
<tr>
<td>Y-</td>
<td>The outward normal is in the negative direction of the local y or η coordinate. It is equivalent to the specification of surface number 3 of Figure 3.51.</td>
</tr>
<tr>
<td>Y+</td>
<td>The outward normal is in the positive direction of the local y or η coordinate. It is equivalent to the specification of surface number 4 of Figure 3.51.</td>
</tr>
<tr>
<td>Z-</td>
<td>The outward normal is in the negative direction of the local z or ζ coordinate. It is equivalent to the specification of surface number 5 of Figure 3.51.</td>
</tr>
<tr>
<td>Z+</td>
<td>The outward normal is in the positive direction of the local z or ζ coordinate. It is equivalent to the specification of surface number 6 of Figure 3.51.</td>
</tr>
</tbody>
</table>
Vertex and Face Number Nomenclature for a Quadrilateral Element

![Quadrilateral Element Diagram]

Vertex and Face number Nomenclature for a Hexahedral Element

![Hexahedral Element Diagram]

FIGURE 3.5.1: BOUNDARY INDEX NOTATION
3.6 SPECIFICATION OF FLUID PHASE

Some of the ACRi software tools can simulate multi-phase flow while other tools are restricted to a single-phase flow. For example, PORFLOW™ can simulate up to three phases for the fluid. Some of the input commands are used to provide input for one or more of these phases. The modifier that specifies the phase in the command itself is symbolically denoted by ‘phase’ in this manual. The choices available for this modifier are summarized in Table 3.6.1. The phase modifier is currently only available with the multi-phase versions of the ANSWER™ and PORFLOW™ Software Tools; it is not available with TIDAL™ series of ACRi software.

<table>
<thead>
<tr>
<th>User Specification of phase</th>
<th>Interpretation For The Corresponding Command</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIRSt</td>
<td>The input is specified for the first phase of the fluid. This is always the default option; if no modifier is specified, then the input is assumed to be for the first phase of the fluid.</td>
</tr>
<tr>
<td>SECONd</td>
<td>The input is for the second phase of the fluid.</td>
</tr>
<tr>
<td>THIRd</td>
<td>The input is for the third phase of the fluid. This modifier is available only for the PORFLOW™ Software Tool.</td>
</tr>
<tr>
<td>GAS</td>
<td>The input is for the GAS Phase of the fluid. The gas phase is always the last of the active fluid phases. Thus this modifier is equivalent to the FIRSt modified for a single-phase gas, the SECONd modifier for a liquid-gas, and the THIRd modifier for a liquid-liquid-gas simulation.</td>
</tr>
<tr>
<td>VAPO</td>
<td>Same as GAS Modifier</td>
</tr>
</tbody>
</table>

TABLE 3.6.1: VALID MODIFIERS FOR PHASE DESIGNATION
3.7 SPECIFICATION OF FREQUENCY FOR OUTPUT

Many of the output commands provide for an option for the user to specify the frequency of output. This input is denoted in this manual by the symbol $V_{frq}$ and may be specified in terms of the number of steps or the time interval. The step interval mode is the default mode and in this case, for example, a specification of 10 will result in output at step number 10, 20, 30, etc. The time interval mode is activated if the modifier TIME is present on the command. In this case, whether or not the output is obtained exactly at the specified interval, depends on the time step specified by the SOLVE command. If an exact time at which the output is due is not simulated, then the output is obtained at the first time step after the due time.
CHAPTER 4

FUNCTIONAL INPUT FOR FREEFORM COMMANDS

This chapter describes the built-in and user-specified functions that can be used to specify key components of the FREEFORM input as functions of other built-in and user specified phase space variables. These functions can be applied to initial and boundary conditions, sources and fluid and host matrix properties. Additionally these functions can be used for extensive user specific pre-and post-processing of input data and results obtained from the ACRI Software Tools.
4.1 GENERAL FUNCTIONAL RELATIONSHIPS

A number of commands allow the use of a functional form for the required input. The general form of the functional relationship is:

$$\Phi = \Phi(\xi)$$  \hspace{1cm} (4.1.1)

where $\Phi$ represents a field variable, or a source or boundary value for a dependent variable, and represents time, a spatial coordinate or a field variable. A library of built-in tabular and analytic functions for $\Phi$ is provided. In addition, it is possible to specify user-defined functions as discussed in Section 4.7. The user should note that the library of built-in functions is constantly being updated and additional options may have been incorporated subsequent to the date of publication of this manual. Please contact ACRi for the latest information. In the description of all these functions the symbols $A_n$, $A$, $B$, $C$, $D$, $E$ and $F$ represent constants.

4.1.1 The Tabular Function

The most powerful and general option available for this purpose is that of a tabular function in which $\Phi$ is specified as an arbitrary function of $\xi$. The desired value is obtained as a step-wise or piece-wise linear, quadratic or cubic approximation over the values of $\Phi$ in the neighborhood of the given value of $\xi$. This can be expressed as:

$$\Phi(\xi_n + \delta \xi) = \Phi_n + \alpha \left( \frac{\partial \Phi}{\partial \xi} \delta \xi \right)_n + \beta \left( \frac{\partial^2 \Phi}{\partial \xi^2} \delta \xi^2 \right)_n + \gamma \left( \frac{\partial^3 \Phi}{\partial \xi^3} \delta \xi^3 \right)_n; \quad \xi_n < \xi < \xi_{n+1}$$  \hspace{1cm} (4.1.2)

where $\alpha=\beta=\gamma=0$ for step wise, $\alpha=1$; $\beta=\gamma=0$ for linear, $\alpha=1$; $\beta=1/2$; $\gamma=0$ for quadratic and $\alpha=1$; $\beta=1/2$; $\gamma=1/6$ for cubic interpolation. For the higher order polynomials, the gradients near the boundaries are computed by one-sided Taylor-Series expansion.

For periodic implementation of the tabular function, the value of $\xi$ used in the above interpolation relation is computed as:

$$\xi_{used} = \text{mod}[\xi, (\xi_N - \xi_1)]$$  \hspace{1cm} (4.1.3)

If extrapolation of the tabular function is specified; then the values are extrapolated by:

$$\Phi(\xi_1 + \delta \xi) = \Phi_1 + \left( \frac{\partial \Phi}{\partial \xi} \delta \xi \right)_1; \quad \xi < \xi_1$$  \hspace{1cm} (4.1.4)

$$\Phi(\xi_N + \delta \xi) = \Phi_N + \left( \frac{\partial \Phi}{\partial \xi} \delta \xi \right)_N; \quad \xi > \xi_N$$

4.1.2 Discrete Point-Wise Function

This function allows the specification of a table of values for a subregion such that for each node of the subregion:

$$\Phi_n = A_n; \quad 1 < n \leq N$$  \hspace{1cm} (4.1.5)

where $A_n$ are arbitrary constants and $N$ is the total number of nodes in the subregion.

4.1.3 Discrete Point-Wise Time-Dependent Function

This function allows the specification of a table of values for a subregion such that for each node of the subregion the values are a function of time. The general form of the given input is:

$$\Phi_n(t) = A_n; \quad 1 < n \leq N$$  \hspace{1cm} (4.1.6)

where $A_n$ are arbitrary constants and $N$ is the total number of nodes in the subregion. The individual values at any given time are computed from sets of values specified at discrete time intervals at $t=t^1, t^2, \ldots, t^M$ from:
\[
\Phi_n^t = \Phi_n^m + \alpha \frac{t-t^m}{t^{m+1}-t^m} (\Phi_n^{m+1} - \Phi_n^m); \quad t^m \leq t < t^{m+1}.
\]

(4.1.7)

Where the coefficient \( \alpha \) is set to 0 for step-wise and 1 for linear interpolation:

### 4.1.4 Discrete Point-Wise Random Functions

The Random functions allow the assignment of values to each node of the subregion such that the overall distribution is random without any recognizable patterns. The well-known examples of random numbers are the results of the roll of an ideal die and the sequence of digits that appear in the number \( \pi \). The set of random numbers generated by the built-in generators is a sequence of Pseudo-Random Numbers (PRN) and should be sufficient for most engineering purposes. If "true" randomness is required then the user is advised to generate such a sequence and specify it through a file with the option defined by Equation 4.1.5 above.

Three distinct PRN options are currently available: these are the Uniform, Normal (Gaussian) and Log-Normal set of random numbers.

#### The Uniform Random number generator

The Uniform Random number generator uses the “Minimal” Pseudo Random Number Generator of Park and Miller (1988) with Bays-Durham Shuffle. This generator belongs to the group of Linear Congruential Generators (LCG). The cycle repeats after 2,147,483,647 numbers. The sequence of normally distributed PNR, \( x_n \), is generated from the uniformly distributed PNR (see Equations 4.1.9) by the Box-Muller Transformation.

\[
pdf(x) = \frac{1}{R}, \quad \mu - \frac{R}{2} \leq x \leq \mu + \frac{R}{2}; \quad \text{0 for all other } x
\]

(4.1.9)

\[
cdf(x) = \frac{x - \mu}{R}, \quad \mu - \frac{R}{2} \leq x \leq \mu + \frac{R}{2}; \quad \text{0 if } x < \mu - \frac{R}{2}; \quad 1 \text{ if } x > \mu + \frac{R}{2}
\]

(4.1.10)

The mean, the median and the variance of the uniform distribution are given by:

\[
E(x) = \mu; \quad m(x) = \mu; \quad Var(x) = \frac{R^2}{12}
\]

(4.1.11)

The Normal or Gaussian probability density function (pdf) is defined by a mean, \( \mu \), and a standard deviation, \( \sigma \). The sequence of normally distributed PNR, \( x_n \), is generated from the uniformly distributed PNR (see Equations 4.1.9) by the Box-Muller Transformation. With \( x \) as the random variable the pdf and its cdf are given by:

\[
pdf(x) = \frac{1}{\sqrt{2\pi} \sigma^2} \exp \left[ -\frac{(x-\mu)^2}{2\sigma^2} \right], \quad \text{(4.1.12)}
\]

\[
cdf(x) = \frac{1}{2} + \frac{1}{2} \text{erf} \left( \frac{x-\mu}{\sqrt{2} \sigma} \right), \quad \text{(4.1.13)}
\]

The mean, the median and the variance of the normal distribution are given by:

\[
E(x) = \mu; \quad m(x) = \mu; \quad Var(x) = \sigma^2
\]

(4.1.14)

The Log-normal distribution is the single-tailed probability distribution of a random variable such that the logarithm of the random variable is normally distributed. It is based on the built-in generator for normally distributed PNR described above and uses the exponential of the random numbers to generate a log-normal distribution. The pdf and cdf of the distribution are:
\[
\text{pdf}(x) = \frac{1}{\sqrt{2\pi \sigma^2}} \exp\left[-\frac{(\ln(x) - \mu)^2}{2\sigma^2}\right],
\]
(4.1.15)
\[
\text{cdf}(x) = \frac{1}{2} + \frac{1}{2} \text{erf} \left( \frac{\ln(x) - \mu}{\sigma \sqrt{2}} \right),
\]
(4.1.16)

The mean, \(E(x)\), the median, \(m(x)\), and the variance of the Log-Normal distribution are given by:
\[
E(x) = e^{\mu + \sigma^2/2}; \quad m = e^\mu; \quad \text{Var}(x) = \left(e^{\sigma^2} - 1\right)e^{2\mu + \sigma^2}
\]
(4.1.17)

The log-normal distribution is also assigned to a sub-domain according to Equation 4.1.12 above.

4.1.5 The Constant Function
\[\Phi = A\]
(4.1.18)

4.1.6 Replacement Function
\[\Phi = \xi\]
(4.1.19)

4.1.7 Multivariate Polynomial Functions
\[
\Phi = A_0 + \sum_{n=1}^{N} A_n \xi_n, \quad 1 \leq N \leq 7
\]
(4.1.20)
\[
\Phi = A_0 + \sum_{n=1}^{N} \left( A_n \xi_n + B_n \xi_n^2 \right), \quad 1 \leq N \leq 7
\]
(4.1.21)
\[
\Phi = A_0 + \sum_{n=1}^{N} \left( A_n \xi_n + B_n \xi_n^2 + C_n \xi_n^3 \right), \quad 1 \leq N \leq 7
\]
(4.1.22)

4.1.8 The Higher Order Polynomial Functions
\[
\Phi = A + B \xi + C \xi^2 + D \xi^3 + E \xi^4 + F \xi^5 + G \xi^6 + H \xi^7,
\]
(4.1.23)
\[
\Phi = A + B \xi + C \xi^2 + D \xi^3 + E \xi^4 + F \xi^5 + G \xi^6,
\]
(4.1.24)
\[
\Phi = A + B \xi + C \xi^2 + D \xi^3 + E \xi^4 + F \xi^5 + G \xi^6 + H \xi^7,
\]
(4.1.25)
\[
\Phi = A + B \xi + C \xi^2 + D \xi^3 + E \xi^4 + F \xi^5 + G \xi^6 + H \xi^7,
\]
(4.1.26)

4.1.9 The Power Functions
\[
\Phi = A \left( \xi + B \right)^C + D,
\]
(4.1.27)
\[
\Phi = A \left| \xi + B \right|^C + D,
\]
(4.1.28)

4.1.10 The Exponential Functions
\[
\Phi = A \exp \left( B \xi + C \right) + D,
\]
(4.1.29)
\[
\Phi = \sum_{n=1}^{N} A_n \exp \left( B_n \xi + C_n \right) + D,
\]
(4.1.30)

4.1.11 The Logarithmic Functions
\[
\Phi = A \ln \left( B \xi + C \right) + D,
\]
(4.1.31)
\[ \Phi = \sum_{n=1}^{N} A_n \ln \left( B_n \xi + C_n \right) + D, \quad (4.1.32) \]

**4.1.12 The Trigonometric Functions**

\[ \Phi = A \sin \left( B \xi + C \right) + D, \quad (4.1.33) \]
\[ \Phi = \sum_{n=1}^{N} A_n \sin \left[ 2\pi \frac{\xi + C_n}{B_n} \right] + D \quad (4.1.34) \]
\[ \Phi = A \cos \left( B \xi + C \right) + D, \quad (4.1.35) \]
\[ \Phi = \sum_{n=1}^{N} A_n \cos \left[ 2\pi \frac{\xi + C_n}{B_n} \right] + D \quad (4.1.36) \]
\[ \Phi = A \tan \left( B \xi + C \right) + D, \quad (4.1.37) \]
\[ \Phi = \sum_{n=1}^{N} A_n \tan \left[ 2\pi \frac{\xi + C_n}{B_n} \right] + D \quad (4.1.38) \]
\[ \Phi = A \arcsin \left( B \xi + C \right) + D, \quad (4.1.39) \]
\[ \Phi = \sum_{n=1}^{N} A_n \arcsin \left[ 2\pi \frac{\xi + C_n}{B_n} \right] + D \quad (4.1.40) \]
\[ \Phi = A \arccos \left( B \xi + C \right) + D, \quad (4.1.41) \]
\[ \Phi = \sum_{n=1}^{N} A_n \arccos \left[ 2\pi \frac{\xi + C_n}{B_n} \right] + D \quad (4.1.42) \]
\[ \Phi = A \arctan \left( B \xi + C \right) + D, \quad (4.1.43) \]
\[ \Phi = \sum_{n=1}^{N} A_n \arctan \left[ 2\pi \frac{\xi + C_n}{B_n} \right] + D \quad (4.1.44) \]

**4.1.13 Rational Functions**

\[ \Phi = \frac{A + B \xi}{C + D \xi}, \quad (4.1.45) \]
\[ \Phi = \left( \frac{A + B \xi}{C + D \xi} \right)^E \cdot \left( \frac{A + B \xi}{C + D \xi} \right)^F, \quad (4.1.46) \]

**4.1.14 Power of Ten Function**

\[ \Phi = A 10^{\xi+C} + D \quad (4.1.47) \]

**4.1.15 Inverse Exponential Function**

\[ \Phi = A \exp \left( \frac{B}{\xi+C} \right) + D, \quad (4.1.48) \]

**4.1.16 Gate Function**

\[ \Phi = \beta AB \sqrt{|\xi-C|}; \quad \beta = 1 \text{ if } \xi > C \text{ otherwise } \beta = 1; \quad (4.1.49) \]
4.1.17 Sutherland Function

\[ \Phi = A \frac{B + C}{\xi + C} \frac{\xi}{B}^{3/2} \]  

(4.1.50)

4.1.18 Multivariate Linear Sum

\[ \Phi = \sum_{n=1}^{N} \xi_n \]  

(4.1.51)

\[ \Phi = \sum_{n=1}^{N} A_n \xi_n + A_{N+1} \]  

(4.1.52)

4.1.19 Multivariate Square Sum

\[ \Phi = \sum_{n=1}^{N} \xi_n^2 \]  

(4.1.53)

\[ \Phi = \sum_{n=1}^{N} A_n \xi_n^2 + A_{N+1} \]  

(4.1.54)

4.1.20 Multivariate Square Root of Sum of Squares

\[ \Phi = \sqrt{\sum_{n=1}^{N} \xi_n^2} \]  

(4.1.55)

\[ \Phi = \sqrt{\sum_{n=1}^{N} A_n \xi_n^2 + A_{N+1}} \]  

(4.1.56)
4.2 COMMAND INPUT OF FUNCTIONAL FORM

The functional form of input can be used with a number of commands. Currently these include the ABSORPTIVITY, BOREHOLE, BOUNDARY, CONDUCTION, DENSITY, DIFFUSION, DISTRIBUTION, FLOW, FRACTURE, GAS, RADIATION, RETARDATION, SET, SOURCE, SPECIFIC heat, STORAGE, SWIRL, TRANSFER, and VISCOSITY commands. These commands are described in detail in the following sections. However, the functional specification for all these commands is identical.

Modifiers on the input command select the specific functional relation and the independent variable. These modifiers are referred to as "func" and $\xi$, respectively. Valid input options for $\text{func}$ and their corresponding interpretations are given in Tables 4.2.1. Valid input options for independent variable $\xi$ are listed in Tables 2.8.1-3. For functions that depend on only a single variable, one of the variables listed in Table 4.2.2 is also allowed as an independent variable.

The numerical input required depends on the type of function selected. For numerical input, these functions may be divided into four categories. The nature of the required input for each category is summarized in Tables 4.2.4 through 4.2.6. By default, the value of the function at a location is computed from the value of the independent variable, $\xi$, at the same location. However, if the modifier “STAC” is present on a command then the function is evaluated with the value of $\xi$ at the most recent location specified by the STACK command.

Most of the commands described above (except the tabular and the discrete point-wise functions) have the additional option that the function may be truncated to retain only the positive or the negative values. This is achieved by specifying the modifiers “POSITIVE” and “NEGATIVE” with the functional relation.
<table>
<thead>
<tr>
<th>Function</th>
<th>Option</th>
<th>Dependent Variable Computed From</th>
</tr>
</thead>
<tbody>
<tr>
<td>TABL</td>
<td></td>
<td>Equation 4.1.2 with STEP, LINE, QUAD or CUBI modifiers</td>
</tr>
<tr>
<td>TABL</td>
<td>PERI</td>
<td>Equations 4.1.2 and 4.1.3 with STEP, LINE, QUAD or CUBI modifiers</td>
</tr>
<tr>
<td>TABL</td>
<td>EXTR</td>
<td>Equations 4.1.2 and 4.1.4 with STEP or LINE or QUAD modifiers</td>
</tr>
<tr>
<td>NODE</td>
<td></td>
<td>Equation 4.1.5</td>
</tr>
<tr>
<td>NODE</td>
<td>TIME</td>
<td>Equation 4.1.7 with STEP (α=0) or LINE (α=1) modifier</td>
</tr>
<tr>
<td>RANDOM</td>
<td>UNIF</td>
<td>Equation 4.1.9</td>
</tr>
<tr>
<td>RANDOM</td>
<td>GAUS</td>
<td>Equation 4.1.12</td>
</tr>
<tr>
<td>RANDOM</td>
<td>LOG</td>
<td>Equation 4.1.15</td>
</tr>
<tr>
<td>CONS</td>
<td></td>
<td>Equation 4.1.18</td>
</tr>
<tr>
<td>EQUAL</td>
<td></td>
<td>Equation 4.1.19</td>
</tr>
<tr>
<td>LINE</td>
<td></td>
<td>Equation 4.1.20</td>
</tr>
<tr>
<td>CUBI</td>
<td></td>
<td>Equation 4.1.21</td>
</tr>
<tr>
<td>QUAD</td>
<td></td>
<td>Equation 4.1.22</td>
</tr>
<tr>
<td>POLY</td>
<td></td>
<td>Equation 4.1.20 through Equation 4.1.26</td>
</tr>
<tr>
<td>POWE</td>
<td></td>
<td>Equation 4.1.27</td>
</tr>
<tr>
<td>POWE</td>
<td>MODU</td>
<td>Equation 4.1.28</td>
</tr>
<tr>
<td>EXP or EXPO</td>
<td></td>
<td>Equation 4.1.29</td>
</tr>
<tr>
<td>EXP or EXPO</td>
<td>SERIes</td>
<td>Equation 4.1.30</td>
</tr>
<tr>
<td>LN or LOG</td>
<td></td>
<td>Equation 4.1.31</td>
</tr>
<tr>
<td>LN or LOG</td>
<td>SERIes</td>
<td>Equation 4.1.32</td>
</tr>
<tr>
<td>SIN or SINE</td>
<td></td>
<td>Equation 4.1.33</td>
</tr>
<tr>
<td>SIN or SINE</td>
<td>SERIes</td>
<td>Equation 4.1.34</td>
</tr>
<tr>
<td>COS or COSI</td>
<td></td>
<td>Equation 4.1.35</td>
</tr>
<tr>
<td>COS or COSI</td>
<td>SERIes</td>
<td>Equation 4.1.36</td>
</tr>
<tr>
<td>TAN or TANG</td>
<td></td>
<td>Equation 4.1.37</td>
</tr>
<tr>
<td>TAN or TANG</td>
<td>SERIes</td>
<td>Equation 4.1.38</td>
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<td>ASIN</td>
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<tr>
<td>ASIN</td>
<td>SERIes</td>
<td>Equation 4.1.40</td>
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<td>SERIes</td>
<td>Equation 4.1.42</td>
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</tr>
<tr>
<td>ATAN</td>
<td>SERIes</td>
<td>Equation 4.1.44</td>
</tr>
<tr>
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</tr>
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<td>Equation 4.1.46</td>
</tr>
<tr>
<td>POWER</td>
<td>TEN</td>
<td>Equation 4.1.47</td>
</tr>
<tr>
<td>EXP or EXPO</td>
<td>INVE</td>
<td>Equation 4.1.48</td>
</tr>
<tr>
<td>GATE</td>
<td></td>
<td>Equation 4.1.49</td>
</tr>
<tr>
<td>SUTHERLAND</td>
<td></td>
<td>Equation 4.1.50</td>
</tr>
<tr>
<td>SUM</td>
<td></td>
<td>Equation 4.1.51 or Equation 5.1.52</td>
</tr>
<tr>
<td>SQUA</td>
<td></td>
<td>Equation 4.1.53 or Equation 5.1.54</td>
</tr>
<tr>
<td>ROOT</td>
<td></td>
<td>Equation 4.1.55 or Equation 5.1.56</td>
</tr>
<tr>
<td>USER</td>
<td>GLOBal</td>
<td>User-defined function called only once for the computational domain.</td>
</tr>
</tbody>
</table>
### TABLE 4.2.2: VALID INDEPENDENT VARIABLES

<table>
<thead>
<tr>
<th>User Specification $\xi$</th>
<th>Denotes Independent Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIME</td>
<td>$t$</td>
</tr>
<tr>
<td>X</td>
<td>Coordinate $x$</td>
</tr>
<tr>
<td>Y or R</td>
<td>Coordinate $y$ (or $r$ for radial geometry)</td>
</tr>
<tr>
<td>Z or THETA</td>
<td>Coordinate $z$ (or $\theta$ for radial geometry)</td>
</tr>
<tr>
<td>Any of the symbols in Table 2.8.1-3</td>
<td>The corresponding variable listed in Table 2.8.1-3</td>
</tr>
</tbody>
</table>

### TABLE 4.2.3: NUMERICAL INPUT FOR THE TABLE SPECIFICATION

<table>
<thead>
<tr>
<th>Numerical Value</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>The number of sets of input in the table that are specified by Equation 4.1.2.</td>
</tr>
<tr>
<td>N2, ... , Nn</td>
<td>The pairs of values, $\xi_n$ and $\theta_n$ (in that order), for Equation 4.1.2. A total of $2^*N_1$ values (N1 sets) must be specified.</td>
</tr>
</tbody>
</table>

### TABLE 4.2.4: NUMERICAL INPUT FOR SIMPLE ANALYTIC FUNCTIONS

<table>
<thead>
<tr>
<th>Numerical Value</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1, ... , Nn</td>
<td>The constants $A_n$ for Equation 4.1.4 or the constants $A$ through $E$ for the functions defined by Equations 4.1.5 through 4.1.18, as appropriate. The number of values must match those required by the function. For Equation 4.1.4, the number of values must equal the number of nodes in the subregion for which the input is specified. The constant function is specified by a single numerical value. Two values are required for the linear relation, five for the polynomial and four for all other functions.</td>
</tr>
</tbody>
</table>

### TABLE 4.2.5: NUMERICAL INPUT FOR THE SERIES FUNCTIONS

<table>
<thead>
<tr>
<th>Numerical Values</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>The number of sets of input in the series specified by Equations given above with the “SERIES” modifier.</td>
</tr>
<tr>
<td>N2, ... , Nn-1</td>
<td>The triplet of values of $A_n$, $B_n$, and $C_n$ (in that order), for the series functions. A total of $3^*N_1$ values (N1 sets) must be specified.</td>
</tr>
<tr>
<td>Nn</td>
<td>The datum $A_0$ for the function.</td>
</tr>
</tbody>
</table>

### TABLE 4.2.6: NUMERICAL INPUT FOR USER SPECIFIED FUNCTIONS

<table>
<thead>
<tr>
<th>Numerical Value</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>The function identification number assigned by the user. Valid values must lie between 1 and 1024 (inclusive). The user must assign a value. For implementation of the function the control is transferred to the USRFNC module and this identification number is returned to the user as the IDUSR variable. The software does not distinguish between the assigned numbers and the same identification number may be assigned more than once, if so desired.</td>
</tr>
<tr>
<td>N2, ... , Nn</td>
<td>The numerical values, if any, which are required by the user to implement the function. These values are returned to the user in the RUSR array when the control is transferred to the USRFNC array.</td>
</tr>
</tbody>
</table>
4.3 SPECIFICATION OF ADDITIONAL OPERATIONS FOR FUNCTIONS

Many commands that allow the use of functions further allow the values to be manipulated according to a number of operations that can be specified on the command. The available operations are denoted by the character string “operation” on the command that can be replaced by one (or more) of the modifiers summarized in the Table below. These options are available with the DENSITY, SET, VISCOSITY and a number of other commands. The availability for a particular command is indicated by the presence of the “operation” on the command.

<table>
<thead>
<tr>
<th>operation</th>
<th>Operation Performed</th>
</tr>
</thead>
<tbody>
<tr>
<td>REPLACE</td>
<td>The computed value replaces the existing value for that variable. This is the default option.</td>
</tr>
<tr>
<td>ADD</td>
<td>The computed value is added to the existing value for that variable.</td>
</tr>
<tr>
<td>SUBTRACT</td>
<td>The computed value is subtracted from the existing value for that variable.</td>
</tr>
<tr>
<td>MULTIPLY</td>
<td>The computed value multiplies the existing value for that variable.</td>
</tr>
<tr>
<td>DIVIDE</td>
<td>The computed value divides the existing value for that variable. A value of 1.E-30 is added to the divisor if it is zero.</td>
</tr>
<tr>
<td>ABS or ABSO</td>
<td>The absolute value of the computed function is taken. This modifier may be present along with one of the REPLACE, ADD, SUBTRACT, MULTIPLY or DIVIDE modifiers</td>
</tr>
<tr>
<td>POSITIVE</td>
<td>The negative values for the computed function are set of zero. This modifier may be present along with one of the REPLACE, ADD, SUBTRACT, MULTIPLY or DIVIDE modifiers</td>
</tr>
<tr>
<td>NEGATIVE</td>
<td>The positive values for the computed function are set of zero. This modifier may be present along with one of the REPLACE, ADD, SUBTRACT, MULTIPLY or DIVIDE modifiers</td>
</tr>
</tbody>
</table>

In case of multiple specification of REPLACE, ADD, SUBTRACT, MULTIPLY and DIVIDE modifiers, the first specification takes precedence over others. Similarly in case of multiple specification of ABS or ABSO, POSITIVE and NEGATIVE, the first specification takes precedence over others.
### EXAMPLES OF FUNCTIONAL FORM OF INPUT

The Tables 4.4.1 through 4.4.3 below provide a number of illustrative examples. The exact interpretation of the input depends upon the particular command and the attributes associated with the command. For example, whereas the **SET** command specifies the value of the dependent variable, the **SOURCE** command would specify the source for that variable and, the **BOUNDARY** command may specify the value of the variable or that of the flux of the variable.

#### TABLE 4.4.1: EXAMPLES OF SIMPLE ANALYTIC FUNCTIONS

<table>
<thead>
<tr>
<th>Illustrative Commands</th>
</tr>
</thead>
<tbody>
<tr>
<td>/// Constant boundary temperature of 30.</td>
</tr>
<tr>
<td>BOUNDARY value at X+ is CONSTANT T = 30.</td>
</tr>
<tr>
<td>/// Source for temperature is a constant value for active subregion</td>
</tr>
<tr>
<td>SOURce for T: = 100 W/m^3 in currently SELECTed subregion</td>
</tr>
<tr>
<td>/// Field values of T set as a power law of pressure in previously identified subregion</td>
</tr>
<tr>
<td>SET T as POWER law: [1.020 * (P + 0.) ^ 0.50 + 100] in subregion ID=ZON1</td>
</tr>
<tr>
<td>/// Boundary temperature is a sinusoidal function of time</td>
</tr>
<tr>
<td>BOUNDary value at Y+: function: T = 10. * SIN (0.003 * TIME +0.5) +10.</td>
</tr>
<tr>
<td>/// Field values of temperature set as a polynomial function of coordinate X</td>
</tr>
<tr>
<td>SET T: POLYnomial in X: (10, 0.5, 0, -0.1, 0.)</td>
</tr>
<tr>
<td>/// Boundary temperature is a linear function of y coordinate</td>
</tr>
<tr>
<td>BOUNdary value at X+ boundary LINEar function: T = 30. -0.015 * Y</td>
</tr>
<tr>
<td>/// Temperature is a cosine function of time</td>
</tr>
<tr>
<td>SET T as 100 * COSIne (0.00274 * TIME)</td>
</tr>
<tr>
<td>/// Temperature is an exponentially decaying function of time</td>
</tr>
<tr>
<td>SET T as 100 * EXP (-0.001 * TIME) +100.</td>
</tr>
<tr>
<td>/// Source for temperature is a linear function of Pressure</td>
</tr>
<tr>
<td>SOURce LINEar function (T = 0. -0.10 * P)</td>
</tr>
<tr>
<td>/// Source for temperature is a cosine function of time</td>
</tr>
<tr>
<td>SOURce T COSIne function of TIME: 100, 0.00274, 0., +10.5</td>
</tr>
<tr>
<td>/// Thermal conductivity for temperature is a linear function of temperature itself</td>
</tr>
<tr>
<td>CONDuctivity for T LINEar function: 0. -0.10 * T</td>
</tr>
<tr>
<td>Illustrative Commands</td>
</tr>
<tr>
<td>-----------------------</td>
</tr>
<tr>
<td>/// Boundary $P$ is a function of $T$ (temperature)</td>
</tr>
<tr>
<td>BOUNDary value for $P$ at $Y$-boundary: COSine SERIes in $T$: 3 sets</td>
</tr>
<tr>
<td>(0, 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.</td>
</tr>
<tr>
<td>/// Field values for temperature set as sinusoidal function of $Y$ coordinate</td>
</tr>
<tr>
<td>SET $T$ as SINE SERIes in $Y$: 3 sets: (0, 5, 1), (100, 10, 1), (200, 20, 3)</td>
</tr>
<tr>
<td>/// Source for temperature is a 3 term cosine series in velocity $U$</td>
</tr>
<tr>
<td>SOURce $T$ as COSIne SERIes in $U$: 3 sets</td>
</tr>
<tr>
<td>(0, 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.</td>
</tr>
<tr>
<td>/// Boundary flux for $T$ is a 3 part sinusoidal function of temperature</td>
</tr>
<tr>
<td>BOUNDary $T$ at $Y$-boundary FLUX type: SINE SERIes in $T$: 3 sets</td>
</tr>
<tr>
<td>(0, 5, 1), (100, 10, 1), (200, 20, 3) datum= 0., $h=1.E-4$</td>
</tr>
<tr>
<td>/// Source for temperature is a function of temperature (itself)</td>
</tr>
<tr>
<td>SOURce $T$ SINE SERIes in $T$: 3 sets: (0, 5, 1), (100, 10, 1), (200, 20, 3)</td>
</tr>
<tr>
<td>/// Source for $T$ as an exponential function of time</td>
</tr>
<tr>
<td>SOURce $T$: EXPOnential SERIes in TIME; with 3 terms</td>
</tr>
<tr>
<td>(0.1, 1.0) (0.05, 0.1) (0.001, 01), base value = 0.</td>
</tr>
<tr>
<td>/// Field value of $U$ velocity is set as a function of Temperature</td>
</tr>
<tr>
<td>SET value for $U$ as COSIne SERIes in $T$: 3 sets</td>
</tr>
<tr>
<td>(0., 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.</td>
</tr>
<tr>
<td>/// Pressure set as a 24 part cosine series; coefficients are contained in file named 'COSVALS'</td>
</tr>
<tr>
<td>SET $P$ as COSIne SERIes of $T$: 24 sets from file 'COSVALS'</td>
</tr>
</tbody>
</table>
### TABLE 4.4.3: EXAMPLES OF TABULAR FUNCTIONS

<table>
<thead>
<tr>
<th>Illustrative Commands</th>
</tr>
</thead>
<tbody>
<tr>
<td>/// The value of P at the boundary is a tabular function of time</td>
</tr>
<tr>
<td><strong>BOUNDary</strong> P value at Y- boundary: <strong>TABLE</strong> of values: 3 sets (TIME, value)</td>
</tr>
<tr>
<td>(0., 0.01), (100, 0.10), (200, -0.20)</td>
</tr>
<tr>
<td>/// The flux of P at the boundary is a tabular function of time</td>
</tr>
<tr>
<td><strong>BOUNDary</strong> P at X+: <strong>FLUX</strong> is <strong>TABLE</strong> in <strong>TIME</strong>: 3 sets</td>
</tr>
<tr>
<td>(0., 5), (100, 15), (200, 3.5), h=0.001</td>
</tr>
<tr>
<td>/// The field values of temperature are set as a tabular function of time</td>
</tr>
<tr>
<td><strong>SET T as <strong>TABLE</strong> of values</strong>: 3 sets: (0., 0.01), (100, 0.10), (200, -0.20)</td>
</tr>
<tr>
<td>/// As above except that step-wise, rather than the linear, interpolation is used</td>
</tr>
<tr>
<td><strong>SET T is <strong>STEP</strong> wise <strong>TABLE</strong>: 3 sets</strong>: (0., 0.01), (100, 0.10), (200, -0.20)</td>
</tr>
<tr>
<td>/// As above except that the values will be repeated after 200 time units</td>
</tr>
<tr>
<td>**SET T is <strong>PER</strong>iodic <strong>TABLE</strong> with <strong>STEP</strong> wise <strong>interpolation</strong>: 3 sets:</td>
</tr>
<tr>
<td>(0., 0.01), (100, 0.10), (200, -0.20)</td>
</tr>
<tr>
<td>/// Table with linear interpolation but time input set to result in steep step-like interpolation</td>
</tr>
<tr>
<td><strong>SET T for as <strong>TABLE</strong> of values</strong>: with 6 sets: (TIME, value)</td>
</tr>
<tr>
<td>(0., 0.0), (1.0000, 0.0), (1.0001, 1.0), (2., 1.0), (2.0001, 0.5), (3.0000, 0.2)</td>
</tr>
<tr>
<td>/// Table with linear interpolation but input from a file</td>
</tr>
<tr>
<td>**SET T for domain as function of <strong>TIME</strong>: 20 sets from file ‘TIMEVALS’</td>
</tr>
</tbody>
</table>
4.5 NODE BY NODE INPUT FUNCTION

The node by node function allows very high flexibility in that individual values can be specified for each node as described in Section 4.1.2. ACRi Software Tools allows for both structured and unstructured grids and input may be provided in either format. The typical input syntax (illustrated with a SET command) is:

```
SET {Φ} {NODE|STRU|UNST|fname} [V₁,…,Vₘ] [subrgn]
```

Φ
A symbol to denote the variable for which the values are specified. The valid symbols include those listed in Table 2.8.1-3.

NODE
The input is specified in a node-by-node manner. By default if is assumed that the input values are given in the STRUCTURED mode if the subrgn was defined with a LOCATE command for a rectangular window in terms of (I,J,K) grid indices or the window coordinates. Otherwise it is assumed to be in the UNSTRUCTURED mode otherwise.

STRU
The input is read in the manner of nested implied FORTRAN DO loops:

```
Read (NUNIT, *) (((VAR (I, J, K), I = ILO, IHI), J = JLO, JHI), K = KLO, KHI)
```

Where NUNIT is an internally assigned unit number, VAR is the variable denoted by Φ, and ILO, IHI, JLO, JHI, KLO, KHI define, respectively, the starting and ending grid index values for the subrgn for a structured grid. For 2D grid, KLO and KHI are set to unity. This mode is available only for a structured grid and only if the subrgn on the corresponding LOCATE command is given in terms of a rectangular window with (I,J,K) or grid coordinates.

The order of the elements is the same as the one specified (or implied) by the corresponding LOCATE command. It should be noted that if the LOCATE command was given with a COOR modifier, then any exterior boundary nodes adjacent to the selected interior nodes will also be selected. Please see further details of specification of subrgn in Section 3.4.

The order of the nodes, and the nodes included in the defined subrgn may be examined by including a file name on the LOCATE command.

UNST
With this modifier is present, then input is read as a simple implied FORTRAN DO loop:

```
Read (NUNIT, *) (VAR (M), M = MLO, MHI)
```

Where NUNIT is an internally assigned unit number, VAR is the variable denoted by Φ, and MLO and MHI are the starting and ending element numbers for the subrgn. The order of the elements is the same as the one specified (or implied) by the corresponding LOCATE command which can be examined by including a file name on the LOCATE command.

fname
The name of the file for numerical values unless the values are directly specified by V₁,…,Vₘ below. See Section 3.3 for additional information.

V₁,…,Vₘ
The values of the variable at each node selected by the subrgn and dir modifiers. These values must be present unless fname is present. In this case, one of the modifiers, NODE, STRU, or UNST must also be specified.

subrgn
The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected. Note that the modifiers FIELD and dir are applicable to this input if specified on the command. These modifiers and further details of specification of subrgn are given in Section 3.4.

EXAMPLES

```
SET T at each subdomain NODE from file ‘ALLVAL’ input for the entire domain of computation
SET T at subdomain NODES for SELECTED region from ‘ACTIVAL’ in STRUCTURED mode
SET T in ID=RGN1 region from file ‘RGN1VAL’ only for the FIELD nodes.
```
4.6 NODE BY NODE INPUT AS A FUNCTION OF TIME

The node by node values may also be set as function of time as described in Section 4.1.3. This generally follows the format of the node by node input (see Section 4.5). The typical input syntax (illustrated by a SET command) is:

\[ \text{SET } \{ \Phi \} \{ \text{TIME} \} \{ \text{LINE|STEP} \} \{ \text{NODE|STRU|UNST} \} \{ \text{fname} \} \{ \text{[subrgn]} \} \]

\( \Phi \) A symbol to denote the variable for which the values are specified. The valid symbols include those listed in Table 2.8.1-3.

\( \text{TIME} \) The presence of this modifier assumes that the user is specifying a set of values at each node that are specified as a function of time.

\( \text{LINE} \) The time step interpolation is linear; this is the default option.

\( \text{STEP} \) The time step interpolation is step function (Equation 4.1.4).

\( \text{fname} \) The name of the file from which numerical values are read. See Section B.1.1 for file format. A file name must be specified; the input cannot be read directly from the command. The number of values for each record at each time step must equal the number of elements for the subdomain; any extra values present in the record are ignored.

\( \text{LINE} \) The time step interpolation is linear (Equation 4.1.7). This is the default option.

\( \text{STEP} \) The time step interpolation is step function (Equation 4.1.7).

The interpretation of all other modifiers is the identical to that described in Section 4.5 for node by node input.

COMMENTS

It is highly recommended that the user examine the input data (for example by running the data set with SOLVE OFF command) to make sure that the input has been properly interpreted.

EXAMPLES

SET T as NODE by node function of TIME rom file ‘ALLVAL’ input for the entire domain of computation
SET T for NODE as function of TIME file=’ACTIVAL’ for SELECTED region in STRUCTURED mode
SET T at NODES function of TIME ID=RGN1 file=’RGN1VAL’ only for the FIELD nodes.
4.7 USER-DEFINED INPUT OPTIONS

Some commands permit input of user-defined functions or options. These options are permitted for all the commands listed in Section 4.2. The user must have a source-code license to exercise these options. The user in terms of FORTRAN 77 statements in a reserved module called USRFNC may supply this input. If the modifier USER is used in the corresponding command, the user must supply FORTRAN 77 statements, functional formulations or numerical values in the USRFNC module. Please contact ACRi for implementation of this option.
CHAPTER 5
KEYWORD COMMANDS

This chapter describes the keyword commands that comprise the user’s interface for all ACRi Software Tools including ANSWER™ PORFLOW™ and TIDAL™ software package. This interface is based on the ACRi format-free command language FREEFORM™. Knowledge of the structure and syntax of this language is essential for understanding the descriptions of keyword commands in this chapter. The command language is fully described in Chapter 1 of this Keyword Command Manual. Descriptive notation for the keyword commands is explained at the beginning of this chapter.
Keyword Commands

**COMMAND**  
**ACRI**

**PURPOSE**  
To select ACRI Software Tool to be used for simulation purposes.

**SYNTAX**  
**ACRI** \{**ANSWER** | **PORFLOW** | **TIDAL**\}

**ANSWER**  
The **ANSWER™** Software Tool is used for simulation of the specified problem.

**PORFLOW**  
The **PORFLOW™** Software Tool is used for simulation of the specified problem.

**ANSWER**  
The **TIDAL™** Software Tool is used for simulation of the specified problem.

**COMMENTS**

Some installations of ACRI Software allow use of multiple tools. Each tool is specialized for a class of fluid flow problems but they collectively cover a wide range of applications in diverse fields. ACRI Software tools are designed so that the optimal tool is automatically selected based on the user input commands. However, there may be certain selections of input commands that can be handled by more than one tool. This command allows the user to select the tool to be used. The dynamic response through a prompt ("?"") character (See section 1.2.7) is not allowed for this command. A valid syntax of the command must be present.

**EXAMPLES**

ACRI tool **ANSWER** to be used for this problem.

ACRI tool **PORFLOW** to be used for this problem.

ACRI tool **TIDAL** to be used for this problem.
COMMAND  ACTIVE

PURPOSE  To set a default subregion for commands that follow.

SYNTAX  ACTI {ID=subrgn | OFF}

ID=subrgn  The subregion that is to become the active default subdomain. The modifier ID must be present. This subdomain must have been previously defined with a LOCATE or SELECT command. See Section 3.4 for further information.

OFF  Any previous active subdomain is deactivated and the active subdomain is again reset to be the total computational domain. This modifier takes precedence over the ID=subrgn modifier.

COMMENTS

This command sets a default subdomain for all commands that follow till the next ACTIVE command is encountered. For a command that requires the specification of a domain, the default option in ACRi Software Tools is to apply the command to the whole of the computational domain if a subrgn modifier is not explicitly specified on the command itself.

Caution must be exercised in the application of this command, since the new default subdomain will apply to ALL commands that do not have an explicit subrgn or LOCATE or SELECT specification.

The recommended practice is to apply this command just before a group of commands that require a default subregion and then immediately follow with another ACTIVE command with OFF modifier to reset the default domain to the whole of the computational domain.

EXAMPLES

ACTIVE default subdomain to be set as ID= LOWER_SUBDOMAIN
ACTIVE default subdomain OFF
ACTIVE previous active ID= LOWER_SUBDOMAIN is now OFF
Keyword Commands

COMMAND  ADAPTIVE

PURPOSE  To compute a new locally refined grid by adaptive methodology from the currently specified grid. The output of this command is an unstructured dataset. This command is effective only for the ANSWER™ and PORFLOW™ Software Tools.

SYNTAX  ADAP {Φ} {N1} [casename]

Φ  One, and only one, symbol for the dependent variable that is used to determine the criterion for adaptive grid refinement. There is no default value.

N1  Any element where the dependent variable is greater than N1 will be a candidate for being refined.

casename  A string, enclosed in quotes, that serves as a filename prefix, to hold the coordinates, vertex connectivity, split connectivity, sub-regions, and initial guesses for the new mesh.

COMMENTS

This command provides a very powerful means to automate the time-consuming gridding process that often precedes the numerical simulation.

A selected variable is used to set a threshold criterion for local grid refinement. If the local value of the variable exceeds the bounds set by the criterion, then the element is split into 4 (for 2D) or 8 (for 3D) elements.

It should be noted that the selected variable does not mean just the phase space variables. Any variable, including those defined by the user can be used. For example, the user can define a combination of gradients of say, velocity, or vorticity, or temperature and density gradients, etc. by appropriate SET commands and then use this defined variable as the criterion for grid refinement.

EXAMPLES

/ The first two commands set-up the flag for mesh refinement.

/ First create DUDY.
ALLOcate 'DUDY- Gradient of U with Y'
SET DUDY GRADient of U with Y

/ Now generate a new unstructured refined dataset.
ADAPt mesh wherever DUDY exceeds 1.2 casename: ‘Level-1’

/ The new connectivity, split connectivity, coordinates, sub-regions, and initial guesses will be generated in files called ‘Level-1.cnc’, ‘Level-1.blk’, ‘Level-1.xyz’, ‘Level-1.loc’, ‘Level-1.init’ etc.
COMMAND  ADIABATIC

PURPOSE  To specify global adiabatic or fixed value boundary conditions at all wall boundaries including internal obstacle walls. This command is effective only for the ANSWER™ Software Tools.

SYNTAX  ADIA [Φ] [OFF]

Φ  The symbol for the dependent variable for which the adiabatic wall conditions are specified. The valid symbols are listed in Table 2.7.1. **One and only one** character string must be specified for each command. If no symbol is specified then the input is assumed to be for the temperature (or enthalpy) variable.

OFF  The wall is assumed to be a fixed value boundary. The boundary value may be specified by a BOUNDARY command or is obtained from default conditions for the variable.

COMMENTS  By default the velocity components, the temperature and, the turbulence variables at all walls and internal obstacles are fixed. The default wall boundary conditions for the species transport variables, on the other hand, are those of adiabatic or zero flux. The actual wall value may vary from one location to another and can be specified by the BOUNDARY, INITIAL, READ or SET commands. The ADIABATIC command provides a convenient means to set the zero flux condition globally at walls and obstacles. The boundary conditions at external walls may also be controlled explicitly by the BOUNDARY command. For the species transport variables, the ADIABATIC OFF command must be used if alternative boundary conditions are to be specified. It should be noted that this command only sets the flux at the wall or the obstacle to zero; it does not update the boundary or obstacle value.

EXAMPLES  

ADIAbatic conditions  ! By default for temperature
ADIAbatic conditions for T at all walls  ! Same as above
ADIAbatic OFF for C transport variable  ! Change from default to fixed type of walls
**COMMAND** ALLOCATE

**PURPOSE** To allocate space for problem-specific input

**MODE 1:** Allocate Space for A New User Defined Variable

**SYNTAX** ALLO {name}

name The name of the user defined variable. It may consist of up to 64 alphanumeric characters of which the 1st character must be an alphabetic (A-Z) character. If more than 32 characters are specified then the name must be enclosed in single or double quotes. If the name is longer than 32 characters but it is not enclosed in quotes then all characters except the first 32 are ignored. **The intended symbol for name must be the first modifier on the ALLOCATE command.**

The 1st string of up to 8 characters is used as the symbolic name to define input for, or properties of, the new variable. If there are more than 8 characters in the 1st string, then the subsequent characters are ignored. No distinction is made between the lower and upper case characters. The allowable set of characters includes the alphabetic (A-Z), the numeric (0-9), the underscore (_), the minus (-), the plus (+) and the period (.) characters. The symbolic name is terminated by the 1st separator character. A list of separator characters is given in Chapter 1.

All operations, which can be performed on the built-in default variables, may be performed on this new variable. For example, a transport equation may be solved for this variable. Alternately, it may be used to build compound functions through SET commands to define complex boundary conditions and sources for another variable.

**COMMENTS**

This command provides the user with a powerful tool to dynamically allocate variables, incorporate new physics, and solve new transport equations without FORTRAN or C programming. This, together with the built-in library of dynamic functions (Section 4.1.6), is an important component of the FORTRANless™ technology built into ACRi Software Tools.

The number of variables that can be allocated by the user varies. The default capability is set such that up to 32 variables can be defined by the user. However, if a particular problem uses the memory resources for other purposes, such as large input tables, then the number of allowable user defined variables may be less.

**EXAMPLES**

ALLOCate VARIABL1 ! VARIABL1 will be used as symbol for this variable
ALLOCate MY_NEW_Variable_that_i_defined ! MY_NEW_V will be used as symbol for this variable
ALLOCate “VARIABL1 - A New Variable Defined Specifically for this Problem”
ALLOCate `R1 ! A variable to hold reaction rates for other variables
ALLOCate ‘R1 - The reaction rate for the first chemical species’
MODE 2: Allocate Space for User Input Tables

SYNTAX  ALLO {TABL}{N1}

TABL By default 10,000-word memory is allocated to store the problem-specific input values by the user. This command should be used to increase the allocated memory if an error message saying insufficient real table space is encountered.

N1 The problem-specific memory space (in words) to be allocated.

EXAMPLES

ALLOcate TABLe space for 50000 words of problem specific input
**COMMAND**  ARRHENIUS

**PURPOSE**  To specify the Arrhenius reaction rate constants for the default 4-step hydrocarbon reaction. This command is effective only for the ANSER™ Software Tool.

**SYNTAX**  ARRH {Φ} [N1, N2, N3, N4, N5]

**Φ**  One of the character strings: FU, CH, CO and H2. It denotes the dependent variable (Table 2.7.1) for which the Arrhenius reaction rate constants are specified.

**N1**  The Arrhenius pre-factor, $C_A (>0)$, of rate expression equation* as given below

$$S_{m_{jk}} = C_A S_o \exp (C_E / T) \rho^{(a+b+c)} m_j^a m_k^b m_l^c$$

**N2**  The Arrhenius activation energy constant, $C_E (\geq 0)$, as shown in above equation.

**N3, N4, N5**  The exponents a, b, and c of the above equation are the primary, secondary and tertiary reaction species.

### TABLE OF DEFAULT VALUES FOR ARRHENIUS COMMAND

<table>
<thead>
<tr>
<th>Symbol</th>
<th>N1</th>
<th>N2</th>
<th>N3</th>
<th>N4</th>
<th>N5</th>
</tr>
</thead>
<tbody>
<tr>
<td>FU</td>
<td>2.0893x10^{22}</td>
<td>2.48x10^{4}</td>
<td>0.50</td>
<td>1.07</td>
<td>0.40</td>
</tr>
<tr>
<td>CH</td>
<td>5.0117x10^{19}</td>
<td>2.50x10^{4}</td>
<td>0.90</td>
<td>1.18</td>
<td>-0.37</td>
</tr>
<tr>
<td>CO</td>
<td>3.9811x10^{19}</td>
<td>2.00x10^{4}</td>
<td>1.00</td>
<td>0.25</td>
<td>0.50</td>
</tr>
<tr>
<td>H2</td>
<td>3.3113x10^{18}</td>
<td>2.05x10^{4}</td>
<td>0.85</td>
<td>1.42</td>
<td>-0.56</td>
</tr>
</tbody>
</table>

**EXAMPLES**

ARRHenus constants for FU: 3.9E11, 1.5E8, 1.0, 1.0, 0.0

* The Rate Expression equation

where

$S_{m_{jk}}$ is the kinetic rate of reaction of $j^{th}$ species, $m_j$, $m_k$ and $m_l$ are mass fractions of the participating species,

$C_A$, $C_E$, a, b and c are empirical constants.

The quantity $S_o$ is unity for all reactions except that for the CO reaction
<table>
<thead>
<tr>
<th>COMMAND</th>
<th>BANNER</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To print a banner page to the output directed to the standard output device (unit 16). The banner page contains the ACRi Software Tool version and date identification, time and date stamp, and user identification.</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>BANN</td>
</tr>
<tr>
<td>EXAMPLES</td>
<td>BANNER page output at this stage</td>
</tr>
</tbody>
</table>
Keyword Commands

COMMAND  BLOCK

PURPOSE  To define a solid object or blockage within the flow domain. This command is effective only for the ANSWER™ and TIDAL™ Software Tools.

MODE 1:  Solid Blocks Immersed in Fluid

SYNTAX  BLOC  {subrgn} [FLUI] [EXCL] [FLOO | DEFA] [ROUG=Z\text{rough}] [TYPE=C\text{rough}]

subrgn  The subregion to be defined as a blocked or solid region. See Section 3.4. The subregion must be interior to the computational domain and must not contain any boundary elements. A subregion must be specified; there is no default value.

FLUI  By default, a blocked region, once defined is assumed to be permanent. If this modifier is present, then the block is treated as a transient object that may be subsequently removed by a BLOCK OFF command.

EXCL  By default the fluid saturation, and hence the volume of the fluid, inside a blocked element is set to zero unless the FLUID modifier is present or the SOLID command is given for conjugate heat transfer. If this modifier is present, then the volume of the fluid saturation and the volume of the fluid in the element are forced to be zero.

FLOO  This mode of the command is operational only for the TIDAL™ software. By default, a blocked region is assumed to be solid block with no fluid. If this modifier is present, then the blocked region can be flooded based on the topographical information specified for the block, if the water level rises above the level of the block.

DEFA  This mode of the command is operational only for the TIDAL™ software. If this modifier is present, then the external boundaries of the region are defined to be blocked region. No fluid can enter or exit from these boundaries. By default, the external boundaries are open for flow.

ROUG  This mode of the command is operational only for the ANSWER™ software. If this modifier is present, then the wall of the block is assumed to be hydro-dynamically rough for turbulent flow. The height and type of roughness is specified by the $Z\text{rough}$ and $C\text{rough}$ constants (below).

$Z\text{rough}$  The average roughness height for the wall. It should be noted that the roughness should be small compared to the grid size in the vicinity of the wall. Further the roughness theory is only valid for the range of $Y+$ values that put it in fully turbulent region of the log-law of the wall.

$C\text{rough}$  The factor that accounts for roughness type. The default value is 0.5 which is generally considered to be suitable for sand-grain type of roughness. The recommended values generally lie between 0.5 and 1.0.

COMMENTS

Multiple BLOCK commands may be specified to accommodate complex or multiple internal obstacles.

EXAMPLES

BLOCK for SELECTED subregion  ! Currently active selected subregion
BLOCK at subregion ID=BLK1  ! Subregion defined with ID=BLK1
BLOCK with FLOODING option for subregion ID=BLK1
BLOCK at subregion ID=BLK1 FLUID  ! Block will be removed later by a BLOCK OFF command
BLOCK at subregion ID=BLK1 ROUGH with height=0.001 and TYPE factor =0.6
### MODE 2: Solid Block Immersed and Moving in Fluid

#### SYNTAX

```
BLOC {subrgn} {MOVE | MOVI} [FLUI] [EXCL] [ROUG=Z_{\text{rough}}] [TYPE=C_{\text{rough}}]
```

#### subrgn

The subregion to be defined as a blocked or solid region. See Section 3.4. The subregion must be interior to the computational domain and must not contain any boundary elements. A subregion must be specified; there is no default value.

#### MOVE

By default, a blocked region is assumed to be stationary in a moving fluid. If this modifier is present, then the block is treated as a moving object. The velocity components for the moving blocks can be specified by `SET`, `INITIAL` or one of the other commands for specification of field values.

#### MOVI

Same as `MOVE`.

#### FLUI

See Mode 1 of command.

#### EXCL

See Mode 1 of command.

#### ROUG

See Mode 1 of command.

#### Z_{ROUGH}

See Mode 1 of command.

#### TYPE

See Mode 1 of command.

#### C_{ROUGH}

See Mode 1 of command.

### APPLICABILITY

This command mode is available only for the ANSWER™ Software Tool. **Current implementation of this option is suitable only for small or oscillatory motions.** It ignores the local changes in fluid volume due to the motion of block. It is assumed that the volume of the surrounding fluid elements stays unchanged. However full account is taken of the effects of the block motion on the surrounding fluid due to momentum and other interaction. It is equivalent to assuming that the fluid displacement is small compared to the total volume of the fluid.

### EXAMPLES

```
BLOCkage at subregion ID=BLK1 is MOVing
```
MODE 3: A Dissolving or Melting Block of Salt or other Material

SYNTAX

```
BLOC {subrgn} [SALT | MELT] [INSO=x] [ALL | NONE] [RATE=λ] [MULT=β] [PLAN=I]
  J | K=N,UK | OFFS=N_{offset} | ISOT | GAMA | [STOR=N_{STOR}]
[ROUG=Z_{rough}] [TYPE=C_{rough}]
```

subrgn
The subregion to be defined as a blocked or solid region. See Section 3.4. The subregion must be interior to the computational domain and must not contain any boundary elements. A subregion must be specified; there is no default value.

SALT
If this modifier is present, then the block is treated as a block of salt that dissolves in water as a function of time. The density of the resulting brine solution, and the parameters used to dissolve the salt may be specified with DENSITY SALT command. The built-in rate of dissolution of salt is computed from a correlation developed at Sandia National Laboratory (Saberian and Podio, 1977). The rate of dissolution of a vertical face in touch with fluid is given by:

\[
\frac{dr}{dt} = α_1 y^4 - α_2 y^3 + α_3 y^2 - α_4 y + α_5 - \frac{α_6}{y}
\]

Where \( y \) is the specific gravity \((=\rho/\rho^*)\) of brine and the superscript * denotes the reference density. This rate is modified for an inclined surface at an angle of \( θ \) \((\theta = 90\) is an upward facing and \( \theta = -90\) is a downward facing surface) by the correlation:

\[
\left[ \frac{dr}{dt} \right]_{θ≥0} = \left[ \frac{dr}{dt} \right]_{θ=0} \left[ \cos θ \right]^{1/2}
\]

\[
\left[ \frac{dr}{dt} \right]_{θ<0} = \left[ \frac{dr}{dt} \right]_{θ=0} \left[ 1 + 0.22 - 0.22 [1 + θ / 45]^{1/3} \right]
\]

The constants for this correlation as recommended in the User’s Manual for SANSMIC code (Russo, 1983) are summarized in the Table below.

<table>
<thead>
<tr>
<th>Units</th>
<th>( α_1 )</th>
<th>( α_2 )</th>
<th>( α_3 )</th>
<th>( α_4 )</th>
<th>( α_5 )</th>
<th>( α_6 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ft/hr</td>
<td>45.654996</td>
<td>232.2931</td>
<td>469.5247</td>
<td>470.37554</td>
<td>232.73686</td>
<td>45.203241</td>
</tr>
</tbody>
</table>

The surface dissolution rate drops off very quickly with the specific gravity of brine. The table below summarizes some of these values for a vertical surface.

<table>
<thead>
<tr>
<th>( ψ = ρ/ρ^* )</th>
<th>1.0</th>
<th>1.05</th>
<th>1.10</th>
<th>1.15</th>
<th>1.20</th>
</tr>
</thead>
<tbody>
<tr>
<td>dr/dt (m/s) x10^6</td>
<td>3.783</td>
<td>2.409</td>
<td>1.368</td>
<td>0.5371</td>
<td>0.01146</td>
</tr>
<tr>
<td>dr/dt (m/day)</td>
<td>0.327</td>
<td>0.208</td>
<td>0.118</td>
<td>0.046</td>
<td>0.001</td>
</tr>
</tbody>
</table>

MELT
Same as SALT.

INSO
If this modifier is present, then it is assumed that a fraction of salt block is composed of insoluble material. As salt dissolves the insoluble material dislocates and becomes part of the brine. A fraction of this insoluble material settles down to the floor of the cavern and the rest leaves with the outflow. With \( V \) as the upward fluid velocity (m/s), the settling fraction by volume, \( f \), is given by the correlation:

\[
f = \frac{0.5}{1. + 27.283 V} + 0.5 \ e^{-23.622 V}
\]

\( ξ \)
The fraction of salt block that is insoluble.

ALL
By default the fraction of the insolubles that settles is computed from the formula given above. If this modifier is specified, then this fraction is set to unity.

NONE
None of the insolubles settle to the floor; all are flushed out of with the outgoing brine.
The specified surface dissolution or melting rate if the modifier RATE is present.

MULT

If this modifier is present, then the rate computed from the built-in correlation is multiplied by the specified factor $\beta$.

PLAN

The computation of dissolution rate ($dr/dt$) requires the location of specific gravity, $\psi$. By default, $\psi$ is computed at the fluid element next to the wall between the fluid and the solid (salt). If this modifier is present, $\psi$ is taken at a location which corresponds to the element directly in line with the wall element but located at the plane defined by the $I$, $J$, $K$, and $N_{IJK}$ (below). This modifier can only be used for a structured grid.

I

The plane is defined by the $I$ (x-direction) grid index of a structured grid.

J

The plane is defined by the $J$ (y-direction) grid index of a structured grid.

K

The plane is defined by the $K$ (z-direction) grid index of a structured grid.

$N_{IJK}$

The $I$, $J$ or $K$ location of the plane at which the specific gravity is computed.

$N_{avg}$

The depth of averaging in the $I$, $J$, $K$ direction. In the absence of the PLAN modifier, the averaging starts from the element located next to the salt wall. If the PLAN modifier is present then the averaging starts from the location on the $N_{IJK}$ plane but in line with the wall element. If $N_{avg}$ is positive, then the averaging is in the increasing direction of the coordinate index $I$, $J$, $K$. If it is negative then it is in the decreasing direction. If any solid block elements are encountered in the averaging, then the averaging process stops at the last element before the solid element; any elements on the other side of the block are ignored. If $N_{avg}$ is too large so that it refers to elements beyond the computational domain, then only the points lying on the transect within the computational domain are selected.

OFFS

The specific gravity is computed from a location that is offset to the reference location.

$N_{offset}$

The offset in the $I$, $J$, $K$ direction. In the absence of the PLAN modifier, the offset refers to the location that is offset in the $I$, $J$, $K$ direction from the element located next to the salt wall. If the PLAN modifier is present then the offset refers to the location on the $N_{IJK}$ plane but in line with the wall element. If $N_{offset}$ is positive, then the offset is in the increasing direction of the coordinate index $I$, $J$, $K$. If it is negative then it is in the decreasing direction. If any solid block elements are encountered then the last element before the solid is selected. If $N_{offset}$ is too large so that it refers to elements beyond the computational domain, then the last element within the computational domain is selected.

ISOT

By default, the computed rate for the dissolution of the wet surface is modified for the inclination of the surface to the vertical direction. If this modifier is present, then the rate is as computed from the correlation without any correction for the angle of inclination.

GAMA

By default, the diffusion coefficient for the governing equation is not modified for the elements that consist partially of brine (fluid) and partially of salt (block). This is reasonable given that the diffusion process is dominated by the gradients normal to the wall and is mostly independent of whether the element is partially or totally filled with brine. If this modifier is present, then the diffusion is proportional to the fluid saturation of the element.

STOR

Memory space is automatically allocated to take account of the changing boundaries (wall facets) of a melting block. By default the amount of space allocated is $N \times N_{23D}$ where $N$ is number of elements in the blocks and $N_{23D}$ is 2 for 2D and 3 for 3D flows. This is typically an overly conservative estimate based on the assumption that every alternate element melts leaving a checkerboard of isolated elements. This can be wasteful for problems with orderly melting at a defined surface. If this modifier is specified, then the amount of memory for wall facets is set to $N_{STOR}$ below.

$N_{STOR}$

The amount of storage allocated for the wall segments of the evolving block if the STOR modifier is present. A fatal error occurs if the amount of allocated memory is not sufficient.
Keyword Commands

ROUG  See Mode 1 of command.
ZROUGH  See Mode 1 of command.
TYPE  See Mode 1 of command.
CROUG  See Mode 1 of command.

APPLICABILITY

This command mode is available only for the ANSWER™ Software Tool.

COMMENTS

The time step for this option must be such that no more than one element (normal to the contact surface) can be fully dissolved in any given time step. If the time step is larger then dissolution will be limited to 1 element. This will appear as an effective slower rate of dissolution than that indicated by the elapsed time.

EXAMPLES

BLOCkage at subregion ID=BLK1 is dissolving SALT
BLOCkage at subregion ID=BLK1 is MELTing at a rate of 0.0001 m/s
BLOCkage SALT subregion ID=BLK1 RATE=0.0001 and STOR 10000 boundary segments.
BLOCkage SALT subregion ID=BLK1 max ISOTropic and MULTiply by 100 the built-in rate
BLOCkage SALT subregion ID=BLK1 max INSOLUBLE fraction=0.08 by volume
BLOCkage MELTing subregion ID=BLK1 PLANE J=20, AVERaging depth =10.
BLOCkage MELTing subregion ID=BLK1 OFFSET by J=20.
BLOCkage MELTing subregion ID=BLK1 max STOR=10000 boundary segments.
MODE 4: A Growing Block with Deposition of Insolubles from a Salt Block

SYNTAX

```
BLOC {subrgn} [GROW] [DEPO] [STOR=N\textsubscript{STOR}] [ROUG=Z\textsubscript{ROUGH}] [TYPE=C\textsubscript{ROUGH}] [DELA=N\textsubscript{DELAY}] [EXCL= subrgn\_ex]
```

subrgn The subregion to be defined as a blocked or solid region. See Section 3.4. The subregion must be interior to the computational domain and must not contain any boundary elements. A subregion must be specified; there is no default value.

GROW The block is treated as a block that receives part of the insoluble material that settles from the dissolving salt blocks. It is assumed that at any time the insolubles fall uniformly on the exposed surface of the block. The elements that have inflow, outflow or mass sources are automatically excluded from deposition.

DEPO Same as GROW.

STOR Memory space is automatically allocated to take account of the evolving block elements of a growing block. The default value is set to assume that the block can grow to be five times the number of initial elements in the block. If this modifier is specified, then the maximum number of elements that the block can grow to is set to the initial number of elements in the block plus \(N_{STOR}\) additional elements.

\(N_{STOR}\) The amount of storage allocated for the maximum number of elements that the block can grow to.

ROUG See Mode 1 of command.

\(Z_{ROUGH}\) See Mode 1 of command.

TYPE See Mode 1 of command.

\(C_{ROUGH}\) See Mode 1 of command.

DELA For formation of caverns by salt or other dissolution, often in the early stages of a computation process, enough surface area is not available for deposition. In this case, it is preferable to delay start of deposition unless a minimum number of elements can participate. This modifier is used to specify the number of minimum elements before deposition can start.

\(N_{DELAY}\) The minimum number of elements before deposition can start. A value of more than 5 is recommended for most cases.

EXCL Some regions may need to be excluded from the deposition process. For example, it may be necessary to exclude additional regions such as in the immediate vicinity of an inflow boundary so that the inflow is not isolated from contact with other computational regions. This modifier is used to specify the sub domain excluded from receiving any deposition.

Subrgn\_ex The subregion to be excluded from receiving any deposition material. See Section 3.4. The subregion must be interior to the computational domain. A subregion must be specified; there is no default value.

APPLICABILITY

This command mode is available only for the ANSWER™ Software Tool.

COMMENTS

The time step for this option must be such that no more than one element (normal to the contact surface) can be added in any given time step. If the time step is larger then the growth will be limited to 1 element. This will appear as an effective slower rate of growth than that indicated by the elapsed time.

EXAMPLES

```
BLOkage at subregion ID=BLK1 is GROWing with time
BLOkage at subregion ID=BLK1 can GROW to be STOR= 1000 max elements.
BLOkage at subregion ID=BLK1 GROW with DELAY=10, EXCLUDE ID=BLK2
```
Keyword Commands

MODE 5: Remove Previously Specified Blocks

SYNTAX

BLOC {subrgn} {OFF}

subrgn The subregion to be defined as a blocked or solid region. See Section 3.4. The subregion must be interior to the computational domain and must not contain any boundary elements. A subregion must be specified; there is no default value.

OFF A previously specified block with the subregion identified above is removed.

EXAMPLES

BLOC Kage ID=BLK1 OFF !Previously specified Block is removed
COMMAND  BOREHOLE

PURPOSE  Define embedded borehole in the porous matrix. This command is effective only for the PORFLOW™ Software Tool.

MODE 1: Specification of a Borehole with fixed Diameter

SYNTAX  BORE  {ID=subrgn} {D_{outer}} {D_{inner}} [INCL] [dir | ALL | NONE] [DETA]

ID  The modifier to indicate that the input is for a previously defined subregion.

subrgn  The subregion in which the borehole is located. The subregion must be previously specified by a LOCATE IJK or LOCATE COOR command.

D_{outer}  The outer diameter of the borehole. There is no default value; a value must be specified.

D_{inner}  Inner diameter of the borehole. By default it is assumed that the inner diameter is zero.

INCL  By default only the boundary faces in the principal direction (determined from the LOCATE command) are included in the definition of the borehole faces. If this modifier is present, together then the boundary faces specified are included based on the dir, ALL or NONE modifier.

dir  One of the direction modifiers (X-, X+, Y-, Y+, Z-, Z+) which indicates the face to be included if the INCL modifier is present.

ALL  All boundary faces in the sub domain are included if the INCL modifier is present.

NONE  No boundary faces in the sub domain are included if the INCL modifier is present.

DETA  If this modifier is present, then a detailed table of the elements and faces that form the fracture is printed out to the Standard Output Device

COMMENTS

Each borehole must be specified by a different LOCATE command. All connected elements in the subdomain are selected to be part of the borehole.

The effective cross-sectional area of the Borehole is computed as:

\[ \text{Area} = \frac{(\pi/4)}{(D_{outer}^2 - D_{inner}^2)} \]

EXAMPLES

BOREHOLE for ID=BOREHOLE_1 dia = 0.2
BOREHOLE ID= BOREHOLE_2 Y: D=0.2, Inner d=0.1 DETA
MODE 2: Specification of a Borehole with Diameter as a Functional Form

SYNTAX

BORE {ID=subrgn} {D_{outer}} [func(\xi)] [N_1, N_2, ..., N_n] [ADJU] [INCL] [dir|ALL|NONE]

ID
The modifier to indicate that the input is for a previously defined subregion.

subrgn
See Mode 1.

D_{outer}
Nominal width of the borehole which is replaced by a value from the specified function.

func
One of the modifiers listed in Table 4.2.1 that denotes the functional form for borehole diameter. If no function is specified, the value is assumed to be constant.

\xi
One of the independent variables listed in Table 4.2.2.

N_1, N_2, ..., N_n
The numerical constants for the selected function. See Section 4.2 for more details. There are no default values for this input.

ADJU
If this modifier is present, and a functional form for the diameter is specified, then the hydraulic conductivity of the fracture is modified as a cubic function.

INCL
See Mode 1.

dir
See Mode 1..

ALL
See Mode 1..

NONE
See Mode 1..

DETA
See Mode 1.

EXAMPLES

BOREHOLE for ID=BOREHOLE_1 dia = 0.2
BOREHOLE ID= BOREHOLE_2 Y: D=0.2; varies LINEARLY as 0.2 +0.00001 P DETAL
COMMAND  BOUNDARY

PURPOSE  To specify boundary conditions for the computational domain.

MODE 1: Constant Boundary Conditions

SYNTAX  BOUN [Φ] [option] [subopt] [dir] [subrgn] {Vs} [h]

Φ  One or more symbols (with a maximum of 10) for the dependent variable(s) for which the boundary conditions are specified. Valid symbols are listed in Table 2.7.1. If no symbol is specified then the boundary condition is applied to ALL dependent variable for which transport equations are solved.

option  The type of the boundary condition.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>VALU</td>
<td>Value of the variable at the boundary node is specified as: $\Phi = \Phi_0$ where $\Phi_0$ is the specified numerical value. This is the default option.</td>
</tr>
<tr>
<td>FLUX</td>
<td>$q$, the flux of the variable at the boundary node is specified according to the equation: $q = -\Gamma \frac{\partial \Phi}{\partial N}$ where $\Gamma$ is the diffusion coefficient for the variable and $N$ is the normal direction at the boundary. The flux is positive if it enters the computational domain and negative if it leaves it.</td>
</tr>
<tr>
<td>GRAD</td>
<td>The normal gradient of the variable at the boundary, $\frac{\partial \Phi}{\partial N}$, is specified. The gradient is taken to be positive in the direction of the outward normal at the surface. A positive gradient will result in a positive flux entering the computational domain.</td>
</tr>
<tr>
<td>MIXE</td>
<td>The flux of the variable at the boundary is specified according to the equation: $q = -\Gamma \frac{\partial \Phi}{\partial N} = \pm h (\Phi - \Phi_0)$ where $h$ is a transfer coefficient, and $\Phi_0$ is the equilibrium (or ambient) value. The sign is chosen based on the direction vector of the boundary so that the incoming flux is positive.</td>
</tr>
<tr>
<td>FLOW</td>
<td>The boundary value depends on the direction of flow. For an incoming flow, the boundary value is fixed (VALU). For an outgoing flow, the normal gradient at the boundary is assumed to be zero.</td>
</tr>
<tr>
<td>EXTR</td>
<td>The normal gradient at the boundary is extrapolated from the neighboring values immediately inside the boundary. In general, this is not a well-posed boundary condition for transport equations. However in certain circumstances it may be used to compute the values of secondary variables.</td>
</tr>
</tbody>
</table>

subopt  The nature of the MIXED boundary condition.

<table>
<thead>
<tr>
<th>subopt</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>FLUX</td>
<td>Mixed boundary condition is specified in terms of the flux of the variable. This is the default option.</td>
</tr>
<tr>
<td>GRAD</td>
<td>Mixed boundary condition is specified in terms of the gradient of the variable (the MIXED condition with $\Gamma = 1$).</td>
</tr>
</tbody>
</table>

dir  The orientation index for the outward normal at the boundary. See Section 3.5 for available choices. If no value is specified, then the boundary condition is implemented at all outermost boundaries of the selected subregion.

subrgn  The subregion for which the input is specified. If no subregion is specified, the outermost boundary of the entire computational domain is selected. See Section 3.4.
The value of the variable $\Phi_0$ if \texttt{VALUE} or \texttt{MIXED} modifier is present, the flux, $q$, if the \texttt{FLUX} modifier is present, and the outward normal gradient $\partial \Phi / \partial N$ if the \texttt{GRAD} modifier is present. If no modifier is specified, then the \texttt{VALUE} modifier is assumed to be present by default. There is no default value.

The transfer coefficient $h$ for the \texttt{MIXED} option. This input is ignored for other options. There is no default value.

**COMMENTS**

In general, boundary conditions at any boundary segment may be specified only once. Two independent \texttt{BOUNDARY} specifications must not refer to the same element for the same boundary orientation index. Unpredictable consequences may arise if the boundary information for any segment is repeated. However, the specification for a boundary segment that was previously identified by a unique identity (\texttt{ID=idsub}; see Section 3.4 and \texttt{LOCATE} command) may be replaced by a new specification provided the previously specified boundary condition is explicitly disabled by the \texttt{BOUNDARY OFF} (see Mode 3 specification) command.

If no boundary conditions are explicitly specified at a particular boundary, then the initial values of the variable at that boundary are used as the boundary conditions. For structured grids, if the number of grid nodes (see \texttt{GRID} command) in any direction is less than or equal to 3, then the boundary conditions at the boundaries normal to that direction are assumed to be those of zero flux.

**EXAMPLES**

- \texttt{BOUNdary for P: at X- boundary, value = 0}
- \texttt{BOUNdary GRADient at X+ boundary for all variables is = 0.}
- \texttt{BOUNdary for T: orientation index X+ value = 10.}
- \texttt{BOUNdary for T at X+: value = 10 at ID=UPPER subregion}
- \texttt{BOUNdary for T at Y- boundary: FLUX = 10 at the selected segment}
- \texttt{BOUNdary for P at Y- boundary: GRAD = -2.5 at the selected segment}
- \texttt{BOUNdary for T at Y+ boundary: MIXEd type: equilibrium value=5 h=0.5}
- \texttt{BOUNdary T: Y+; MIXEd FLUX: v=1, h=0.1 for segment with ID=MIDDLE}
- \texttt{BOUNdary T: Y+; MIXEd GRAD: v=-1, h=0.1 for SELECTed subregion}
MODE 2: Boundary Condition as a Function of another Variable

SYNTAX

BOUN \([\Phi]\) [func[\xi]] \{N_1, N_2, .., N_n\} [fname] [option] [subopt] [dir] [subrgn] [h]

\(\Phi\)
One, and only one, symbol for the dependent variable for which the boundary conditions are specified. The valid symbols are listed in Table 2.7.1.

func
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the boundary value, flux or gradient of the dependent variable based on the presence of one or more of the VALUE, FLUX, GRAD and MIXED modifiers. If no function is specified then the value is assumed to be constant.

\(\xi\)
One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

\(N_1, N_2, .., N_n\)
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname
The name of the file containing numerical values \(N_2\) through \(N_n\). This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

option
See Mode 1 specification.

subopt
See Mode 1 specification.

dir
See Mode 1 specification.

subrgn
See Mode 1 specification.

h
The transfer coefficient. In the FLUX mode, the input units are those of velocity, heat or mass flux divided by the units of the dependent variable, \(\Phi\). In the GRADIENT mode, the input units are those of \(\Phi\) divided by those of distance. The default value is 0. In the presence of the fname modifier, the input value must be the 2nd numerical value in the command because all-functional input is obtained from the file.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (BOUNDARY) must replace the keyword used in these examples. The boundary orientation (dir) identifier and the transfer coefficient must also be specified, if appropriate.

///// Some additional examples
BOUNDary value at X+ boundary LINEar function: T = 30 -0.015 * Y
BOUNDary for T: at X+ boundary FLUX given by USER function #7
BOUNDary value for P at Y- COSine SERIES in T: 3 sets: (0., 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.
BOUNDary P GRADient: Y- boundary: TABLE of values: 3 sets (TIME, value) (0., 0.01), (100., 0.10 ), (200, -0.20)
BOUNDary P at X+: TABLE of 32 sets (TIME, value) from file='BVALUES'

///// Examples with transfer coefficient for MIXEd type
BOUNDary T: X+: MIXEd: POLYnomial in Y: (10, 0.5, 0, -0.1, 0): h_F=0.01
// Next 2 lines specify boundary T as a function of T
BOUNDary T at Y- boundary MIXEd type: SINE SERIES in T: 3 sets
(0., 5, 1), (100, 10, 1), (200, 20, 3) datum= 0., h=1.E-4
// Next 2 lines specify mixed type P boundary as a function of time
BOUNDary T at X-: MIXEd GRADient TABLE of Z: 3 sets: (0., 5), (100, 15), (200, 7.5), h=0.001
BOUNDary MIXEd GRAD P at Y+: SINE SERIES in TIME 24 sets 'BMIXEDV' h=0.01
**Keyword Commands**

**MODE 3:** Total Pressure Boundary Condition

**SYNTAX**

```
BOUN {TOTA} {P} {func[], ξ} {N₁, N₂, ..., Nₙ, fname} [Nₙ₊₁, ..., Nₙ₊ₘ] [dir] [subrgn]
```

**TOTA**
The total pressure at the boundary is specified. The pressure and velocity components at the boundary are computed such that these satisfy the relation:

\[
P_{\text{Total}} = P + \frac{1}{2} \rho (u^2 + v^2 + w^2),
\]

Where \( P_{\text{Total}} \) is the total pressure, \( P \) is the local pressure, \( ρ \) is the density, and \( u, v, \) and \( w \) are Cartesian velocity components. There is no default value; this modifier must be present on the command.

**P**
The symbol to denote that the input is for the pressure variable. There is no default value; this symbol must be present on the command.

**func**
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the value of total pressure. If no function is specified then the value is assumed to be constant.

**ξ**
One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

**N₁, ..., Nₙ**
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

**fname**
The name of the file containing numerical values \( N₂ \) through \( Nₙ \). This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

**Nₙ₊₁, ..., Nₙ₊ₘ**
If present, these specify the relative values of the Cartesian velocity components at the total pressure boundary. If these are not present, then either a zero gradient or a normal flow at the boundary is assumed. If present, then 2 values are required for 2D and 3 for 3D flow.

**dir**
See Mode 1 specification.

**subrgn**
See Mode 1 specification.

**APPLICABILITY**

This mode of the command is only available with the ANSWER™ Software Tool.

**EXAMPLES**

Generic examples for this command are given in Section 4.4. The command keyword (BOUNDARY) must replace the keyword used in these examples. The boundary orientation (dir) identifier and the transfer coefficient \( μ \) must also be specified, if appropriate.

```
/// Some additional examples
BOUNDary TOTAL P at X+ boundary = 2.E5
BOUNDary TOTAL P at X- boundary = 1.E6; velocity components (0.5, 0.5, 0.) ! flow at 45 deg to x-axis
BOUNDary TOTAL P X-: POLYNomial in Y: (10, 0.5, .. -0.1, 0.)
BOUNDary TOTAL P X-: POLYNomial in Y: (10, 0.5, 0., -0.1, 0.) (1, 0., 0.) ! flow at 0 deg to x-axis
```

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**MODE 4:** Discharge Coefficient or Gate Boundary Conditions for Velocity Components

**SYNTAX**

```plaintext
BOUN \{ \phi \} \{ \text{DISC|GATE} \} \{ \text{dir} \} \{ \text{subrgn} \} \{ \text{C_D} \} \{ \text{P|PRES=P_B} \} \{ \text{AREA=A_B} \} \{ \text{IN|OUT} \}
```

**DISC|GATE** The modifier to denote that the discharge coefficient or gate type of boundary condition is being specified. This mode is not available for the PORFLOW™ software tool. The boundary velocity component is computed from:

\[ v = C_D \sqrt{\frac{2(P_B - P)}{\rho}} \frac{A_B}{A} \]

Where \( v \) is the boundary value of the velocity component, \( C_D \) is a discharge or drag coefficient, \( P_B \) is the boundary pressure, \( P \) is the computed pressure in the flow field interior to the boundary, \( \rho \) is the density at the boundary, \( A_B \) if the specified area and \( A \) is the actual area of the boundary face for the element.

\( \phi \) One of the symbols U, V or W to denote the velocity component to be set by the command.

\( \text{dir} \) See Mode 1 specification.

\( \text{subrgn} \) See Mode 1 specification.

\( C_D \) The discharge coefficient for the boundary

\( P|PRES \) The modifier to indicate that the pressure at the boundary is being specified explicitly.

\( P_B \) By default it is assumed that the boundary pressure is equal to zero. If the \( P \) or \( PRES \) modifier is present, then this is taken to be the value of the boundary pressure.

\( \text{AREA} \) The modifier to indicate that the effective flow at the boundary is being specified explicitly.

\( A_B \) By default it is assumed that the area through which the flow occurs is the actual area of the boundary segment; that is \( A_B=A \). If the modifier \( \text{AREA} \) is present, then this is taken to be area through which the flow occurs.

\( \text{IN} \) If this modifier is present, then only inflow is allowed at the boundary. Any pressure gradient that indicates an outflow is set to zero.

\( \text{OUT} \) If this modifier is present, then only outflow is allowed at the boundary. Any pressure gradient that indicates an inflow is set to zero.

**APPLICABILITY**

This mode of the command is only available with the ANSWER™ and TIDAL™ Software Tools.

**EXAMPLES**

- **BOUN for U at ID=GATE surface:** DISCHARGE coef = 0.5
- **BOUN for V at ID=OPEN surface:** DISCHARGE coef = 0.5, \( P=100 \)
- **BOUN for U at ID=OPEN surface:** DISCHARGE coef = 0.5, \( P=100 \), \( \text{AREA}=0.02 \)
MODE 5: Gate boundary conditions for Tide Height

SYNTAX

```
BOUN {ETA} {GATE} {IN|OUT} [func] {N1, N2, ..., Nn} [fname] [dir] [subrgn]
```

ETA
The boundary condition is for water elevation or tide height for TIDAL™ Software Tool.

GATE
The boundary is considered to be operated by a gate that allows the water to go in or out based on the nature of the gate (see IN and OUT below).

IN
The gate is assumed to open inwards. When the specified water elevation (η) exceeds the elevation just inside the boundary, the flow is allowed to go in; otherwise the normal velocity at the boundary (Vn) is assumed to be zero. Let S denote the elevation computed from the specification above, B the value at the boundary node, and F that at the field node immediately inside; then the conditions imposed are:

\[
\eta_S > \eta_F \rightarrow \eta_B = \eta_S; \quad V_nB = V_nF \\
\eta_S \leq \eta_F \rightarrow \eta_B = \eta_F; \quad V_nB = 0
\]

OUT
The gate is assumed to open outwards. When the elevation just inside the boundary exceeds the specified water elevation (η), the flow is allowed to go out; otherwise the normal velocity at the boundary (Vn) is assumed to be zero. The imposed boundary conditions are:

\[
\eta_F > \eta_S \rightarrow \eta_B = \eta_S; \quad V_nB = V_nF \\
\eta_F \leq \eta_S \rightarrow \eta_B = \eta_F; \quad V_nB = 0
\]

func
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the value of elevation, η, at the boundary. If no function is specified then the value is assumed to be constant.

ξ
One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N1,...,Nn
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname
The name of the file containing numerical values N2 through Nn. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

dir
See Mode 1 specification.

subrgn
See Mode 1 specification.

APPLICABILITY
This mode of the command is only available with the TIDAL™ Software Tool.

EXAMPLES
Generic examples for this command are given in Section 4.4. The command keyword (BOUNDARY) must replace the keyword used in these examples and the ETA, GATE and one of the IN or OUT modifiers must be specified. The dir boundary orientation must also be specified.

\\
An additional example (2 lines)

BOUnDary ETA at X+ is GATE IN type: SINE function of TIME
Amplitude=0.1 frequency: 1.405634E-4; phase=0; offset=0, for region ID=SOUTH
**MODE 6:** Disable Previously Specified Boundary Conditions

**SYNTAX**

```
BOUN {Φ} {OFF} {dir} {ID=idsub}
```

**Φ**
One, and only one, symbol for the dependent variable for which the boundary conditions were previously specified. The valid symbols are listed in Table 2.7.1.

**OFF**
Previously specified boundary conditions for Φ for the identified subregion and the boundary direction identified by the orientation index N1 are deactivated. A new specification for this subregion may follow.

**dir**
See Mode 1 specification.

**idsub**
Identifier for the boundary segment which must have previously appeared with the same identity on a LOCATE or SELECT command.

**REMARKS**
The OFF command can only be used to disable previous commands that were specified for a single dependent variable. The boundary conditions specified with multiple list of variables (Mode 1) cannot be disabled by this command. These can however be superseded by new specifications.

**EXAMPLES**

```
BOUNDRY for T at Y+ boundary for ID=UPPER turned OFF
```
Keyword Commands

COMMAND   BRINKMAN-FORCHHEIMER

PURPOSE   To include Brinkman-Forchheimer terms in the governing Momentum equations. This command is effective only for the ANSWER™ and PORFLOW™ Software Tools.

SYNTAX    BRIN [C_F] [subrgn]

C_F       The Forchheimer coefficient for the non-linear drag terms for flow in a porous medium. The default value is 0.55.

If this command is present then the Brinkman-Forchheimer terms are included in the governing momentum equations.

For ANSWER™ the governing equation for momentum is modified to account for porosity of the medium as shown below.

\[
\frac{\partial}{\partial t}(\rho \theta V_j) + \frac{\partial}{\partial x_i}(\rho \theta V_i V_j) = \frac{\partial}{\partial x_i}(\mu \frac{\partial V_j}{\partial x_i}) - \theta \frac{\partial p}{\partial x_j} + \rho \theta g_j \cdot S_{BF} + S_j
\]

\[
S_{BF} = \theta^2 (1 + C_F \text{Re}_K) \frac{\mu}{K} V_j
\]

\[
\text{Re}_K = \frac{\rho \theta |V| \sqrt{K}}{\mu}
\]

Where the dimensions are given in square brackets and

- \( t \) is the time [\( t \)],
- \( X_i \) is the coordinate in the \( i^{th} \) direction [\( L \)],
- \( \rho \) is the mass density of the fluid, [\( M/L^3 \)],
- \( \theta \) is the porosity of medium, [0]
- \( V_j \) is the \( j^{th} \) component of fluid (particle) velocity [\( L/t \)]
- \( \mu \) is fluid viscosity [\( M/(Lt) \)]
- \( p \) is the fluid thermodynamic pressure [\( M/(L^2 t^2) \)],
- \( g_j \) is gravitational acceleration in the \( j^{th} \) direction [\( L/t^2 \)],
- \( S_{BF} \) is Brinkman-Forchheimer drag term [\( M/(L^2 t^2) \)],
- \( S_j \) is the source (or sink) term of the \( j^{th} \) component of velocity [\( M/(L^2 t^2) \)],
- \( C_F \) is Forchheimer-Ergun drag coefficient [0],
- \( \text{Re}_K \) is the Reynolds number based on permeability length scale [0],
- \( K \) is the permeability of the medium [\( L^2 \)],

For PORFLOW™ the governing equation for momentum is modified as follows:

\[
V_{dj} = - \frac{K_H}{1 + C_F \text{Re}_K} \left( \frac{\partial p}{\partial x_j} + \frac{\rho g_j}{\rho^* g} \right)
\]

\[
K_H = \frac{\rho^* g}{\mu} K ; \quad P = \frac{p - p^*}{\rho^* g}
\]

Where the superscript “*” denotes a reference value and

- \( V_{dj} \) is the Darcy velocity
- \( K_H \) is the hydraulic conductivity of porous medium [\( L/t \)],
- \( P \) is the hydraulic head [\( L \)]

**subrgn** The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.
REMARKS

For ANSWER™ Software Tool the permeability of the porous medium must be specified for this command to be effective. See the PERMEABILITY command. For the PORFLOW™ Software Tool, the hydraulic conductivity specified through the HYDRAULIC or CONDUCTIVITY command is used to compute these terms.

EXAMPLES

BRINKMAN terms to be included. For whole of domain
BRINKMAN terms to be included. For whole of domain
BRINKMAN terms to be included. For whole of domain
Keyword Commands

COMMAND  CAPILLARY

PURPOSE  To specify the coefficients for modification of capillary pressure due to changes in temperature or species concentration. This command is effective only for the PORFLOW™ Software Tool.

SYNTAX  CAPI {func[ξ]} {N₁, N₂, .., Nₙ | fname} [ZERO] [SECO] [subrgn]

func  One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input for capillary pressure. The function specifies the capillary pressure that is used to determine the phase saturation by the MULTIPHASE command. See COMMENTS below.

ξ  One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,..,Nₙ  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  The name of the file containing numerical values N₂ through Nₙ. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

ZERO  If this modifier is present, then the capillary pressure is set to zero.

SECO  By default the specification is assumed to be for the 1st phase fluid. If this modifier is present, then the input is applied to the capillary pressure of the 2nd phase.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

APPLICABILITY

This command is effective only for the PORFLOW™ Software Tool.

COMMENTS

The capillary pressure is meaningful only for vadose or multiphase problems (MULTIPHASE command), where the phase saturation is a function of the capillary pressure. By default, the capillary pressure is computed from the computed values of the pressures for the different phases of the fluid. With $P_n$ as the pressure of the nth phase fluid, the capillary pressure, $Ψ_n$, is computed from:

$$Ψ_n = P_n - P_{n+1}$$

If the CAPILLARY command is present, then the computed value is further modified as per the specification on the command. The nth phase saturation, $S_n$, is then computed from the specified soil-characteristic by the MULTIPHASE command. Though specifics of the $S''(Ψ_n)$ depend on the command, in general, the following conditions prevail for most characteristics.

$$Ψ^1 < 0 \rightarrow S^1 < 1; \ Ψ^1 \geq 0 \rightarrow S^1 = 1$$

$$Ψ^2 < 0 \rightarrow S^1 + S^2 < 1; \ Ψ^2 \geq 0 \rightarrow S^1 + S^2 = 1$$

The above guidelines may be violated for special cases especially those when hysteresis is present.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (CAPI) must replace the keyword used in these examples.
COMMAND  CLOSE

PURPOSE  To close output devices.

SYNTAX  CLOS  [filename] [SAVE | TABL | NUNIT]

filename  The name of the file to be closed. See Section 3.3 for additional information. If filename is specified, then the named file, if connected to a unit, will be closed. If NUNIT refers to a different file unit, then that unit, if open, will also be closed.

SAVE  Currently active archive file (SAVE) is closed; the default unit number for this file is 11.

TABL  Currently active Tabulated archive file (SAVE TABLE) is closed; the default unit number for this file is 12.

NUNIT  The file or I/O device unit number for the file for which the operation is performed. The unit number is ignored if one of the SAVE or TABL modifier is present.

COMMENTS

In general FORTRAN language does not differentiate between lower and upper case characters. However that is not true of many operating systems (O/S). It is in fact the O/S that performs all file handling. O/S peculiarities have been reported where, for example, there was no case distinction for read/write operations but the O/S distinguished between upper and lower case for file closing. It is therefore strongly recommended that the user should be consistent in using the same case characters if a previous file is referred to during file operations.

EXAMPLES

CLOS e  SAVE file
CLOS e  archive TABLe output file now
CLOS e  file by name “MYOLDFILE”
Keyword Commands

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>COMPRESSIBLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To select compressible flow option. This command is effective only for the ANSWER™ Software Tool.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>Mild Compressibility Option</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>COMP {MILD} [ATMO] [N1]</td>
</tr>
</tbody>
</table>

**MILD**
By default, the COMPRESSIBLE command invokes the fully compressible mode where density is assumed to be a function of the local pressure. If, this modifier is present then the mildly compressible mode of the equations is invoked. In this mode $\frac{\partial \rho}{\partial p}$ is assumed to be given from the gas law and, the variation of density due to pressure is taken account of only in the accumulation (time-dependent) term of the continuity equation. The fluid density is computed with a reference pressure rather than the local pressure. This form of the equations is primarily useful for acoustic purposes.

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial t} \frac{\partial p}{\partial t} = \alpha \rho \frac{\partial p}{\partial t}$$

In this equation the constant $\alpha$ has the units of $1/p$.

**ATMO**
The constant $\alpha$ is assumed to be equal to $1./101325$; the denominator being the value of the standard atmosphere in metric units.

**N1**
If a value greater than zero is specified then constant $\alpha$ is assumed to be equal to the specified value. If this value is omitted or is less than or equal to zero, and the ATMO is not specified, then $\alpha$ is assumed to be a local variable and is computed as:

$$\alpha = \frac{1}{\gamma(p + p^*)}$$

Where $\gamma$ is the specific heat ratio, $p$ is the local density, $p$ is the local pressure and $p^*$ is the reference pressure.

**COMMENTS**

For the compressible mode of solution, the enthalpy equation is modified to solve for stagnation enthalpy, $h_s$, rather than enthalpy, $h_T$. That is, the mean and turbulence kinetic energy of fluid is added to the enthalpy as defined by the below equation

$$h_s = h_T + \frac{1}{2} (U^2 + V^2 + W^2) + k$$

$$h_T = \sum_j m_j h_j ; \quad \sum_j m_j = 1 ,$$

$$h_j = h_j^0 + \int \frac{C_p_j}{T} dT ,$$

$$k = \frac{1}{2} (\overline{uu} + \overline{vv} + \overline{ww})$$

where

- $h_s$ is the enthalpy,
- $m_j$ the mass fraction, of the $j^{th}$ chemical species,
- $h_j^0$ is the heat of formation of the $j^{th}$ species,
- $C_p_j$ is the specific heat of the $j^{th}$ species at constant pressure,
- $T$ is the fluid temperature,
- $U, V, W$ are the mean, and $u,v,w$ the fluctuating, velocity components, and
- $k$ is the turbulence energy of fluid.
EXEMPLARY

COMPRESSIBLE FLOW
COMPRESSIBLE FLOW WITH C=1.0
COMPRESSIBLE FLOW WITH MILD COMpressibility
COMPRESSIBLE ISENthalpic FLOW
COMPRESSIBLE FLOW WITH INVIScid AND ISOPressure Assumptions
COMPRESSIBLE FLOW WITH INVIScid AND ISOPressure Assumptions; USE Fixed Pressure Option
Keyword Commands

MODE 2: Full Compressibility Option

SYNTAX COMP [DENS|SIMP|SYMM|DIRE|COUP] [ISEN|ISOT|ISOP] [INVI] [FIXE] [RHOU] [N₁]

DENS The density correction based DEFCON method is employed to solve the fully compressible version of the continuity equation. This is the default option.

SIMP The pressure correction based SIMPLE method is employed.

SYMM It is assumed that the changes in convective fluxes are directly proportional to changes in pressure gradient. This may lead to more robust numerical method for transonic flows. This option is not recommended for high Mach number flows.

DIRE By default after a new estimate of the pressure is computed at a given step, the velocity field, and therefore, convective mass flux, is updated to account for changes in pressure before going on to the next step. If this modifier is present, then no corrections are performed. This essentially leads to a direct sequential solution of the momentum and continuity equations.

COUP This is a reserved modifier. It implements a coupled solution method that is not yet available for general use.

ISEN By default, the temperature is computed from the stagnation enthalpy equation. If, this modifier is present then the stagnation enthalpy, hₛ, is assumed to be conserved and the temperature is computed from:

\[ T = \left( h_s - 0.5 V^2 \right) / C_p \]

where V is the flow speed and Cₚ is the specific heat at constant pressure. In this case, the stagnation enthalpy of the fluid must be supplied as input by the user.

ISOT The flow is assumed to be isothermal. Temperature is not computed; it is maintained at the initially specified value.

ISOP By default, the contribution of the \( \partial p / \partial t \) term is included in the computation of the enthalpy equation. If this modifier is present then this term is ignored.

INVI By default, the viscous heating terms are included in the computation of the enthalpy equation. If this modifier is present then the viscous heating effect in the stagnation enthalpy equation is ignored.

FIXE By default, for mildly compressible flow, the pressure is assumed to be in relative mode. The actual gas (datum) pressure is specified by the GAS P command. If this modifier is present, then the all input and output of pressure is in absolute mode.

RHOU By default, the convective flux at the interfaces of elements is computed from a product of averages of density and velocity. If this modifier is present, then the interface flux is computed as the average of the product of density and velocity.

N₁ The constant C (>0) of the pressure perturbation equation as given below. The default value is 1.4.

\[ P' = \rho' CRT \]

Where C is equal to unity for an isothermal process, and is equal to, \( \gamma \), the ratio of the specific heat at constant pressure to that at constant temperature, for an isentropic process.

COMMENTS

For the compressible mode of solution, the enthalpy equation is modified to solve for stagnation enthalpy rather than enthalpy. See the comments under Mode 1.
EXAMPLES

COMPressible flow
COMPressible flow with C=1.0
COMPressible flow with MILD compressibility
COMPressible ISENthalpic flow
COMPressible flow with INVIscid and ISOPressure assumptions
COMPressible flow with INVIscid and ISOPressure assumptions; use FIXED pressure option
**Keyword Commands**

**COMMAND**  CONDUCTIVITY

**PURPOSE**  To specify conductivity or diffusivity and the treatment of interface diffusion.

**MODE 1:**  Constant Hydraulic Conductivity in Principal Directions

**SYNTAX**  COND {P} {Γxx, Γyy, Γzz} [SATU|TOTA] [option] [subrgn]

**P**  Hydraulic conductivity is specified.  *This symbol must be specified.*

**Γxx, Γyy, Γzz**  The numerical values (>0) for the conductivity.  Two values must be specified for 2D geometry and three for 3D geometry.  The default units are [L/t] such as [m/s].

**SATU**  If this modifier is present, then it is assumed that the specified values are for the saturated hydraulic conductivity of the porous matrix.  The saturated value is multiplied with the relative conductivity (e.g. of unsaturated media see MULTIPHASE and COND RELATIVE commands) to compute the effective conductivity.  *This is the default option.*

**TOTA**  If this modifier is present, then the input is assumed to be the absolute or the effective hydraulic conductivity.  No multiplication by relative conductivity takes place.

**option**  Option selected for the operation to be performed.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>REPL</td>
<td>The computed value replaces the existing value. <em>This is the default option.</em></td>
</tr>
<tr>
<td>ADD</td>
<td>The computed value is added to the existing value.</td>
</tr>
<tr>
<td>SUBT</td>
<td>The computed value is subtracted from the existing value.</td>
</tr>
<tr>
<td>MULTI</td>
<td>The computed value multiplies the existing value.</td>
</tr>
<tr>
<td>DIVI</td>
<td>The computed value divides the existing value. A value of 1.E-30 is added to the divisor if it is zero.</td>
</tr>
</tbody>
</table>

**subrgn**  The subregion for which the input is specified.  See Section 3.4.  If *no* subregion is specified, the entire computational domain is selected.

**APPLICABILITY**

This input is applicable only for the PORFLOW™ Software Tool.

**EXAMPLES**

CONDUCTIVITY for P = 0.02, 0.01, 0.01 meters per year
CONDUCTIVITY for P = 0.02, 0.01, 0.01 meters per year ADD to existing value in ID=BLK1
MODE 2: **Hydraulic Conductivity in a Specified Direction**

**SYNTAX**

```
COND {P} [xyz] {func {ξ}} {N₁, N₂, ..., Nₙ} [fname] [SATU|TOTA][option] [subrgn]
```

- **P**
  - The hydraulic conductivity is specified.

- **xyz**
  - One of the character strings: **XX**, **YY**, **ZZ**, **XY**, **YX**, **XZ**, **ZX**, **YZ**, and **ZY**. It denotes the component of the conductivity tensor to which the input is applied. The first 3 denote the diagonal components of the tensor while the others denote the off-diagonal components. Since the tensor is symmetric, **XY** and **YX**, **XZ** and **ZX**, and **YZ** and **ZY** are equivalent. If no direction is specified, then the input is applied to all components of the tensor.

- **func**
  - One of the modifiers listed in Table 4.2.1 that denotes the functional form of the value of the appropriate component(s) of hydraulic conductivity. If no function is specified then the value is assumed to be constant.

- **ξ**
  - One of the independent variables listed in Table 4.2.2. If a function is explicitly specified but no variable is specified, then the independent variable is assumed to be time.

- **N₁,...,Nₙ**
  - The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

- **fname**
  - The name of the file containing numerical values **N₂** through **Nₙ**. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

- **SATU**
  - See Mode 1 of the command.

- **TOTA**
  - See Mode 1 of the command.

- **option**
  - See Mode 1 of the command.

- **subrgn**
  - See Mode 1 of the command.

**APPLICABILITY**

This input is applicable only for the **PORFLOW™** Software Tool.

**EXAMPLES**

Generic examples for this command are given in Section 4.4. The command keyword (**COND**) must replace the keyword used in these examples and the modifier **P** must appear on the command.
**MODE 3:** Hydraulic Conductivity in a Specified Direction

**SYNTAX**

\[ \text{COND} \ (P) \ \{\text{RELA}\} \ \{\text{func}[\xi]\} \ \{N_1, \ N_2, \ldots, \ N_n\ | \text{name}\} \ \{\text{option}\} \ \{\text{GRAD}\} \ \{\text{subrgn}\} \]

**P**
The hydraulic conductivity is specified.

**RELA**
The input is assumed to be for the relative hydraulic conductivity. The actual hydraulic conductivity is obtained by multiplying the saturated conductivity with the relativity conductivity.

**func**
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the value of the appropriate component(s) of hydraulic conductivity. If no function is specified then the value is assumed to be constant.

**\(\xi\)**
One of the independent variables listed in Table 4.2.2. If a function is explicitly specified but no variable is specified, then the independent variable is assumed to be time.

**\(N_1,\ldots,N_n\)**
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

**fname**
The name of the file containing numerical values \(N_2\) through \(N_n\). This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

**option**
See Mode 1 of the command.

**GRAD**
By default the relative hydraulic conductivity at boundaries is computed from the specified function. If this modifier is present, then the value of relative conductivity at all external boundaries is set equal to the field value at the nearest neighbor.

**subrgn**
See Mode 1 of the command.

**APPLICABILITY**
This input is applicable only for the PORFLOW™ Software Tool.

**EXAMPLES**
Generic examples for this command are given in Section 4.4. The command keyword (COND) must replace the keyword used in these examples and the modifiers P RELA must appear on the command
MODE 4: Thermal Conductivity of Primary Fluid Phase

SYNTAX

```
COND {HT | T} [xyz] {func(ξ)} {N₁, N₂, .., Nₙ} [fname] [MOLE | TOTA] [ALWA] [option] [subrgn] [FIEL | dir]
```

**HT**

The symbol that denotes that the value specified is the thermal conductivity of fluid. The thermal conductivity must be specified in mass units [e.g. J/(m·s·K)].

**T**

Same as above.

**xyz**

One of the character strings: XX, YY, ZZ, XY, YX, XZ, ZX, YZ and ZY. It denotes the component of the conductivity tensor to which the input is applied. The first 3 denote the diagonal components of the tensor while the others denote the off-diagonal components. Since the tensor is symmetric, XY and YX, XZ and ZX, and YZ and ZY are equivalent. If no direction is specified, then the input is applied to all components of the tensor.

**func**

One of the modifiers listed in Table 4.2.1 that denotes the functional form for the value of the thermal conductivity.

**ξ**

One of the independent variables listed in Table 4.2.2. If a function is explicitly specified but no variable is specified, then the independent variable is assumed to be time.

**N₁,..,Nₙ**

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

**fname**

The name of the file containing numerical values N₂ through Nₙ. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

**MOLE**

If this modifier is present, then it is assumed that the specified value is for the molecular component of the thermal conductivity. The dispersion (see DISPERSION command) is added to the computed value.

**TOTA**

If this modifier is present, then it is assumed that the specified value is for the total thermal conductivity of the system. No dispersion is added and no account is taken of the fact that the total system may consist of multiple fluid phases or a solid-fluid matrix. This is the default option.

**ALWA**

If this modifier is present, then the thermal conductivity is computed at every step of calculation. By default, the value is computed once (at the time the command is encountered) and stored in the thermal conductivity array. This modifier is only required if the computed value is a function of a variable that will change during computations.

**option**

See Mode 1 of the command.

**subrgn**

See Mode 1 of the command.

**FIEL**

See Mode 1 of the command.

**dir**

See Mode 1 of the command.

**REMARKS**

If the computed system has multiple fluid phases or is a fluid-solid matrix, then the effective value of thermal conductivity is computed as the weighted sum of the fluid and solid components. The weighting function is the volumetric saturation of each phase. The dispersion, if any, is then added to this effective value to arrive at the total thermal conductivity of the system.

**EXAMPLES**

Generic examples for this command are given in Section 4.4. The command keyword (COND) must replace the keyword used in these examples and the modifier T or HT must appear on the command.
MODE 5: Thermal Conductivity of the Second Fluid Phase

SYNTAX

COND {HT | T} {SECO} {Γ}

HT
The symbol that denotes that the value specified is the thermal conductivity of fluid. The thermal conductivity must be specified in mass units [e.g. J/(m·s·°K)].

T
Same as above.

SECO
The thermal conductivity of the 2\text{nd} fluid phase is specified.

Γ
The constant and uniform value of the thermal conductivity for the 2\text{nd} phase fluid. The default value is zero.

REMARKS

Current versions of the ACRi Software Tools only allow a constant and uniform value for the thermal conductivity of the 2\text{nd} phase fluid. If a 3\text{rd} fluid phase is present then the thermal conductivity for the 3\text{rd} phase is assumed to be zero; user can not specify a value for the 3\text{rd} phase.

EXAMPLES

CONDUCTIVITY for T SECOND phase value = 1.E-5
MODE 6: Thermal Conductivity of the Solid Component of a Fluid-Solid Matrix

SYNTAX 
COND {HT | T} {SOLI} {func[3]} {N₁, N₂, .., Nₙ} | fname | [option] | [subrgn] | [FIEL | dir]

HT The symbol that denotes that the value specified is the thermal conductivity of fluid. The thermal conductivity must be specified in mass units [e.g. J/(m·s⁻¹·K)].

T Same as above.

SOLI The thermal conductivity of the solid component of a fluid-solid matrix is specified.

func One of the modifiers listed in Table 4.2.1 that denotes the functional form for the value of the thermal conductivity.

ξ One of the independent variables listed in Table 4.2.2. If a function is explicitly specified but no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname The name of the file containing numerical values N₂ through Nₙ. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

option See Mode 1 of the command.

subrgn See Mode 1 of the command.

FIEL See Mode 1 of the command.

dir See Mode 1 of the command.

REMARKS
If the computed system has multiple fluid phases or is a fluid-solid matrix, then the effective value of thermal conductivity is computed as the weighted sum of the fluid and solid components. The weighting function is the volumetric saturation of each phase. The dispersion, if any, is then added to this effective value to arrive at the total thermal conductivity of the system.

EXAMPLES
Generic examples for this command are given in Section 4.4. The command keyword (COND) must replace the keyword used in these examples and the modifier T or HT and SOLI must appear on the command.
MODE 7: Conductivity or Diffusivity of a Mass Species

SYNTAX  
COND {Φ} [xyz] {func[ξ]} {N₁, N₂, ..., Nₙ} [fname] [MOLE|TOTA] [KINE|MASS] [option] [subrgn] [FIEL|dir]

Φ  
A symbol that denotes the dependent variable for which the conductivity or diffusivity is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

xyz  
One of the character strings: XX, YY, ZZ, XY, YX, XZ, ZX, YZ, and ZY. It denotes the component of the conductivity or diffusivity tensor to which the input is applied. The first 3 denote the diagonal components of the tensor while the others denote the off-diagonal components. Since the tensor is symmetric, XY and YX, XZ and ZX, and YZ and ZY are equivalent. If no direction is specified, then the input is applied to all components of the tensor.

func  
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the value of the appropriate conduction or diffusion coefficient for the corresponding Φ variable. If no function is specified then the value is assumed to be constant.

ξ  
One of the independent variables listed in Table 4.2.2. If a function is explicitly specified but no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ  
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  
The name of the file containing numerical values N₂ through Nₙ. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

MOLE  
If this modifier is present, then it is assumed that the specified value is for the molecular component of the diffusivity. The dispersion (see DISPERSION command) is added to the computed value.

TOTA  
If this modifier is present, then it is assumed that the specified value is for the total diffusivity. No dispersion is added to the computed value. This is the default option.

KINE  
By default the units of diffusivity are mass units [e.g. kg/m-s] for ANSWER™ and TIDAL™ Software Tools. If KINE modifier is present, the specification is assumed to be in kinetic units (e.g. m²/s). The kinetic units are converted to mass units by multiplication with reference density (see REFERENCE command).

MASS  
By default PORFLOW™ input for mass species is assumed to be in kinetic units (e.g. m²/s). If this modifier is present, then the input is assumed to be in mass units [e.g. kg/m-s]. The conversion to kinetic units is done by division with reference fluid density (see REFERENCE command).

option  
Option selected for the operation to be performed.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>REPL</td>
<td>The computed value replaces the existing value. This is the default option.</td>
</tr>
<tr>
<td>ADD</td>
<td>The computed value is added to the existing value.</td>
</tr>
<tr>
<td>SUBT</td>
<td>The computed value is subtracted from the existing value.</td>
</tr>
<tr>
<td>MULT</td>
<td>The computed value multiplies the existing value.</td>
</tr>
<tr>
<td>DIVI</td>
<td>The computed value divides the existing value. A value of 1.E-30 is added to the divisor if it is zero.</td>
</tr>
</tbody>
</table>

subrgn  
The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.
APPLICABILITY

For PORFLOW™ Software Tool the vector (with diagonal components) mode of the command is operational for all equations. The tensor (with off-diagonal components) mode is applicable only for the thermal and species transport equations.

For ANSWER™ Software Tool this command can be employed for all equations. However, if the vector or tensor mode (dir modifier) is invoked, then the skew diffusion terms (see Mode 6) are ignored and the wall diffusive flux is set to zero for all except the momentum equations.

For TIDAL™ Software Tool this command is implemented only for the species transport equations.

COMMENTS

The conductivity for a species is generally a tensor. This command allows the components of the tensor to be specified in many different forms. For flow in porous media, the conductivity is often modified by dispersivity and tortuosity. See the DISPERSIVITY and TORTUOSITY commands for further information.

EXAMPLES

CONDUCTIVITY for C =1.E-6 ! Diffusivity for the species transport equation

See also generic examples for functional specification in Section 4.4. The command keyword (COND) must replace the keyword used in these examples. The modifier XX, YY or ZZ may be additionally specified on the command.
Keyword Commands

MODE 8: Specification of Conductivity or Diffusivity on a Node by Node Basis

SYNTAX

```
COND {Φ} {NODE|STRU|UNST|fname} [V₁...Vₘ] [KINE|MASS] [option] [subrgn] [FIEL] [dir]
```

**Φ**
A symbol that denotes the dependent variable for which the conductivity or diffusivity is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

**NODE**
The input is specified in a node-by-node manner. By default if is assumed that the input values are given in the STRUCTURED mode if the subrgn was defined with a LOCATE command in terms of grid indices or in the UNSTUCTURED mode otherwise.

**STRU**
The input is read in the manner of nested implied FORTRAN DO loops:

```
Read (NUNIT, *) (((VAR (I, J, K), I = ILO, IHI), J = JLO, JHI), K = KLO, KHI)
```

Where NUNIT is an internally assigned unit number, VAR is the variable denoted by Φ, and ILO, IHI, JLO, JHI, KLO, KHI define, respectively, the starting and ending grid index values for the subrgn for a structured grid. For 2D grid, KLO and KHI are set to unity.

**UNST**
The input is read in the manner of a simple implied FORTRAN DO loop:

```
Read (NUNIT, *) (VAR (M), M = MLO, MHI)
```

Where NUNIT is an internally assigned unit number, VAR is the variable denoted by Φ, and MLO and MIHI are the starting and ending element numbers for the subrgn. The order of the elements is the same as the one specified (or implied) by the corresponding LOCATE command which can be examined by including a file name on the LOCATE command.

**fname**
The name of the file for numerical values unless the values are directly specified by V₁...Vₘ below. See Section 3.3 for additional information.

**V₁...Vₘ**
The values of the variable at each node selected by the subrgn and dir modifiers. These values must be present unless fname is present. In this case, one of the modifiers, NODE, STRU, or UNST must also be specified.

**KINE**
See Mode 1 of command..

**MASS**
See Mode 1 of command..

**option**
See Mode 1 of command..

**subrgn**
The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

**dir**
One of the character strings: XX, YY, ZZ, XY, YX, XZ, ZX, YZ and ZY. It denotes the component of the conductivity tensor to which the input is applied. The first 3 denote the diagonal components of the diffusion tensor while the others denote the off-diagonal components. Since the tensor is symmetric, XY and YX, XZ and ZX, and YZ and ZY are equivalent. The off-diagonal components are only allowed for the PORFLOW™ software; their specification automatically and simultaneously invokes Mode 6 of the command. If no direction is specified, then the input is applied to all components of the tensor.

**APPLICABILITY**

See Mode 2 of the Command.

**EXAMPLES**

CONDuctivity by NODE for P variable for ID=SUBRGN1 ! 3 nodes in this region – PORFLOW™

```
1.5, 11.5, 10.
```

CONDuctivity for P NODE in STRUctured mode from File “KHYD.FIL”

CONDuctivity for P STRUctured mode from File “KHYD.FIL” for Field NODES only

CONDuctivity by NODE ID=MIDDLE T from file ‘SPATIAL’ in UNSTructured mode from ‘KT.FIL’
MODE 9: Specification of Contact or Film Transfer Coefficient

SYNTAX

```
COND {CONT|FILM} {Φ} {func[ξ]} {N₁, N₂, ..., Nₙ} {fname} [REPL|ADD|TOTA] {subrgn} [dir]
```

CONT

The contact or film transfer coefficient at a surface is specified. This transfer coefficient can replace or augment the conduction or diffusion that occurs at a surface.

FILM

Same as CONTACT Modifier.

Φ

A symbol that denotes the dependent variable for which the input is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

func

One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the value of the appropriate transfer coefficient for the specified Φ variable. If no function is specified then the value is assumed to be constant.

ξ

One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname

The name of the file containing numerical values N₂ through Nₙ. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for additional information.

REPL

This is the default mode. Any internal computations for the conductive (diffusive) flux between two nodes across a surface are replaced by:

\[
q_Φ = \frac{A_f (Φ_1 - Φ_2)}{ds_1 + \frac{ds_2}{Γ} + h}
\]

where, \(q_Φ\) is flux from node “1” to node “2”, \(A_f\) is the interface area, \(ds_1\) and \(ds_2\) are distances, \(Γ\) is the diffusion coefficient and, \(h\) is the specified transfer coefficient.

ADD

The transfer flux is added to the internally computed flux (which may have been modified by effects such as wall functions for turbulent flow). In this case:

\[
q_Φ = q_Φ_{intena} + hA_f (Φ_1 - Φ_2)
\]

TOTA

The diffusive flux at the surface is computed as:

\[
q_Φ = hA_f (Φ_1 - Φ_2)
\]

subrgn

The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

dir

The orientation index for the element boundary associated with the transfer coefficient. See Section 3.5 for available choices. If no dir is specified, then all surfaces of the selected subrgn are selected.

APPLICABILITY

This command mode is not available for the TIDAL™ Software Tool.

EXAMPLES

```
CONDuction for T with contact heat transfer coefficient of 0.01 at Y+ of ID=WALL
CONDuction for T with contact heat transfer coefficient of 0.01 at Y+ of ID=WALL TOTAl
```

Generic examples for this command are given in Section 4.4. The command keyword (COND) must replace the keyword used in these examples. The modifier FILM or CONTACT must appear in the command.
MODE 10: Modification of Diffusion Coefficient by Richardson Number

SYNTAX

COND {RICH | [dir]} [UNLI | ZERO] [α, β, αφ, βφ]

RICH
The viscosity and diffusion coefficient in the specified direction are modified due to the effects of density gradient for the Richardson number effect. The viscosity, \( \mu \), and the diffusion coefficient, \( \Gamma \), in the selected direction are computed from:

\[
\mu_i = \frac{\mu}{[1 + \beta_Ri]^\alpha}, \quad \Gamma_i = \frac{\Gamma}{[1 + \beta_{\varphi}Ri]^\phi}
\]

Where subscript "i" denotes the direction specified by the \( \text{dir} \) modifier, \( \mu \) and \( \Gamma \) are, respectively, the scalar values of the viscosity and diffusion coefficients (specified by user or computed from built-in formulae), and \( \alpha \), \( \beta \), \( \alpha_{\varphi} \) and \( \beta_{\varphi} \) empirical constants. The Richardson number, \( Ri \), is defined as:

\[
Ri = \frac{1}{g_i \rho} \frac{\partial \rho}{\partial x_i} \left( \sum_{j \neq i} \left( \frac{\partial u_j}{\partial x_i} \right)^2 \right)
\]

where \( g_i \) is the gravitational acceleration in the \( i^{\text{th}} \) direction (specified by the \( \text{dir} \) modifier), \( \rho \) is the fluid density and \( u_j \) represents the velocity components in directions other than the \( i^{\text{th}} \) direction.

A final consequence of Richardson number modification is that the production term in the turbulence kinetic energy equation is modified to include the additional term for production/destruction of turbulence energy due to buoyancy:

\[
- \frac{\mu_{\alpha} \partial \rho}{\rho^2} \frac{\partial \rho}{\partial x_i} \frac{\partial P}{\partial x_i}
\]

If this command with a \( \text{RICH} \) modifier is not specified, then this additional term is excluded from the turbulence kinetic energy equation.

dir
One of the \( X \), \( Y \), \( Z \), \( R \) or \( \text{THETA} \) modifiers that, respectively, denotes directional viscosity and diffusivity that are modified. If no direction is specified, then y-direction in the 2D and Z direction in the 3D geometry is automatically selected.

UNLI
By default the modification of the production term in the turbulence kinetic equation is performed with the constraint that the net production term is not less than zero; that is the total production can never become negative. However if the \( \text{UNLIMITED} \) modifier is present, then the production term is allowed to become negative. If this option is activated, then it is possible that turbulence kinetic energy, \( k \), may become negative. This is physically unrealistic; it is therefore strongly recommended that the \( \text{LIMIT} \) command should be specified to place a reasonable lower limit on \( k \).

ZERO
The additional term in the turbulence production is identically set to zero.

\( \alpha, \beta, \alpha_{\varphi}, \beta_{\varphi} \)
The empirical constants for the Richardson number formula. The default values are 0.5, 10, 1.5 and 3.33, respectively.

APPLICABILITY

This command mode is available only for the \( \text{ANSWER}^{TM} \) Software Tool
EXAMPLES

CONDuction modified by RICHardson Number
CONDuction modified by RICHardson Number with constants: 0.67, 6.67, 1., 5
Keyword Commands

MODE 11 Treatment of Skew Diffusion Terms

SYNTAX COND {SKEW|SECO} [POSI] [Φ]

SKEW Skew conduction or diffusion terms at the element interfaces, that arise if the grid arrangement is non-orthogonal, are included in computing interface diffusive fluxes. Typically these are 2nd order terms and have very little influence in convection-dominated flow but the computing time is generally increased by 10 to 20 percent. In many practical situations, these terms can be ignored. By default these terms are not included; hence this modifier must be specified to account for skew diffusion.

SECO Same as SKEW modifier.

POSI The total diffusive flux for the variable Φ at the face “f” between two elements shown in the picture below is given by:

\[ Q_D = -\Gamma_{ij} \frac{\partial \Phi}{\partial x_j} n_i A_f, \]

where summation convention is implied, and \( \Gamma_{ij} \) is the diffusion coefficient for the variable Φ at face f, \( A_f \) is the area of the face and \( n_i \) is the direction vector in the \( i^{th} \) direction. The direction of flux is positive if it is incoming for the element at P (aligned with the normal vector at face f).

In general, for numerical robustness of the algorithm, it is preferable that:

\[ \frac{Q_D}{\Phi_B - \Phi_P} > 0; \quad \Phi_B - \Phi_P \neq 0 \]
\[ Q_D = 0; \quad \Phi_B - \Phi_P = 0 \]

For highly skewed grids, above relation may be violated. If the modifier POSI is specified, then the diffusive flux \( Q_D \) is computed only from the values of \( \Phi_B \) and \( \Phi_P \) and any contribution of the 2nd order skew terms is ignored.

Φ One or more of the symbols that denote the dependent variables for which the skew terms are to be included. The valid symbols are listed in Table 2.7.1. If no symbol is specified, then skew terms are included for all variables.

APPLICABILITY

This command mode is not available for the TIDAL™ Software Tool

EXAMPLES

CONDuction due to SKEW terms to be included for all variables
CONDuction due to SECOndary terms to be included for U and T
CONDuction due to SECOndary and enforce POSItive relation between flux and node values.
MODE 12: Tensor Diffusivity with off-Diagonal Terms

SYNTAX

COND {TENS} [USER] [POSI] [Φ]

TENS

By default only the diagonal components of the diffusion tensor $\Gamma_{ij}$ are included in computations. It is assumed that the off-diagonal components ($i \neq j$) are zero. If this modifier is present, the off-diagonal components of the diffusion tensor are also included (see Mode 4 for mathematical expression of diffusive flux). It should be noted, that this mode automatically and simultaneously invokes Mode 4 of command.

This mode of the command is currently available only for the PORFLOW™ software. Unless individual values of the diffusion components are specified by Mode 2 of the command, the general form of the diffusivity tensor is that given by Scheidegger (1961):

$$\Gamma_{ij} = \alpha_T \delta_{ij} V + (\alpha_L - \alpha_T) \frac{v_i v_j}{V},$$

$$V = (v_i v_j)^{1/2}; v_i = \frac{V_i}{\theta_E}$$

where $\alpha_L$ and $\alpha_T$ are, respectively, the longitudinal and transverse dispersivities for the porous matrix, $\delta_{ij}$ is the Kronecker delta function, $v_i$ is the fluid particle velocity vector, $V$ is its magnitude, $V_i$ is the Darcy velocity vector and $\theta_E$ is the soil moisture.

USER

By default the tensor diffusivity components are computed from Scheidegger (1961) relations as given above. If this modifier is present, then this computation is by-passed. In this case, each component of the diffusivity tensor must be explicitly specified by the user through Mode 1 of this command.

POSI

See Mode 4 of the command.

Φ

One or more of the symbols that denote the dependent variables for which the skew terms are to be included. The valid symbols are listed in Table 2.7.1. If no symbol is specified, then skew terms are included for all variables.

APPLICABILITY

This command mode is not available for the TIDAL™ Software Tool

EXAMPLES

CONDuction due to SKEW terms to be included for all variables
CONDuction with TENSOR diffusivity
CONDuction TENSOR diffusivity with USER specified values and POSITive relation with del_phi
CONDuction due to SECOndary terms to be included for U and T
MODE 13: Treatment of Conductivity and Diffusivity at External Boundary

SYNTAX COND {BOUN} [Φ]

BOUN For elements that lie next to the exterior boundary, the conductivity or diffusivity at the external boundary (edge of the element) may differ from the value specified at the interior (node) of the element. The user is therefore expected to specify these properties. If the BOUNDARY modifier is specified, then the boundary value of conductivity or diffusivity, for all elements next to boundary, is set equal to the value at the interior node of the element.

Φ One or more of the symbols that represent the variables for which the boundary conductivity or diffusivity is specified. The valid symbols are listed in Table 2.7.1. If no symbols are specified then the boundary conductivity or diffusivity for all the variables is set equal to the interior node value.

APPLICABILITY This command mode is not available for the TIDAL™ Software Tool

EXAMPLES

CONDuctivity BOUNdary for T : Set boundary value equal to interior.
CONDuctivity BOUNdary for C : Set boundary value equal to interior. value
MODE 14: Elimination of Diffusion Terms

SYNTAX COND {OFF} [Φ]

OFF The conduction or diffusion terms for the specified variable are completely omitted from the governing equation.

Φ A symbol that denotes the dependent variable for which the diffusion terms are to be eliminated. The valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

EXAMPLES

CONDuction OFF for the temperature variable: T
Keyword Commands

**COMMAND**

**CONNECTIVITY**

**PURPOSE**
To specify element to vertex connectivity for unstructured grid. This command is effective only for the ANSWER™ and PORFLOW™ Software Tools.

**MODE 1:**
Vertex Connectivity for Quad or Hex Elements

**SYNTAX**

`CONN {VERT} {fname}`

**VERT**
The element to vertex connectivity is specified. The file must contain as many records as the number of elements specified on the GRID command. Each record consists of the element number followed by 4 (for 2D) or 8 (for 3D) vertex numbers of the element corners. Each record is read by the FORTRAN statement:

```
READ (IFILE,*) M,( NV(K),K = 1, NBRMX )
```

where IFILE is an internally assigned file unit number, M, is the element number, NBRMX takes the value of 4 in 2D and value of 8 in 3D, and NV are the vertex numbers for the element corners.

For 2D geometry, the vertices must be specified in a **counter-clock wise fashion in the x-y plane**, such that the local ($\xi$, $\eta$) and the direction normal to the plane form a right handed system. For 3D geometry, the vertices on “bottom” side must be specified first (in counter-clockwise order) followed by the corresponding vertices on “top” side, such that the local ($\xi$, $\eta$, $\zeta$) direction forms a right handed system. (Any side may be chosen as the “bottom”, then the topologically opposite side is considered to be the “top”). The local ($\xi$, $\eta$, $\zeta$) direction for each element is defined by the order in which the vertices appear on this record. The local $\xi$ axis is oriented from vertex 1 to vertex 2, the $\eta$ axis from vertex 1 to vertex 4, and the $\zeta$ axis from vertex 1 to vertex 5. These then determine the local side number (1, 2, 3, 4) or the local X-, X+, Y-, Y+, Z- Z+ sides which are used to specify the boundary and boundary conditions. These concepts are illustrated in Figures 1 and 2. Some further details are also given in Section 3.5. This is the default option.

**fname**
The name of the file containing the numerical input for the connectivity. **There is no default value; a file name must be specified.**

**COMMENTS**

An unstructured mesh is defined by:

(a) A list of vertex numbers (integer) and their space coordinates (real), and
(b) A list of element numbers (integer) and their vertex numbers (integer).
(c) The list (b) defines the “mapping” from each element to its vertices in list (a).

**EXAMPLES**

CONNnectivity information on file “VERT2ELM.CNC”
CONNnectivity of VERTices to elements on file “VERT2ELM.CNC”
Assume that the vertex connectivity record for this element reads as follows:

<table>
<thead>
<tr>
<th>Cell #</th>
<th>Cell Type</th>
<th># of Corners</th>
<th>Vertex List</th>
</tr>
</thead>
<tbody>
<tr>
<td>?</td>
<td>2</td>
<td>4</td>
<td>1, 2, 3, 4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Side Number</th>
<th>Vertex Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 4</td>
</tr>
<tr>
<td>2</td>
<td>2, 3</td>
</tr>
<tr>
<td>3</td>
<td>1, 2</td>
</tr>
<tr>
<td>4</td>
<td>3, 4</td>
</tr>
</tbody>
</table>

The right hand rule implies that: $(\vec{r}_{12} \times \vec{r}_{13}) \cdot \vec{k} > 0$, where $\vec{r}_{12}$ is the position vector from vertex 1 to vertex 2.

Figure 1: Relation between Vertex Numbers and Side Numbers for a Quadrilateral illustrating the application of the right hand rule. (2D only).
Hexahedron

Assume that the vertex connectivity record for this element reads as follows:

<table>
<thead>
<tr>
<th>Cell #</th>
<th>Cell Type, # of Corners</th>
<th>Vertex List</th>
</tr>
</thead>
<tbody>
<tr>
<td>?</td>
<td>6, 8</td>
<td>1, 2, 3, 4, 5, 6, 7, 8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Side Number</th>
<th>Vertex Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 4, 8, 5</td>
</tr>
<tr>
<td>2</td>
<td>3, 2, 6, 7</td>
</tr>
<tr>
<td>3</td>
<td>2, 1, 5, 6</td>
</tr>
<tr>
<td>4</td>
<td>4, 3, 7, 8</td>
</tr>
<tr>
<td>5</td>
<td>1, 2, 3, 4</td>
</tr>
<tr>
<td>6</td>
<td>5, 8, 7, 6</td>
</tr>
</tbody>
</table>

The right hand rule implies that: \((\mathbf{r}_{12} \times \mathbf{r}_{14}) \cdot \mathbf{r}_{15} > 0\), where \(\mathbf{r}_{12}\) is the position vector from corner 1 to corner 2.

Note that the side numbering scheme in the hexahedron follows a different scheme from that of other shapes. Here, the opposite sides are numbered consecutively.

**Figure 2:** Relation between Vertex Numbers and Side Numbers for a Hexahedron illustrating the application of the right hand rule. (3D only).
MODE 2: Vertex Connectivity for Mixed Hybrid Elements.

SYNTAX

```
CONN {HYBR} {fname}
```

HYBR
The element to vertex connectivity is specified for a grid with mixed type of elements. Currently 6 different types of elements are allowed. These are given in the Table below.

<table>
<thead>
<tr>
<th>Element Type</th>
<th># of Vertices</th>
<th># of Sides</th>
<th>Geometry</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3</td>
<td>3</td>
<td>2D</td>
<td>Triangle</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>4</td>
<td>2D</td>
<td>Quadrilateral</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>4</td>
<td>3D</td>
<td>Tetrahedron</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>5</td>
<td>3D</td>
<td>Quad-Based Pyramid</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>5</td>
<td>3D</td>
<td>Triangle-based Prism</td>
</tr>
<tr>
<td>6</td>
<td>8</td>
<td>6</td>
<td>3D</td>
<td>Hexahedron</td>
</tr>
</tbody>
</table>

The file must contain as many records as the number of elements specified on the GRID command. Each record must specify (in order), the element number, element type (given in the Table above), the total number of vertices for that element (given in Table above) and the vertex numbers for the element corners. Each record is read by the FORTRAN statement:

```
READ (IFILE,*) M, MTYPE, NVRTX,( NV(K),K=1,NVRTX)
```

where IFILE is an internally assigned file unit number, M, is the element number, MTYPE is the element type, NVRTX is the number of vertices for the element, and NV are the vertex numbers for the element corners.

Schematic of each element type and its connectivity describing the relationship of the local side numbering to the vertex connectivity is illustrated in Figures 1 through 6. Further details are given in Section 3.5).

fname
The name of the file containing the numerical input for the connectivity. There is no default value; a file name must be specified.

EXAMPLES

```
CONNectivity for HYBRID elements on file "MIXED_ELEMENTS.CNC"
```
Triangle

Assume that the vertex connectivity record for this element reads as follows:

<table>
<thead>
<tr>
<th>Cell #</th>
<th>Cell Type</th>
<th># of Corners</th>
<th>Vertex List</th>
</tr>
</thead>
<tbody>
<tr>
<td>?</td>
<td>1</td>
<td>3</td>
<td>1, 2, 3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Side Number</th>
<th>Vertex Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 2</td>
</tr>
<tr>
<td>2</td>
<td>2, 3</td>
</tr>
<tr>
<td>3</td>
<td>3, 1</td>
</tr>
</tbody>
</table>

The right hand rule implies that: \((\vec{r}_{12} \times \vec{r}_{13}) \cdot \hat{k} > 0\), where \(\vec{r}_{12}\) is the position vector from vertex 1 to vertex 2.

**Figure 3: Relation between Vertex Numbers and Side Numbers for a Triangle illustrating the application of the right hand rule. (2D only).**
Tetrahedron

Assume that the vertex connectivity record for this element reads as follows:

<table>
<thead>
<tr>
<th>Cell #</th>
<th>Cell Type</th>
<th># of Corners</th>
<th>Vertex List</th>
</tr>
</thead>
<tbody>
<tr>
<td>?</td>
<td>3</td>
<td>4</td>
<td>1, 2, 3, 4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Side Number</th>
<th>Vertex Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 3, 4</td>
</tr>
<tr>
<td>2</td>
<td>1, 4, 2</td>
</tr>
<tr>
<td>3</td>
<td>4, 3, 2</td>
</tr>
<tr>
<td>4</td>
<td>1, 2, 3</td>
</tr>
</tbody>
</table>

The right hand rule implies that: \((\vec{r}_{12} \times \vec{r}_{13}) \cdot \vec{r}_{14} > 0\), where \(\vec{r}_{12}\) is the position vector from vertex 1 to vertex 2.

**Figure 4:** Relation between Vertex Numbers and Side Numbers for a Tetrahedron illustrating the application of the right hand rule. (3D only).
Figure 5: Relation between Vertex Numbers and Side Numbers for a Pyramid illustrating the application of the right hand rule. (3D only).

Pyramid

Assume that the vertex connectivity record for this element reads as follows:

<table>
<thead>
<tr>
<th>Cell #, Cell Type, # of Corners, Vertex List:</th>
</tr>
</thead>
<tbody>
<tr>
<td>4, 5, 5, 1, 2, 3, 4, 5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Side Number</th>
<th>Vertex Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 4, 5</td>
</tr>
<tr>
<td>2</td>
<td>1, 5, 2</td>
</tr>
<tr>
<td>3</td>
<td>3, 2, 5</td>
</tr>
<tr>
<td>4</td>
<td>4, 3, 5</td>
</tr>
<tr>
<td>5</td>
<td>1, 2, 3, 4</td>
</tr>
</tbody>
</table>

The right hand rule implies that: 

\[ \vec{r}_{12} \times \vec{r}_{14} \cdot \vec{r}_{15} > 0 \],

where \( \vec{r}_{12} \) is the position vector from vertex 1 to vertex 2.
Assume that the vertex connectivity record for this element reads as follows:

<table>
<thead>
<tr>
<th>Cell #</th>
<th>Cell Type</th>
<th># of Corners</th>
<th>Vertex List:</th>
</tr>
</thead>
<tbody>
<tr>
<td>?</td>
<td>5</td>
<td>6</td>
<td>1, 2, 3, 4, 5, 6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Side Number</th>
<th>Vertex Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 3, 6, 4</td>
</tr>
<tr>
<td>2</td>
<td>2, 1, 4, 5</td>
</tr>
<tr>
<td>3</td>
<td>3, 2, 5, 6</td>
</tr>
<tr>
<td>4</td>
<td>1, 2, 3</td>
</tr>
<tr>
<td>5</td>
<td>4, 6, 5</td>
</tr>
</tbody>
</table>

The right hand rule implies that: \( \overrightarrow{r_{12}} \times \overrightarrow{r_{13}} \bullet \overrightarrow{r_{14}} > 0 \), where \( \overrightarrow{r_{12}} \) is the position vector from vertex 1 to vertex 2.

**Figure 6**: Relation between Vertex Numbers and Side Numbers for a Triangular Prism illustrating the application of the right hand rule. (3D only).
MODE 3: Connectivity for Quad or Hex Elements with Split Sides

SYNTAX CONN \{SPLI\} \{fname\}

SPLI The vertex and element connectivity for the split elements is specified. This is a supplementary mode of the command to enable local grid refinement or adaptation of the mesh in selected parts of the domain, based on solution features. (Split sides are element sides with more than one attached neighboring element). It can be used in conjunction with Mode 1 but is not available with Mode 2 of the command.

By default all ACRi Software Tools assume that each element is connected to 4 other elements in 2D and 6 other element in 3D geometry. However if the grid is locally refined then a element may be split into multiple “child” elements and some of the elements may be connected to more than the default number of neighboring elements. This supplementary connectivity is specified in the following manner.

The 1st record in the file consists of a header with two numbers: the number of split elements and the total number of data items in the rest of the file. The header is followed by a number of sets of data equal to the number of split elements. The 1st record of each set consists of the element number that is split followed by a side index for each side (4 for 2D and 6 for 3D) of the element which denotes the number of neighboring elements (if > 1) connected to that face. The index is zero if there is only one element connected to the side (no split). This record is followed by a list of element numbers that adjoin the split side in the order of the side index. The final record of the set consists of the local side number (from 1 to 6) for the adjoining elements that are attached to the split side.

The entire file is read in using the following two FORTRAN statements:

```
READ(IFILE,*) N_SPLIT_M, N_ITEMS
READ(IFILE,*) ( N_SPL(K), K = 1, N_ITEMS )
```

fname The name of the file containing the numerical input for the split connectivity. There is no default value; a file name must be specified.

EXAMPLES

```
1 2 3
4 5 6
7 8 9
10 11 12
13 14 15
16
```

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If the (Mode 1) vertex connectivity for the above mesh is as follows:

<table>
<thead>
<tr>
<th>Element #</th>
<th>Vertex Connectivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 2 6 5</td>
</tr>
<tr>
<td>2</td>
<td>2 3 7 6</td>
</tr>
<tr>
<td>3</td>
<td>3 4 8 7</td>
</tr>
<tr>
<td>4</td>
<td>5 6 10 9</td>
</tr>
<tr>
<td>5</td>
<td>6 20 17 18</td>
</tr>
<tr>
<td>6</td>
<td>7 8 12 11</td>
</tr>
<tr>
<td>7</td>
<td>9 10 14 13</td>
</tr>
<tr>
<td>8</td>
<td>10 11 15 14</td>
</tr>
<tr>
<td>9</td>
<td>11 12 16 15</td>
</tr>
<tr>
<td>10</td>
<td>20 7 19 17</td>
</tr>
<tr>
<td>11</td>
<td>17 19 11 21</td>
</tr>
<tr>
<td>12</td>
<td>18 17 21 10</td>
</tr>
</tbody>
</table>

Then the SPLIT connectivity command is:

CONNection SPLIT on file “SPLIT.CON.

Contents of the file SPLIT. CON are: *(the text in red is for clarity and must NOT be present in the file)*

```
4 36 ! 4 Split elements; 36 numeric items follow
2
0 0 0 2 ! Face # 4 is split in to 2 segments
5 10 ! Element numbers that split face connects to
3 3 ! Face # 3 (of Element 5) and Face # 3 (of Element 10)
4
0 2 0 0 ! Face # 2 is split in to 2 segments
5 12 ! Element numbers that split face connects to
3 1 ! Face # 1 (of Element 5) and Face # 1 (of Element 12)
6 ! Split Element Number
2
10 11 ! Element numbers that split face connects to
2 2 ! Face # 2 (of Element 10) and Face # 2 (of Element 11)
8 ! Split Element Number
0 0 2 0 ! Face # 3 is split in to 2 segments
12 11 ! Element numbers that split face connects to
4 4 ! Face # 4 (of Element 12) and Face # 4 (of Element 12)
```
COMMAND  CONVERGENCE

PURPOSE  To specify the convergence criterion for solution of the system of equations.

MODE 1:  Specification of Convergence Tolerance and Iterations

SYNTAX  CONV [Φ] [phase] (GLOB | LOCA | DIFF | NORM) [OLD | NEW] [εTol, NITER, NMIN Xref]

Φ  A symbol that denotes the dependent variable for which input is specified. The valid symbols are listed in Table 2.7.1. If no symbol is specified then the input is applied to control the outer (total) flow loop, which consists of all the momentum (velocity) and mass equations that are active.

phase  The fluid phase for which the input is specified. See Section 3 for available options. By default the input pertains to the 1st phase of the fluid. This modifier is currently available only for the PORFLOW™ Software Tool.

GLOB  Convergence is judged by the average residual defined by one of the following equations:

\[ ε = \frac{1}{N} \sum_{i=1}^{N} \left| A_{ij} X_j - B_i \right| \]

\[ ε = \frac{1}{N} \sum_{i=1}^{N} \left| X_j^{\text{new}} - X_j^{\text{old}} \right| \]

\[ ε = \frac{1}{N} \sum_{i=1}^{N} \frac{X_j^{\text{new}} - X_j^{\text{old}}}{X_j^{\text{old}}} ; \left| X_j^{\text{old}} \right| ≥ X^{\text{ref}} \]

where A is coefficient matrix, X is the variable vector and B is the forcing function. By default this option is active unless the LOCA modifier is specified. Also, by default, the 1st equation is used unless the DIFF modifier is present.

LOCA  Convergence is judged by the maximum of the local residual defined by one of the following equations:

\[ ε = \max_i \left| A_{ij} X_j - B_i \right| \]

\[ ε = \max_i \left| X_j^{\text{new}} - X_j^{\text{old}} \right| \]

\[ ε = \max_i \left| \frac{X_j^{\text{new}} - X_j^{\text{old}}}{X_j^{\text{old}}} \right| ; \left| X_j^{\text{old}} \right| ≥ X^{\text{ref}} \]

By default the first equation is used unless the DIFF modifier is present.

DIFF  Convergence is judged on the basis of the 2nd or 3rd equation above based on whether the GLOB or LOCA mode of the command is selected. In each case, the 2nd equation is used by default unless the NORM modifier is present.

NORM  This modifier is effective only in the presence of the DIFF modifier. In this case, the convergence residual is normalized as given by the 3rd equation based on whether the GLOB or LOCA mode of the command is selected.

OLD  This modifier is effective only for PORFLOW™ and then only if the automatic time step mode is invoked. In this case, if the time step is decreased, then, by default, the most recent computed values (with a larger time step) are retained if the convergence residue was decreasing monotonically for the previous 3 iterations. However, if this modifier is present, then the computations are restarted from the values at the end of the previous time step.

NEW  This modifier is effective only if the automatic time step mode of PORFLOW™ is invoked. If the time step is decreased, then computations restart from the most recent computed values (with a larger time step) rather than the values at the end of the previous time step.

εTol  The maximum threshold tolerance of the residual ε of equations. The default value is 1.E-6. If the computed ε exceeds this value, then the matrix solution process is repeated for the
specified number of iterations. For steady state flow, the solution is assumed to have converged if the computed $\varepsilon$ falls below this value for the chosen REFERENCE variable (see Mode 2).

**N_{ITER}**

Maximum number of “outer” iterations for convergence (see comments below). The default value may change for each installation. For most installations, the value is set to 1 with one exception. For the PORFLOW™ Software Tool, the number of iterations is set to 100 for the mass balance equation if the multi-phase or free-surface mode of the flow (pressure) equation is invoked.

**N_{MIN}**

Minimum number of iterations for the specified variable. The default value is 1.

**X_{ref}**

The $X_{ref}$ of the normalized residual equations above. The default value is 1.E-7.

**COMMENTS**

If the matrix coefficients are independent of the values of the dependent variable (linear equation) then a solution of the algebraic matrix equations ensures that the differential equation is satisfied. However, if the coefficients are functions of the dependent variable (non-linear equation), then the solution of the matrix equation does not guarantee that the differential equation is satisfied.

This command controls the “outer” iterations. The term “outer” refers to a complete pass through the governing transport equation where (1) the coefficients of the matrix are assembled, (2) the matrix is solved and (3) the convergence norm is checked against the convergence tolerance. For non-linear equations, it is necessary to iteratively perform these 3 steps till the differential equation is satisfied. The $N_{ITER}$ on this command specifies the number of passes through these steps. The solution of the algebraic matrix of equations is referred to as the process of “inner” iteration and is controlled by the MATRIX command.

If no variable ($\Phi$) is specified on this command, then the convergence tolerance applies to the total flow loop consisting of the momentum and mass flow equations (see also Mode 2 of this command). In this case, the number of iterations is interpreted as the total number of times the whole set of velocity and flow equations are sequentially solved till the convergence constraints are met.

The default options and values may depend on your installation. The defaults may be configured differently based on installation-specific optimizations.

**EXAMPLES**

CONvergence tolerance = 1.E-6
CONvergence criterion = 1.E-6 for SECOnd phase of fluid
CONvergence for U in LOCAI mode: value = 1.E-4
CONvergence for U in DIFFerence mode: value = 1.E-3
CONvergence for T as REFERENCE variable in GLOBal mode: value = 1.E-4
CONvergence for T in GLOBal SUM mode: tolerance = 1.E-4
CONV for U: LOCAI mode, value = 1.E-4, max iterations 10, min iter= 5; min value 1.E-5
CONV for flow: LOCAI mode, epsilon = 1.E-2, max iterations = 5
CONV LOCAI, eps=0.001, max iter=50, min = 10, F_threshold=1.e-5;
CONvergence epsilon = 1.E-6, 20 iterations; always use OLD values
MODE 2: Reference Option for Overall Convergence of Solution Process

SYNTAX

CONV {REFE} [MOME | FLOW | ALL | Φ] [ε_Tol, NITER]

REFE

The specified variable is used as a reference variable for monitoring the convergence of the solution process. The default options and values may depend on your installation. For most installations the default is set as:

(1) The MOMEntum option if the velocity and mass balance equations are solved.
(2) The 1st dependent variable, if no flow equations are solved.

MOME

The convergence of the solution process is judged on the basis of the individual convergence criteria specified for the momentum and mass balance equation. The process is assumed to converge only when the criteria for the momentum and mass equations are all simultaneously satisfied.

FLOW

The convergence of the solution process is judged on the basis of mass balance. The flow equations must be solved for this option to be active.

ALL

The convergence of the solution process is judged on the basis of the individual convergence criteria specified for all active equations. The process is assumed to converge only when the criteria for all equations are simultaneously satisfied.

Φ

The convergence of the solution process is judged on the basis of the dependent variable denoted by the specified symbol. The valid symbols are listed in Table 2.7.1.

ε_Tol

The convergence tolerance ε for the reference variable or quantity. The default value is 1.E-6.

NITER

Maximum number of iterations for convergence for the iteration process for the selected variable or quantity. If the quantity is flow or momentum then the process consists of the total set of active momentum (velocity) and mass balance equations. The default value is 1.

COMMENTS

The default options and values may depend on your installation. The defaults may be configured differently based on installation-specific optimizations.

EXAMPLES

CONVergence REFErence based on FLOW with Tolerance = 1.E-6
CONVergence REFErence FLOW with Tolerance = 1.E-6 with 10 outer loop iterations
CONVergence REFErence based on MOMEntum with Tolerance = 1.E-5
CONVergence REFErence based on ALL equations with tolerance = 1.E-6
CONVergence REFErence based on ALL equations with tolerance = 1.E-6 and 5 outer iterations
MODE 3: Coupled Convergence Test for Species Transport Equations

SYNTAX

CONV {COUP} {SPEC} [N_ITER]

COUP
By default, at any time step, the species equations are solved sequentially only once. This means that though inner iteration may be performed on any equation (see Mode 1 of command), each species equation is visited only once at each time step. If COUPLED modifier is present then an iterative loop is set up over the complete set of species equations. The equations are solved up to N_ITER times to meet the convergence criteria set up by Mode 1 of the command. The iterative loop is terminated only if either all of the convergence criteria for all the equations are met or the number of specified iterations has been completed.

SPEC
This modifier must be present along with the COUPLED modifier for this mode of the command to be effective.

N_ITER
Maximum number of iterations for convergence. If a value less than 2 is specified, then NITER is set to 2. The default value is 2.

EXAMPLES

CONvergence for SPECies in COUPLEd mode
CONvergence for SPECies in COUPLEd mode with a maximum of 10 iterations
MODE 4: Convergence Based on Averaged Convergence Index

SYNTAX

```
CONV {AVER} [ NShort ] [ NLong ] [ NStart ] [ α ] [ SHOR|LONG ]
```

**AVER**

The convergence is judged by long and short term average of the convergence index computed according to one of the previous modes of the command. Two averaged values of computed:

\[
\varepsilon_{\text{Long}} = \frac{1}{N_{\text{Long}}} \sum_{i=1}^{N_{\text{Long}}} \varepsilon_i
\]

\[
\varepsilon_{\text{Long}} = \frac{1}{N_{\text{Long}}} \sum_{i=1}^{N_{\text{Long}}} \varepsilon
\]

Where \( \varepsilon \) is the convergence index computed for the reference variable (See Mode 2 of command). The computations are terminated if:

\[ \varepsilon > \varepsilon_{\text{Short}} > \varepsilon_{\text{Long}} \]

and

\[ \varepsilon > \alpha \varepsilon_{\text{Short}} \]

Where \( \varepsilon_{\text{Tol}} \) is the maximum tolerance for the reference variable or quantity (see Mode 2)

**NShort**

The number of time (or iteration) steps over which the running short-time average is computed. After this number of steps is reached, the old avenge is discarded and the averaging process starts again. The default value is 7.

**NLong**

The number of time (or iteration) steps over which the running long-time average is computed. After this number of steps is reached, the old avenge is discarded and the averaging process starts again. The default value is 31

**NStart**

The time step or iteration number at which the averaging criterion starts to apply. Often, there are large fluctuations in the matrix residuals at the start due to poor initial conditions. It may be optimal then to start the averaging criteria after the solution process is stabilized. The default value is 1

**α**

The multiplying factor for termination criterion as in the equation above. The default value is 2

**SHOR**

By default, the convergence index (defined as \( \varepsilon / \varepsilon_{\text{Tol}} \)) is printed out as a diagnostic output (see DIAGNOSTICS Command). If this modifier is present, then the short-term average is printed out.

**LONG**

If this modifier is present, then the long-term average is printed out.

**EXAMPLES**

```
CONVERGENCE AVERAGE over 31 and 151 steps
CONVERGENCE AVERAGE over 31 and 151 steps. Start at 50 steps and print LONG term average
CONVERGENCE AVERAGE over 31 and 151 and start at 50 steps. Alpha=1.5 ; LONG term average
```
MODE 5: Convergence Threshold for Termination of Solution Process

SYNTAX

CONV {TERM} [Φ_BIG]

TERM

By default, the solution process is terminated if the selected convergence index (CONVERGENCE REFERENCE command) exceeds a value of $10^{30}$ at any stage of the solution process. If this command is present, then the convergence threshold for termination is set to the value specified by $Φ_BIG$.

Φ_BIG

The threshold value for termination of solution process. The default value is $10^{30}$.

EXAMPLES

CONVergence TERMinate if value exceeds 1.E50.
CONVergence TERMinate if value reaches 1.E16.
Keyword Commands

COMMAND: COORDINATE

PURPOSE: To specify the grid locations for Cartesian (x, y, z) or cylindrical (x, y, θ) coordinates.

MODE 1: Structured Grid: Coordinate Range

SYNTAX: COOR {RANG} {dir} [CYLI] [DEGR] [NODE] {N1} [N2]

RANG: The total range (total domain length in the corresponding direction) is specified. The coordinates are calculated internally with a geometric ratio between the successive grid intervals. It is assumed that the coordinate system is structured and orthogonal.

dir: One of the X, Y, Z, R or THETA modifiers that, respectively, denotes the x, y, z, r or θ coordinates for which input is specified.

CYLI: By default the coordinate system is assumed to be Cartesian. If this modifier is present, then a cylindrical coordinate system is selected.

DEGR: By default, the angular input for θ is assumed to be in radian. If the modifier DEGREE is present, then the input values are in degrees.

NODE: By default, the total range is divided into the specified number of elements and the internal grid nodes are placed at the geometric center of each of these elements. If this modifier is present then the total range is divided such that the grid nodes are placed at appropriate spacing and the element interfaces are positioned at the middle of the grid nodes.

N1: The desired range for the computational domain length in the specified direction for an orthogonal grid. There is no default value. A value must be specified.

N2: The geometric ratio by which the size of the grid element (or grid interval) changes between successive elements (or nodes). The default value is 1.

EXAMPLES

COORDinate X: RANGE = 10.
COORDinate X: RANGE = 10, increase ratio = 1.05!!! Expanding grid
COORDinate X: RANGE = 10, decrease ratio = 0.95!!! Contracting grid
COORDinate Z: RANGE = 6.28 implement in the NODE mode
COORDinate R: RANGE = 10, ratio = 0.95
COORDinate R: RANGE = 10, ratio = 0.95 CYLindrical
COORDinate THETA: RANGE = 270. DEGREes
MODE 2: Structured Grid: Coordinate Minimum and Maximum

SYNTAX

```
COOR {MINI | MAXI} {dir} [CYLI] [DEGR] [NODE] {N1} {N2, N3}
```

**MINI**
The minimum and maximum values are specified. The coordinates are calculated internally, with a geometric ratio between the successive grid intervals.

**MAXI**
Same as MINI modifier.

**dir**
See Mode 1 specification.

**CYLI**
See Mode 1 specification.

**DEGR**
See Mode 1 specification.

**NODE**
See Mode 1 specification.

**N1**
The 1st coordinate value. **There is no default value; a value must be specified.**

**N2**
The last coordinate value. **There is no default value; a value must be specified.**

**N3**
The geometric ratio by which the size of the grid element (or grid interval) changes between successive elements (or nodes). **The default value is 1.**

EXAMPLES

```
COORDinate X: MINImum = 0., maximum = 10.
COORDinate X: NODE values: MINImum = 0., maximum = 10. ratio = 1.05
COORDinate X: MINImum = 0., maximum = 10, ratio = 1.05 in NODE mode
COORDinate Z: MINImum = 0., maximum = 6.28
COORDinate THETA: MINImum 0., max = 270. DEGrees for the NODEs
```
MODE 3: Structured Grid: Corners Points of the Computational Domain

SYNTAX COOR [CYLI] [DEGR] {N1, .., Nn}

CYLI See Mode 1 specification.

DEGR See Mode 1 specification.

N1, .., Nn The coordinates of the corners of a quadrilateral for 2D simulation or those of a hexahedral for 3D simulations. Thus 8 values (x, y for each of 4 corners) must be specified for 2D and 24 values (x, y, z for each of the 8 corners) for a 3D simulation. In 2D mode, the coordinate values must be in the following order: the lower left, the lower right, the upper left, and the upper right corners. In 3D mode, the values must be in the same order as for the 2D first for the front plane (K=1) and then for the last plane (K=KMAX) of the grid nodes. For each grid line the computational domain is divided into equal length elements. The nodes are then placed in the middle of each of the element except for the boundary nodes that are placed at the middle of the boundary face.

EXAMPLES

ODERdate corners are: (0., 0.) (1., 0.), (0., 1.) and (1., 1.) !! Unit Square
COODinate: (0,0) (0.707,0.707), (-0.707,0.707) and (0,1.414)! 45 Deg Square
COODinate: (0,0) (1., 0.), (0., 1.) and (1,1) CYLindrical system
COODinates: 0,0,0 1,0,0 0,1,0 1,1,0 0,0,1 1,0,1 0,1,1 1,1,1 !! Unit Cube
COODinates: CYLindrical in DEGREes 0,0,0 1,0,0 0,1,0 1,1,0 0,0,45 1,0,45 0,1,45 1,1,45
MODE 4:  Structured Grid: Individual Coordinates for Orthogonal Grids

SYNTAX  COOR {dir} [CYLI] [DEGR] [NODE] {N1, .., Nn}

dir  See Mode 1 specification
CYLI  See Mode 1 specification.
DEGR  See Mode 1 specification.
NODE  By default, the numerical values specify the coordinates of the vertices of the elements for an orthogonal grid. For an orthogonal grid these are the same as the coordinates of the element interfaces. If the modifier NODE is present then the numerical values are assumed to be the coordinates of the node points.

N1, .., Nn  The 1st through Nth coordinate values for the specified direction. The number of values must equal the corresponding number of grid nodes or element interfaces in that direction as specified by the GRID command. In the presence of the NODE modifier, the number of values must be equal to the number of nodes (IMAX, JMAX or KMAX) in the specified direction. If NODE modifier is omitted, then the number of values must be equal to the number of vertices (IMAX-1, JMAX-1 or KMAX-1) in the specified direction.

EXAMPLES

COORDinate X: 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100  !!! element interfaces
COORDinate Y: 0, 5, 15, 25, 35, 45, 55, 65, 75, 85, 95, 100 at NODES
COORDinate R: 0, 5, 15, 25, 35, 45, 55, 65, 75, 85, 95, 100 at NODES
COORDinate Y: 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100 CYLindrical mode
COORDinate THETA: 0, 5, 15, 25, 35, 45, 60, 75, 90, 105, 120 DEGREes
Keyword Commands

**MODE 5:** Structured or Unstructured Grid: Element Vertex or Grid Node Coordinates

**SYNTAX**

```
COOR  {fname} {dir} [CYLI] [DEGR][BLOC] [NODE] [PLAN] [JIK][KJI][KIJ][IKJ][N1]
```

- **fname**: The name of the file that contains the coordinate values. See Section 3.3 for additional information. The number of values specified must equal the number of specified directions times the number of grid vertices or grid nodes, as applicable. The specification of grid node coordinates (NODE modifier) is available only for a structured grid.
- **dir**: One or more of the X, Y, Z, R or THETA modifiers that, respectively, denote the x, y, z, r or θ coordinates. Up to two symbols may be specified for 2D and, 3 for 3D simulations.
- **CYLI**: See Mode 1 specification.
- **DEGR**: See Mode 1 specification.
- **BLOC**: By default, the coordinate values are assumed to be specified as sets of (x, y) or (x, y, z) for each vertex (or node) starting with the 1st vertex (or node) and ending with the last one. In the presence of this modifier, it is assumed that the values are specified in “block” mode; that is first all the x-coordinates, followed by the y and z coordinates, respectively.
- **NODE**: See Mode 1 specification; this modifier is applicable only for a structured grid.
- **PLAN**: This modifier is applicable only for a structured grid. By default, the number of coordinate values must equal the number of corners (or number of nodes). In the presence of this modifier, for a 3D grid, the input is assumed to be for a single z-plane; the other z-planes are assigned the same x and y values.
- **JIK**: This modifier is applicable only for a structured grid. By default, the values are read according to the FORTRAN DO loop convention (I, J, K) corresponding to the x, y and z direction respectively. For example, if only x coordinate for a 2D grid is specified, then the grid values xi must be in the order: x11, x21, x31, ...xn1; x12, x22, x32, ...xn2; ... and so on. If, say, both x and y coordinates for a 2D grid are simultaneously specified, then the set of values (xij, yij) must be in the order: (x11, y11), (x21, y21), (x31, y31), ... (xn1, yn1); (x12, y12), (x22, y22), (x32, y32), ... (xn2, yn2); ... and so on. However, if the JIK modifier is present, then it is assumed that the input data is in the order xijk. The I and J values are then transposed internally to the ACRi xijk format.
- **JKI**: This modifier is applicable only for a structured grid. Similar to the JIK modifier, except that the input is assumed to be in the (J, K, I) format.
- **KIJ**: This modifier is applicable only for a structured grid. Similar to the JIK modifier, except that the input is assumed to be in the (K, I, J) format.
- **KJI**: This modifier is applicable only for a structured grid. Similar to the JIK modifier, except that the input is assumed to be in the (K, J, I) format.
- **IKJ**: This modifier is applicable only for a structured grid. Similar to the JIK modifier, except that the input is assumed to be in the (I, K, J) format.
- **N1**: The number of header records at the beginning of the file. These header records are read and ignored. The coordinate values are assumed to start with the N1+1st record. The default value is 0.
COMMENTS

If this command is used for cylindrical geometry in unstructured mode, then the vertices for elements must be defined such that the local element (ξ, η, ζ) coordinates are identical with the global (X, R, θ) coordinates. It is required that the external normal at Face number 3 points in the R⁻ direction and that at Face number 4 in the R⁺ direction. Further details are given in Section 3.5 and the CONNECTIVITY command.

EXAMPLES

COORDinate X from file 'XGRID'
COORDinate X, Y and Z from file 'XYZGRID'
COORDinate X, Y and Z from file 'XYZGRID' in BLock mode; ignore 7 records
COORDinate X, Y and Z from file 'XYZGRID' in BLock IJK mode; ignore 7 records
COORDinate X, Y from file 'XRGRID' in CYLindrical mode
COORDinate X, R, THETA (DEGRees) from file 'XRTHTGTA'
COORDinate X, Y and Z from file 'XYZ' in JIK mode for grid NODEs
MODE 6: Structured or Unstructured Grid: Vertex Coordinates

SYNTAX COOR {'VERT'}{fname}

VERT The grid coordinates for a set of numbered vertices are specified in the input file.

fname The name of the file that contains the vertex numbers and their corresponding coordinate values. See Section 3.3 for additional information.

COMMENTS

The file format must consist of a number of records each of which must specify a vertex number followed by the set of x, y (for 2D) or x, y, z (for 3D) coordinates of that vertex. The vertex numbers on the record may be in arbitrary order but the total number of records must equal the number of vertices for the problem. A unique set of coordinate values must be specified for each vertex; no two vertices may be co-located at the same point in space.

EXAMPLES

COORDinates of VERTices on file ‘PROBGRID’
**COMMAND**  
CORIOLIS

**PURPOSE**  
To specify the Coriolis parameter for the momentum balance equations. This command is effective only for the TIDAL™ Software Tool.

**SYNTAX**  
CORI \{Ω\}

Ω  
The value of Ω (≥0) the Coriolis parameter. The default value is 0.

**COMMENTS**  
This command is implemented only for the TIDAL™ Software Tool.

**EXAMPLES**  
CORIolis parameter for this location is 0.05
COMMAND  CORRELATION

PURPOSE  Compute and output auto and cross correlations for dependent variables.

MODE 1:  Auto Correlation for the Variables

SYNTAX  CORR  {Φ} [subrgn] [fname] [TIME] [NOW] [Vfrq] [OFF]

Φ  A symbol that denotes the variable for which correlation is desired. Valid symbols are listed in Table 2.7.1. If Φ denotes the instant value of a variable at a given location, Φ^n its value at n^{th} time (or iterative) step, then its 1^{st} and 2^{nd} mean over N steps are defined as:

\[ \langle \Phi \rangle = \frac{1}{N} \sum_{n=1}^{N} \Phi^n \]

\[ \langle \Phi^2 \rangle = \frac{1}{N} \sum_{n=1}^{N} (\Phi^n)^2 \]

The following correlation quantities are then computed and printed:

\[ R_{11} = \langle \Phi^2 \rangle - \langle \Phi \rangle \langle \Phi \rangle \]

\[ C_{11} = \frac{R_{11}}{\langle \Phi \rangle \langle \Phi \rangle} \]

\[ D_{11} = \Phi - \langle \Phi \rangle \]

subrgn  The subregion for computations. If no subregion is specified, the entire domain is selected.

fname  The file name for output. If a file name is specified then the output is directed to the named file, otherwise the output is directed to the standard output device. If a file name is specified, it must be different from any previously specified file name. The total number of open files in any simulation cannot exceed 64.

TIME  By default, Vfrq is interpreted as the frequency of output in terms of number of steps. In the presence of TIME this is the time intervals between successive outputs.

NOW  A record of is written to the output device at the next time step. This is in addition to the output from the Vfrq specification.

Vfrq  The frequency (step or time interval) at which the output is written to the output device. In the step interval mode, a specification of 10 results in output at step number 10, 20, 30, etc. In the time interval mode, whether or not the output is obtained exactly at the specified interval depends on the time step specified by the SOLVE command. If an exact time at which the output is due is not simulated, then the output is obtained at the first time step after the due time. By default the output is obtained only at the end of simulations.

OFF  Any previously specified CORRELATION commands for the specified variable and subregion are disabled. New commands may be subsequently specified.

EXAMPLES

CORR elation for variable U for the SELEcted subregion at the end of simulations
CORR elation for variable U for the ID=LOC_AUTO every 25 steps
CORR elation OFF for variable U for the ID=LOC_AUTO
MODE 2: Cross Correlation for Two Variables

SYNTAX

\[ \text{CORR} \{ \Phi_1, \Phi_2 \} \text{[subrgn]} \text{[fname]} \text{[TIME]} \text{[NOW]} \text{[Vfrq]} \text{[OFF]} \]

**Φ₁, Φ₂** Two symbols that denote the variables for which correlation is desired. Valid symbols are listed in Table 2.7.1. If \( \Phi_k \) denotes the instant value of the \( k \)th variable at a given location, \( \Phi_k^n \) its value at \( n \)th time (or iterative) step, then the means over \( N \) steps are defined as:

\[
\langle \Phi_k \rangle = \frac{1}{N} \sum_{n=1}^{N} \Phi_k^n \\
\langle \Phi_k^2 \rangle = \frac{1}{N} \sum_{n=1}^{N} (\Phi_k^n)^2 \\
\langle \Phi_1 \Phi_2 \rangle = \frac{1}{N} \sum_{n=1}^{N} (\Phi_1 \Phi_2)
\]

The following correlation quantities are then computed and printed:

\[
R_{12} = \langle \Phi_1 \Phi_2 \rangle - \langle \Phi_1 \rangle \langle \Phi_2 \rangle \\
C_{12} = \frac{R_{12}}{\sqrt{\langle \Phi_1^2 \rangle - \langle \Phi_1 \rangle^2} \sqrt{\langle \Phi_2^2 \rangle - \langle \Phi_2 \rangle^2}} \\
D_{12} = (\Phi_1 - \langle \Phi_1 \rangle)(\Phi_2 - \langle \Phi_2 \rangle)
\]

**subrgn** The subregion for computations. If no subregion is specified, the entire domain is selected.

**fname** The file name for output. If a file name is specified then the output is directed to the named file, otherwise the output is directed to the standard output device. If a file name is specified, it must be different from any previously specified file name. The total number of open files in any simulation can not exceed 64.

**TIME** By default, \( V_{frq} \) is interpreted as the frequency of output in terms of number of steps. In the presence of **TIME** this is the time intervals between successive outputs.

**NOW** A record of is written to the output device at the next time step. This is in addition to the output from the **Vfrq** specification.

**Vfrq** The frequency (step or time interval) at which the output is written to the output device. In the step interval mode, a specification of 10 results in output at step number 10, 20, 30, etc. In the time interval mode, whether or not the output is obtained exactly at the specified interval depends on the time step specified by the **SOLVE** command. If an exact time at which the output is due is not simulated, then the output is obtained at the first time step after the due time. By default the output is obtained only at the end of simulations.

**OFF** Any previously specified **CORRELATION** commands for the specified variable and subregion are disabled. New commands may be subsequently specified.

**EXAMPLES**

**CORR**elation for variable U and V for the SELEcted subregion at the end of simulations
**CORR**elation for variable U and T for the ID=LOC_AUTO every 25 steps
**CORR**elation OFF for variable U and T for the ID=LOC_AUTO
MODE 3: Two Point Correlation for One or Two Variables

SYNTAX

```
CORR {TWO} { Φ₁ } [Φ₂] [subrgn] [fname] [TIME] [NOW] [Vfrq] [OFF]
```

TWO

Two point correlation with matched sets of pairs of elements is specified. The subregion for this option must be previously specified with a LOCATE CORRELATION command.

Φ₁, Φ₂

One or Two symbols that denote the variables for which correlation is desired. Valid symbols are listed in Table 2.7.1. The correlation formulae are identical to the two-variable cross-correlation described in Mode 2 except for the definition Φ₁ and Φ₂. The Φ₁ is always taken to be the values of the 1st specified variable at the elements of the 1st set of paired elements. If only one variable is specified then Φ₂ is taken to be the values at the 2nd set of paired elements. If two symbols are specified then Φ₂ is defined to be values of the 2nd variable at the 2nd set of elements.

subrgn

The subregion for computations. The subregion must be previously specified with a LOCATE CORRELATION command. There is no default value.

fname

The file name for output. If a file name is specified then the output is directed to the named file, otherwise the output is directed to the standard output device. If a file name is specified, it must be different from any previously specified file name. The total number of open files in any simulation cannot exceed 64.

TIME

By default, Vfrq is interpreted as the frequency of output in terms of number of steps. In the presence of TIME this is the time interval between successive outputs.

NOW

A record of is written to the output device at the next time step. This is in addition to the output from the Vfrq specification.

Vfrq

The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the output is obtained only at the end of simulations.

OFF

Any previously specified CORRELATION commands for the specified variable and subregion are disabled. New commands may be subsequently specified.

EXAMPLES

```
CORR elation is TWO point type for variable U at ID=LOC_CORR2 at the end of simulations
CORR elation is TWO point type for variables U and V at ID=LOC_CORR2 output on file 'TWOPCORR.UV'
CORR elation is TWO point type for variables U and V at ID=LOC_CORR2 at the end of simulations
CORR elation is TWO point OFF for variable U and T for the ID=L OC CORR2
```
COMMAND   CPU

PURPOSE  To specify the number of Central Processing Units for parallel processing.

SYNTAX   CPU   \{N_{CPU}\}

$N_{CPU}$  The number of CPU's for parallel processing. The defaults value is the smaller of the number of physical processors present and the number of permitted licenses for the software installation.

EXAMPLES

CPU  4 CPU's for this computer system
Keyword Commands

**COMMAND** DATUM

**PURPOSE** To specify datum coordinates, \( x \), which are used to define the total hydraulic head, \( \bar{H} \). This command is effective only for the ANSWER™ and PORFLOW™ Software Tools.

**SYNTAX** DATU \{N1, N2, N3\}

**N1, N2, N3** The \((x, y, z)\) or \((x, r, \theta)\) datum elevation coordinate values, respectively, which are used to define the total hydraulic head. The default value for all of these is 0.

**COMMENTS** The datum coordinates enter the computations only if the multi-phase or free-surface flow options are used, or if the gravitational field is explicitly set to a non-zero value by the GRAVITY command.

**EXAMPLES**

DATUm is at zero
DATUm coordinates for this problem are: \( x=0 \), \( y=1000 \), \( z=50 \)
**COMMAND**  DEBUG  

**PURPOSE**  To obtain debug output related to specification of geometrical features, the error indicators and the matrix coefficients.

**MODE 1:**  Check Validity of Geometric and Grid Input

**SYNTAX**  

```
DEBU {GEOM} [FILE] [OFF]
```

**GEOM**  The geometrical features specified by the user explicitly or by default (such as inlets, outlets, walls, blocked elements, sources and, open, cyclic or symmetric boundaries) are checked for compatibility and validity. Any elements or surfaces with conflicts (such as duplicate or ambiguous assignments) are identified and listed in the standard output file.

Also the grid is checked for orthogonality and uniformity and a summary of grid statistics is written to the standard output file.

**FILE**  A detailed output of non-orthogonality angle and grid nodal distance for each element is written to a file. The output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by "\_GRID\_QUALITY.TMP". For example, if the Standard Output file is "PROBLEM.OUT", then the file is named "PROBLEM\_GRID\_QUALITY.TMP".

The orthogonality index for any element is defined as the maximum of the skewness angles for the faces of the element. For each face the skewness angle is defined as the angle between the normal vector at the face and the vector connecting the two grid nodes, one on either side of the face. The angle is expressed in degrees. A value of 0 implies that the grid vector is orthogonal to the face.

\[ \alpha_i = \cos^{-1} \frac{\sum_{i=1}^{N^{23}} A_i \delta x_i}{A_i \delta S} \]

The nodal distance for any element is defined as the maximum of the Euclidean distance for the nodes straddling the element faces. For any face, the Euclidean distance is the magnitude of the vector connecting the two grid nodes, one on either side of the face.

**OFF**  By default these checks are always performed if this modifier is present, then the diagnostic and grid checks are omitted.

**EXAMPLES**  

```
DEBU GEOMetry is on by default
DEBU GEOMetry checks OFF
```
MODE 2: Diagnostic Output of Numerical Error Indicators

SYNTAX

DEBU \{\Phi\} [fname] [subrgn] [Vfrq] [TIME]

Φ One and only one symbol for the dependent variable for debug output; valid symbols are listed in Table 2.7.1. There is no default value. A valid symbol must be specified.

fname The name of the output file. If no name is specified then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by “.DEBUG.TMP”. For example, if the Standard Output file is “PROBLEM.OUT”, then the debug file is named “PROBLEM_DEBUG.TMP”. A summary of output is also printed to the standard output device at the end of simulations.

subrgn The subregion for computation of the error parameters. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

Vfrq The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the output is obtained only at the end of simulations.

TIME By default, Vfrq is the computation (and output) frequency in terms of number of steps. If this modifier is present, then Vfrq is the time interval between successive outputs.

COMMENTS

The debug output consists of the local Peclet and Courant numbers. These error-indicators provide a measure of the numerical error in the solution. Peclet number, the ratio of the convection to the diffusion term, is generally considered to be indicative of the “numerical diffusion” in the solution. The Courant number, the ratio of the convection to the accumulation term, is generally considered to be indicative of the “dispersion” in the transient component of the solution. These error indicators are based on the Taylor series analysis of the governing equation and are known to be inadequate for prediction of numerical error in many practical situations. Therefore caution should be exercised in the interpretation of these error indicators. Peclet number can not be defined for the pressure equation since it does not have a convection term. Similarly, no Courant number can be defined for steady state computation since the accumulation term is identically equal to zero.

EXAMPLES

DEBU output of error indicators for T
DEBU output for T every 12 steps
DEBU output for T for SELECTed subregion at TIME interval of 1.5 units
DEBU output for T for subregion with ID=SUBZone at TIME interval of 1.5 units
DEBU specified output: for T on 'MYFILE.DBG'
MODE 3: Diagnostic Output of Matrix Coefficients

SYNTAX

DEBU {MATR} [N\text{Step}]

MATR

The debug output pertaining to the matrix of the algebraic equations is produced on a file at the computation step specified by the N1 input. The governing algebraic matrix equation is:

\[ A_{ij} X_j = B_i \]

where, for the \( i^{th} \) element, \( A_{ij} \) are the matrix coefficients, \( X_j \) are the values of the dependent variable and \( B_i \) is the forcing function.

One file is generated for each governing transport equation. Each file is named \texttt{acr\_MATRXxxxx.TMP} where “xxxx” are replaced by the non-blank characters of the 1st four characters of the symbolic name of the corresponding variable. If the name of the variable has fewer than 4 non-blank characters, then the trailing characters will stay as \texttt{xx}. The records on each file are in the order described below.

The first record consists of: the symbolic name of the variable, the order number of the variable in the master storage array, the step number at which the output is produced, the number of internal field elements, the number of neighbors for each element, the grid dimensions in each direction and, the total number of nodes.

This is followed by one record for each field element in sequence. Each record consists of: the value of the variable \( (X_j) \), the source term (part of \( B_i \) that pertains to the source or sinks in physical units), the forcing function \( (B_i) \), the diagonal component of the matrix coefficients \( (A_{ii}) \) and, the negative of the matrix coefficient for each neighbor \( (-A_{ij}, i \neq j) \).

\texttt{N\text{Step}}

The step number at which output is required. There is no default value; a value must be specified.

EXAMPLES

DEBU MATRix information at step #9 for each equation in turn
COMMAND  DECAY

PURPOSE  To specify rate constants and mode of decay of a dependent variable due to physical, chemical or radioactive decay.

MODE 1:  Direct Linear Decay

SYNTAX  DECA  {Φ}  [RATE]  [LIFE]  [FIEL]  [λ]

Φ  A symbol that denotes the dependent variable for which the decay or reaction rate constant is specified. The valid symbols are listed in Table 2.7.1.

RATE  The decay rate of Φ is specified; the units are those of inverse of time. This is the default option.

LIFE  The half-life of v is specified; the units are those of time.

FIEL  If the modifier FIEL is present, then the decay reaction is assumed to occur only inside the field and not at the boundaries. The boundary values are maintained at the specified conditions.

λ  The decay rate of Φ in the presence of the RATE modifier or the half-life of decay in the presence of the LIFE modifier. The default value is set so that no decay occurs.

EXAMPLES

DECAY rate of C is 0.001
DECAY rate of FU is 0.001; only for FIELd values
DECAY half - LIFE of C is 1.632
DECAY half - LIFE of C is 15.00 in the FIELd only
MODE 2: Drag Type Of Decay Based On Flow Speed

SYNTAX

DECA {Φ} [DRAG] [option] [subrgn] [C0] [α] [N1, Nk] [Nk+1]

Φ See Mode 1 specification.

DRAG The decay of dependent variable Φ is according to the drag law based on the flow speed. This adds a source, SΦ, in the transport equation for Φ given by:

$$S\Phi = -0.5 \rho \Phi C_D C_\Phi (U^2 + V^2 + W^2)^{\alpha/2},$$

where C_D is the drag coefficient, C_Φ is a scaling factor, and U, V and W are components of flow velocity. C_D and C_Φ are dimensional constants such that SΦ has appropriate units [e.g. M L T^{-2}]. For example, if N=1, and C_Φ is an area, then C_D is non-dimensional.

option Options selected for implementation of the source.

<table>
<thead>
<tr>
<th>option</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>VOLU</td>
<td>The coefficient C_Φ in the S_Φ term is set equal to the volume (δV) of the element.</td>
</tr>
<tr>
<td>AREA</td>
<td>The coefficient C_Φ in the S_Φ term is set equal to the area (δA) of the element face indicated by the dir modifier.</td>
</tr>
<tr>
<td>dir</td>
<td>The orientation index for the element boundary associated with the source. See Section 3.5 for available choices. There is no default value for this input.</td>
</tr>
</tbody>
</table>
| NORM   | The coefficient C_Φ in the S_Φ term is computed as:

$$C_\Phi = \sum A_i \cdot V_i$$

where A_i is the i-th direction component of the element boundary area specified by dir. V_i are the values specified by N3 through Nk (2 for 2D, and 3 for 3D). |
| DENS   | The computed source, C_Φ, is further multiplied by density. The density may be specified as the last value, Nk+1, on the command. If this value is omitted, then the boundary value in the dir direction is used if the AREA or NORMAL modifiers are present, otherwise the local density for the element is used. |

subrgn The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

C_D The drag coefficient, C_D, in the drag law (see Comments). The default value is 0.

α The power exponent, N, in the drag law (see Comments). The default value is 1.

N_1, .., N_k The normalizing vector components, V_i, if the NORMAL modifier is present. Two values must be specified for 2D and 3 for 3D flows. There are no default values for this input.

N_k+1 The density value that multiplies the computed source, if the DENSITY modifier is present. There is no default value for this input.

EXAMPLES

DECAy of U: DRAG law: cf=0.001, for previously SELECTed subregion
DECAy of T: DRAG law: cf=0.002, N = 0.80 for subregion ID=OBSTRUCTION
DECAy for T: DRAG type: cf=0.001, N=0.5 multiply by AREA in X- direction for SELECTed subregion
DECAy for T: DRAG type: cf=0.1, N=0.5 X- dir & multiply by VOLUME. DENSITY for SELECTed subregion
DECAy for T: DRAG type: cf=0.1, N=0.5 X- direction NORMALized 1.0. DENSITY for SELECTed subregion

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**COMMAND**  DEFINE

**PURPOSE**  To define the value of a symbolic variable as a numeric or character expression.

**MODE 1:**  Assign Numeric Values to Symbolic Variables

**SYNTAX**  \( \text{DEFI } \{X_1=V_1\} [X_2=V_2], \ldots, [X_n=V_n] \ [\text{OFF}] \)

- **X\(_1\), X\(_2\), \ldots, X\(_n\)**  A list of symbolic variables that at run-time is replaced by the corresponding numerical value, \(V_1, V_2, \ldots, V_n\) in the same order. Once variable has been defined, the corresponding numeric value will replace any occurrence of this variable in the user input.

  The symbolic variable appearing on a DEFINE command must be distinct and must not be one of the defined field variables listed in Tables 2.7.1 or 2.8.1-3. Neither should it conflict with any command Keyword or modifier that appears on these commands. Only the first 8 characters in the symbolic variables are meaningful; any subsequent characters are ignored.

- **V\(_1\), V\(_2\), \ldots, V\(_n\)**  The numerical values that replaces every occurrence of the \(X_1, X_2, \ldots, X_n\) in the user input in the order of assignment.

- **OFF**  The previously defined variables are deactivated. New variables may be defined for input that follows.

**COMMENTS**

This command provides a powerful means of performing symbolic math and/or creating 'prototype' data input files in which symbolic variables may be used to denote problem-specific input data. These symbolic variables may then be defined at the beginning of the input or they can be replaced by character or numeric data at run time by using the interactive input feature described in Section 3.2. Up to 256 symbolic variables may be defined at any time.

**EXAMPLES**

- `DEFINE XXX = 1.2345` in all input that follows
- `DEFINE TWOPi = 2.2830, PI = 3.1415, PIBY2 = 1.57075. PIBYFOUR = 0.785375.`
- `DEFINE OFF` for all previous variables
MODE 2: Assign Symbolic Values to Symbolic Variables

SYNTAX

```
DEFI {X_1=Y_1, X_2=Y_2, ..., X_n=Y_n} [OFF]
```

- **X_1, X_2, ..., X_n**: Symbolic variables that at run-time are replaced by the corresponding character strings Y_1, Y_2, ..., Y_n in the same order. Once variable has been defined, the corresponding symbol will replace any occurrence of this variable in the user input.

- **Y_1, Y_2, ..., Y_n**: The symbols that replace every occurrence of the corresponding X_1, X_2, ..., X_n in the user input in the order of assignment.

- **OFF**: The previously defined variables are deactivated. New variables may be defined for input that follows.

**COMMENTS**

This command provides a powerful means of performing symbolic math and/or creating 'prototype' data input files in which symbolic variables may be used to denote problem-specific input data. These symbolic variables may then be defined at the beginning of the input or they can be replaced by character or numeric data at run time by using the interactive input feature described in Section 3.2. Up to 256 symbolic variables may be defined at any time.

**EXAMPLES**

```
DEFINE XXX = P in all input that follows
DEFINE XXX = U234, YYY = U235 and ZZZ = U238.
DEFINE OFF for all previous variables
```
Keyword Commands

MODE 3: Multiple Simulations of a Given Input for a Series of Assigned Values

SYNTAX

```
DEFI {variable} {LIST} {V1, V2, .., Vn}
```

variable
A symbolic variable, that at run-time, is replaced by user specified input value to create multiple sets of data (See COMMENTS below). The 'variable' must be the 1st modifier following the DEFINE command. Only the first 8 characters are meaningful; any subsequent characters are ignored. The symbolic variable for each DEFINE statement must be distinct and must not be one of the defined field variables listed in Tables 2.7.1 or 2.8.1-3. Once a variable has been defined, a numeric value selected from the specified list replaces ALL occurrences of this variable in the user input.

LIST
A list of values to generate a sequence of inputs with assigned values is specified. A DEFINE LIST command must not appear if a metafile for input is specified (see META command).

V1, V2, .., Vn
The numerical values that sequentially replace the variable in each data set. See COMMENTS below. A maximum of 32 values can be specified, excess values are discarded.

COMMENTS

This command provides a powerful means of performing multiple simulations with a given data set where one or more symbolic variables in the input are sequentially replaced with the specified values to generate multiple input data sets. Up to 8 DEFINE LIST or DEFINE DO commands can occur in a data set and these can generate up to 256 simulations from a given data set. The resulting "unfolded" data set is saved in a file that has the same name as the input file but with "_DEFINE_UNFOLD.DAT" appended to the file name. For example, if the input file is called "PROB.DAT", then the unfolded input file will be called "PROB_DEFINE_UNFOLD.DAT".

Output for all the simulations is directed to a single Standard Output Unit file) with the name as specified by the user or the default name generated automatically (see OUTPUT Command). A separate archive file is generated for each of the problems. If a SAVE command is present then the name of the archive file for each problem is the file name given in the command with the string "0nnn" appended to the name of the file where "nnn" represents the problem number in the sequence. For example if the file name on the SAVE command is "PROB.SAV", then the names of the archive files will be "PROB_0001.SAV", "PROB_0002.SAV", etc. in order for each problem. If no file name is present then a default file name for the archive file is generated (see SAVE command). If no SAVE command is present, then a default SAVE command is automatically added.

Consider a set of statements in an input file, "PROB.DAT":

```
TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data
GRID:  22 in x and 12 in y direction
DEFINE VAL_LEFT LIST 100, 120, 130
BOUNDARY T at X- value = VAL_LEFT
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
END
```

The above input data will result in 3 problems being solved where the symbolic variable VAL_LEFT will be successively assigned the value of 100, 120 and 130. The resulting unfolded data set is saved in file named "PROB_DEFINE_UNFOLD.DAT" with 3 problems as follows:

```
!*************************************************************************
! Problem #    1 Created from DEFINE DO or LIST Command
!*************************************************************************
TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data
GRID:  22 in x and 12 in y direction
DEFINE VAL_LEFT LIST 100
BOUNDARY T at X- value = VAL_LEFT
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE inserted “PROB_0001.SAV”
END
```
EXAMPLES

DEFINE XXX LIST of values: 1., 2., 3., 4
MODE 4: Multiple Simulations of a Given Input for a Series of Assigned Values

SYNTAX  
\texttt{DEFI \{variable\} \{DO\} \{V_1, V_2, V_3\}}

\textbf{variable}  
A symbolic variable, that at run-time, is replaced by user specified input value to create multiple sets of data (See COMMENTS below). The 'variable' must be the 1\textsuperscript{st} modifier following the DEFINE command. Only the first 8 characters are meaningful; any subsequent characters are ignored. The symbolic variable for each DEFINE statement must be distinct and must not be one of the defined field variables listed in Tables 2.7.1 or 2.8.1-3. Once a variable has been defined, a numeric value selected from the specified list replaces ALL occurrences of this variable in the user input.

\textbf{DO}  
A DO Loop is specified to generate a sequence of inputs from the assigned values. A DEFINE DO command must not appear if a metafile for input is specified (see META command).

\textbf{V}_1, \textbf{V}_2, \textbf{V}_3  
The numerical values that generate a sequence of values to replace the variable in each data set. \textbf{V}_1 is the starting value, \textbf{V}_2 the ending value, and \textbf{V}_3 the increment at which the values are generated. See COMMENTS below. All 3 numerical values must appear on the command; continuation records are not allowed. A maximum of 32 values are computed from the DO loop; any excess values are discarded.

\textbf{COMMENTS}  
This command provides a powerful means of performing multiple simulations with a given data set where one or more symbolic variables in the input are sequentially replaced with the specified values to generate multiple input data sets. \textbf{Up to 8 DEFINE LIST or DEFINE DO commands can occur in a data set and these can generate up to 256 simulations from a given data set.} The resulting "unfolded" data set is saved in a file that has the same name as the input file but with "_DEFINE_UNFOLD.DAT" appended to the file name. For example, if the input file is called "PROB.DAT", then the unfolded input file will be called "PROB_DEFINE_UNFOLD.DAT".

Output for all the simulations is directed to a single Standard Output Unit file) with the name as specified by the user or the default name generated automatically (see OUTPUT Command). A separate archive file is generated for each of the problems. If a SAVE command is present then the name of the archive file for each problem is the file name given in the command with the string "0nnn" appended to the name of the file where "nnn" represents the problem number in the sequence. For example if the file name on the SAVE command is “PROB.SAV”, then the names of the archive files will be “PROB_0001.SAV”, “PROB_0002.SAV”, etc. in order for each problem. If no file name is present then a default file name for the archive file is generated (see SAVE command). If no SAVE command is present, then a default SAVE command is automatically added.

Consider a set of statements in an input file, “PROB.DAT”:

\begin{verbatim}
ITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data
GRID:  22 in x and 12 in y direction
DEFINE VAL_LEFT DO 100, 125, 150
BOUNDARY T at X- value = VAL_LEFT
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
END
\end{verbatim}

The above input data will result in 3 problems being solved where the variable VAL_LEFT will be successively assigned the value of 100, 125 and 150. The resulting unfolded data set is saved in file named “PROB_DEFINE_UNFOLD.DAT” with 3 problems as follows:

\begin{verbatim}
ITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data
GRID:  22 in x and 12 in y direction
DEFINE VAL_LEFT LIST 100
BOUNDARY T at X- value = VAL_LEFT
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE inserted “PROB_0001.SAV”
\end{verbatim}
END
!
*************************************************************************
Problem #  2 created from DEFINE DO or LIST Command
*************************************************************************
TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data
GRID:  22 in x and 12 in y direction
DEFINE VAL_LEFT LIST 125
BOUNDARY T at X- value = VAL_LEFT
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE inserted “PROB_0002.SAV”
END
!
*************************************************************************
Problem #  3 created from DEFINE DO or LIST Command
*************************************************************************
TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data
GRID:  22 in x and 12 in y direction
DEFINE VAL_LEFT LIST 150
BOUNDARY T at X- value = VAL_LEFT
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE inserted “PROB_0003.SAV”
END

EXAMPLES

DEFINE XXX DO  start at 100, end at 200, interval =20  ! 5 sets (100 120,140,160, 200) generated
COMMAND  DENSITY

PURPOSE  To specify the options and constants used to calculate fluid density.

MODE 1:  Fluid Density as a Constant or General Function

SYNTAX  DENS  {func[ξ]} {N₁, N₂, ..., Nₙ} [fname] [phase] [subrgn] [STAT]

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

func  One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. For this input, the function specifies the value of the density for the corresponding phase. If no function is specified then the value is assumed to be constant.

ξ  One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

phase  The phase for which the input is specified. See Section 3.6 for available options. By default the input pertains to the 1st phase of the fluid. This modifier is available only for the multi-phase versions of the PORFLOW™ and ANSWER™ Software Tools.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

STAT  By default for transient flows, the volumetric change due to ∂ρ/∂t term is automatically accounted for. If this modifier is present, then the effect of this term in the continuity equation is ignored. This modifier is effective only for the ANSWER™ Software Tool. The use of this modifier is not recommended; it is being retained for backward compatibility.

APPLICABILITY

The general functional from of this command is currently available only for the ANSWER™ and PORFLOW™ Software Tools. Only the constant density option is available for TIDAL™ Software Tool.

EXAMPLES

DENSITY of fluid = 1.18 Kg/m^3
DENSITY of fluid is = 1000

Generic examples for this command are given in Section 4.4. The command keyword (DENS) must replace the keyword used in these examples.
**MODE 2:** Special Density Functions

**SYNTAX**

DENS \{POWE|POLY|LINE\} [phase] [\(p^*\)] [\(\alpha\)] [\(\beta\)] [\(\gamma\)]

**POWE**

Density varies according to the power law:

\[
\frac{\rho}{\rho^*} = \left[ \frac{\beta - T}{\beta - T^*} \right]^\alpha
\]

**POLY**

Density varies according to the polynomial Equation:

\[
\frac{\rho}{\rho^*} = 1 + \alpha (T^* - T) + \beta (T^* - T)^2 + \gamma (T^* - T)^3
\]

**LINE**

Density varies according to the linear relation:

\[
\frac{\rho}{\rho^*} = 1 + \alpha (T^* - T) + \gamma (\beta - C)
\]

**phase**

The fluid phase for which the input is specified. See Section 3.6 for available options. By default the input pertains to the 1\(^{st}\) phase of the fluid. This modifier is available only for the multi-phase versions of the PORFLOW™ and ANSWER™ Software Tools.

**\(p^*\)**

Reference density for the fluid, \(\rho^*\).

**\(\alpha\)**

The exponent for the POWER law or the coefficient for the POLYNOMIAL and LINEAR relations. The default value is 0.2 for the POWER law equation and 0 otherwise.

**\(\beta\)**

The critical temperature for the of the POWER law, the coefficient for the POLYNOMIAL relation or the reference concentration for the LINEAR relation. The default value is 374.15 for POWER law and 0 otherwise.

**\(\gamma\)**

The coefficient in the POLYNOMIAL and LINEAR relations. The default value is 0.

**APPLICABILITY**

This mode of the command is available only for the ANSWER™ and PORFLOW™ Software Tools.

**EXAMPLES**

DENSITY by POWER law: \(\rho^* = 1.\), Exponent = 0.25, \(T_c = 374.15\) K

DENSITY POLYNOMIAL law: \(\rho^* = 1000\), \(a=1000\), \(b=0.05\), \(c=0\), \(d=3.0E-5\)

DENSITY LINEAR function: \(997\), Beta=1.0E-4

DENSITY LINEAR function \(789\), Beta=1.0E-4 for SECOND phase
MODE 3: Density from Gas Law

SYNTAX DENS {GAS}[phase] [INCO | COMP] [REAL] [A, B]

GAS Density varies according to the gas law Equation:

\[ \rho = \frac{p + p^*}{R_u (T + T_a) \sum \frac{m_j}{M_j}} \]

In this equation, \( p \) is the gas pressure, \( p^* \) is a reference datum pressure, \( R_u \) is the universal gas constant, \( T \) is the temperature, \( T_a \) is the base to convert temperature to absolute units, \( m_j \) is the mass fraction of the \( j \)th component of the gas species and \( M_j \) is the corresponding molecular weight.

phase The fluid phase for which the input is specified. See Section 3.6 for available options. By default the input pertains to the 1st phase of the fluid. This modifier is available only for the multi-phase versions of the PORFLOW™ and ANSWER™ Software Tools.

INCO The incompressible form of the gas law is used where the local pressure, \( p \), is ignored in comparison to \( p^* \) in the gas law equation. This modifier is effective only if the GAS modifier is present. This is the default option for all ACRI Software Tools except PORFLOW™.

COMP The compressible form of the gas law equation is used. The local pressure, \( p \), is added to the reference pressure, \( p^* \), in computing density. This modifier is effective only if the GAS modifier is present. This is the default option for the PORFLOW™ Software Tool.

REAL The gas is assumed to be real and not ideal; the density is given by:

\[ \rho = \frac{(p + p^* + A)(1 - B \rho)}{R_u (T + T_a) \sum \frac{m_j}{M_j}} \]

A The pressure coefficient if the REAL modifier is specified.

B The density coefficient if the REAL modifier is specified.

APPLICABILITY This mode of the command is available only for the ANSWER™ and PORFLOW™ Software Tools.

EXAMPLES

DENSITY from GAS law: reference value = 0.960 kg/m^3
DENSITY from GAS law reference value computed from other input
DENSITY GAS law in INCOMPRESSIBLE mode
MODE 4: Density of Brine as a Function of Salt Concentration

SYNTAX

DENS {SAND} [p*] [α] [ρ_max] [ρ_salt] [CS_Sat]

SAND

Density varies according to the exponential law correlation:

\[ \frac{ρ}{ρ^*} = \min\{ \exp(α C_S), ρ_{max} \} \]

Where \( C_S \) is the mass concentration of salt (0 ≤ \( C_S \) ≤ 1) in the brine mixture which is computed from a transport equation.; other symbols are defined below.

\( ρ^* \)

Reference density for the fluid, \( ρ^* \). The default value is 998.2.

\( α \)

The exponent for the function; the default value is 0.6995.

\( ρ_{max} \)

The maximum density of the mixture fluid; the default value is 1200.9.

\( ρ_{salt} \)

The density of solid salt; the default value is 2165 (see Comments below).

\( C_{S_Sat} \)

The maximum saturation mass fraction of salt in solution; the default value is 0.2643 (see Comments below).

APPLICABILITY

This mode of the command is available only for the ANSWER™ and PORFLOW™ Software Tools.

COMMENTS

This relationship for the density of saline mixture of water is based upon the correlations developed for Sandia national Laboratory. (Anthony J. Russo, 1983. A User’s Manual for the Salt Solution Mining Code, SANSMIC, UC-94e, Sandia National Laboratories, Albuquerque, NM 87185).

The input of \( ρ_{salt} \) and \( C_{S_Sat} \) is not used for computing fluid density. However, if the solution mining algorithm is activated (see BLOCK SALT command), then these values are used to compute the amount of salt that dissolves from the salt blocks into the water.

EXAMPLES

DENSITY SANDIA function
DENSITY SANDIA function; \( ρ^* = 998.2 \), \( α = 0.6995 \), \( ρ_{max} = 1209 \)
DENSITY SANDIA function; \( ρ^* = 998.2 \), \( α = 0.6995 \), \( ρ_{max} = 1209 \), \( ρ_{salt} = 2165 \), \( C_{sat} = 0.2643 \)
Keyword Commands

MODE 5: Density of Solid or Particle Material

SYNTAX
DENS {SOLID|PART} {func[ξ]} {N₁, N₂, ..., Nₙ|fname} [ALWA] [subrgn]

SOLID|PART
The solid material or particulate density is specified. The density is assumed to be for the dry particulate material.

func
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. For this input, the function specifies the value of the density of the solid phase. If no function is specified then the value is assumed to be constant.

ξ
One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname
The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

ALWA
By default the DENS command is implemented immediately and only once – as soon as the command is encountered. If this modifier is present then the command is executed immediately as well as repeatedly at the beginning of each time step (or iterative step in steady state mode) of the solution procedure.

subrgn
The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

APPLICABILITY
This command is currently available only for the ANSWER™ and PORFLOW™ Software Tools.

COMMENTS
If specification for a fracture subdomain (FRAC TURE command) is missing, then the value is assumed to be that for the host matrix at the first element of the subdomain.

EXAMPLES
DENSITY of SOLID is = 1
DENSITY of SOLID is 2200 kg/m^3

Generic examples for this command are given in Section 4.4. The command keyword (DENS) must replace the keyword used in these examples.
COMMAND  DIAGNOSTIC

PURPOSE  To specify the options for diagnostic output of the values of variables, flux balances or convergence residual values.

SYNTAX  DIAG \( [\Phi] \) \( [\text{NOW \| OFF}] \) \( [\text{ELEM}] \) \( [\text{OPEN}] \) \( [\text{HIGH}] \) \{\( N_1, \ldots, N_n \)\} \( [N_{\text{freq}}] \) \( [N_{\text{file}}] \) \( [\text{fname}] \) \( n=1 \) for unstructured, \( n=2 \) for 2D and \( n=3 \) for 3D input mode

\( \Phi \)  One or more symbolic character strings. Each string denotes a desired diagnostic output for a corresponding variable. The valid symbols are:

1) The symbols listed in Table 2.8.1-3,
2) The symbols listed in Table 2.8.1-3 preceded by 'D',
3) The symbols listed in Table 2.7.1 preceded by a 'B'
4) The symbols listed in Table 2.7.1 preceded by an 'R',
5) The modifiers TIME or DTIM.

The prefix 'D' denotes difference (change) of the variable from the previous value, 'B' denotes the normalized flux balance disparity over the whole domain, and 'R' denotes the matrix residue. The diagnostic variables appear in the output in the same order as on the command. A maximum of 9 variables are written to the output file. The first 5 of these also appear on the screen (see \text{SCREEN } command) by default. All 9 variables are directed to the screen if the \text{WIDE } modifier is present on the \text{SCREEN } command.

The default diagnostic output depends on the equations being solved and the nature of the problem. For transient problems, time is always printed as the first value. Then up to 8 (for transient) or 9 (for steady state) other diagnostic indicators are selected. The order of selection is: values of the active field variables, flux balances and matrix residue for the variables for which the governing equations are solved.

OFF  Diagnostic output is suppressed.

NOW  Diagnostic output is produced immediately.

ELEM  By default for structured grids, the input of \( N_1, \ldots, N_n \) specifies the grid indices. If this modifier is present, then \( N_1 \) specifies the element number at which diagnostic output is produced. This modifier has no effect for unstructured grids.

OPEN  If this modifier is present, and the user specifies an element for diagnostic output (see \( N_1, \ldots, N_n \)) that is located in a blocked region (\text{BLOCK } command), then the diagnostic element will be moved to a neighboring open element.

HIGH  If this modifier is present then additional diagnostics is provided about the allocation of memory for the storage of variables.

\( N_1, \ldots, N_n \)  The grid index location for the element for which the output is obtained. For unstructured grids, the input is that of the element number. For structured grids the input consists of the grid indices \((I, J, K)\) in the 3D or \((I, J)\) in the 2D mode or the element number (if the \text{ELEM } modifier is present). If the specified node is located at the domain boundary, it is automatically adjusted to fall within the domain of computation.

\( N_{\text{freq}} \)  The frequency of diagnostic output in terms of time steps. A value of 0 is treated as identical to 1. The default value is 1.

\( N_{\text{file}} \)  The frequency of output to the extended diagnostic file described by \text{fname} below. If no value is specified, then the default value is set equal to \( N_{\text{freq}} \).
fname

By default a file with extended diagnostic output is generated with the same name as the Standard Output file but with the extension as “DGN”. For example, if the Standard Output file is “PROBLEM.OUT”, then the diagnostic file is named “PROBLEM.DGN”. If a file name is specified, then the diagnostic output is directed to the named file. This file contains the mass balance residuals and fluxes for each variable for which a transport equation is solved.

COMMENTS

The 1st column of the output for the diagnostic command contains a “Convergence Index”. This index is representative of a measure of the residue of matrix equations and is controlled by the CONVERGENCE command. The residue in turn is related to the flux balance disparity in the solution of the differential equations. The flux balance disparity is composed of four components: The cumulative changes in storage, inflow, outflow and decay (see FLUX command).

The convergence index is normalized by a used specified error tolerance (CONVERGENCE REFERENCE command). A value of less than unity for this index means that the residue for the reference matrix equation(s) is smaller than the specified tolerance.

If the equations are solved in the steady state mode, then steady state is assumed to be reached when the index reaches a value of less than unity. However, caution should be exercised and the solution should also be examined for changes in the values of the key variables. The step-to-step values (or changes) of selected variables at a diagnostic node are also printed by this command. At steady state, there should be no further changes in the values of variables. In practice, often a true steady state (except for simple flows) can only be approached asymptotically. In this case a steady state is assumed to prevail provided the changes in the values of the variables are negligible compared to some norm of the solution.

If the equations are solved in the transient mode, then the index is a measure of the accuracy of the solution at each intermediate time step.

EXAMPLES

DIAGnostic node (4,8) ! 2D input mode; diagnostic printout every step
DIAGnostic node (4,8,7) ! 3D input mode; diagnostic printout every step
DIAGnostic output at element number 25 ! Unstructured mode
DIAGnostic output at element number 25 every 10 steps; also file ‘Diagnostics.eqn’
DIAGnostics at (7,2,5) every 10 steps
DIAGnostic output for U, P and T at node (7,2) print every 10 steps; also ‘EQUATIONS.DGN’
DIAGnostic output for TIME, U, BP and RT at node (7,2) print every 10 steps
DIAGnostic output HIGH level with TIME, U, BP and RT at node (7,2) print every 10 steps
DIAGnostic output for TIME, DTIME, P, DP & RP at node (7,2) every 10 steps
DIAGnostic output: U, BP, RT and TIME in that order at (7,2) every 10 steps
DIAGnostic output: TIME, U, BP and RT at node (7,2) print every 10 steps but every 20 steps for file output
DIAGnostic output OFF
DIAGnostic output NOW
COMMAND  DIFFUSION

PURPOSE  To specify diffusivity and the treatment of interface diffusion.

COMMENTS  This command is identical to the CONDUCTION command.

EXAMPLES  See CONDUCTION command
Keyword Commands

COMMAND  DISABLE

PURPOSE  To disable built-in default options.

MODE 1:  Disable Global Options

SYNTAX  DISA  [FLOW] [ENTH] [VELO] [DPDX] [DENS] [ALL]

FLOW  By default, the equations for the velocity components U, V, W and the density/pressure correction variable are always solved. This modifier may be used to disable flow calculations. Flow computation may also be disabled by appropriate specification of variables on the SOLVE command.

ENTH  By default if enthalpy is read from an archive file by a READ command, then any user input of temperature is ignored. Any new specification of temperature by the user is ignored. However, in some cases, it may be desirable to overwrite the specified enthalpy value by computing a new value from the temperature field. If this modifier is present, then enthalpy at the start of the solution process is recomputed from the temperature field. This modifier is active only for the ANSWER™ Software Tool.

VELO  By default velocity, pressure and density are corrected based on the continuity equation. If this modifier is present, then only the pressure and density are corrected; velocity is retained at its value computed from the momentum equations. This modifier is active only for the ANSWER™ Software Tool.

DPDX  The pressure gradient terms in the momentum equations for ANSWER™ software are set to zero. This is primarily a diagnostic tool to check the relative importance of various terms in the governing momentum equations. This modifier is active only for the ANSWER™ Software Tool.

DENS  If this modifier is present then the effect of density in the pressure equation is ignored everywhere except in the buoyancy term. This is equivalent to the so-called Boussinesq assumption. This modifier is active only for the PORFLOW™ Software Tool.

ALL  If this modifier is present along with the DENSity modifier, then the effect of density changes is ignored in all the heat and mass transport equations; that is the fluid density appearing in these equations is set equal to its reference value. This modifier is active only for the PORFLOW™ Software Tool.

EXAMPLES

DISABLE FLOW
DISABLE FLOW computations
DISABLE ENTHalpy values read from the file for ANSWER software
DISABLE FLOW
DISABLE VELOcity correction for ANSWER
DISABLE DENSity variations in flow equation (Boussinesq assumption)
DISABLE DENSity variations in ALL equations for PORFLOW
DISABLE FLOW and DENSity variation in ALL equation
MODE 2: Disable Options for Specific Variables

SYNTAX DISA {Φ} [CONV] [OFF]

Φ One or more symbols that denote the dependent variables for which the specified feature is disabled. There is no default value.

CONV In the absence of the OFF modifier, the convection term in the transport equation for the specified variable is set to zero. If the OFF modifier is present, then the convection term is reinstated.

OFF Any previously disabled CONV option is reinstated.

COMMENTS

This command may be used to explore the effect of each individual component of the transport equation for a selected variable. At any given time at least one of the three (storage, convection and diffusion) terms in the transport equation must stay active, otherwise the transport equation has no solution.

EXAMPLES

DISAble CONvection term for T and C
DISAble CONvection term for T is OFF (reinstate convection)
Keyword Commands

**COMMAND**  DISPERSIVITY

**PURPOSE**  To specify the dispersion coefficients for dispersion of thermal and species equations. This command is effective only for the PORFLOW™ Software Tool.

**MODE 1:**  Uniform Dispersion Coefficients

**SYNTAX**  DISP {Φ} [LONG] [α_L] [TRAN] [α_T] [subrgn]

Φ  The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are those for thermal and species equations listed in Table 2.7.1. There is no default value; a symbol must be specified.

LONG  The longitudinal dispersion coefficient is specified.

α_L  The longitudinal dispersion coefficient. The default value is 0.

TRAN  The transverse dispersion coefficient is specified.

α_T  The transverse dispersion coefficient. The default value is 0.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

**COMMENTS**

The dispersion coefficients are used to compute the effective diffusivity tensor for a species due to diffusion and dispersion (see e.g. Freeze & Cherry, 1979). Typical formulation due to Scheidegger (1961) is:

\[
\Gamma_{ij} = \varphi_D \xi_{ij} \Gamma_M + \varphi_E \Delta_{ij},
\]

\[
D_{ij} = \alpha_T \delta_{ij} V + (\alpha_L - \alpha_T) \frac{|V_i V_j|}{V},
\]

Where:

Γ_{ij}  is the effective diffusivity tensor,

φ_D  saturated diffusional porosity,

ξ_{ij}  is the tortuosity,

Γ_M  is the molecular diffusivity,

φ_E  saturated effective porosity,

Δ_{ij}  is the hydrodynamic dispersion,

δ_{ij}  is the Kronecker delta,

V_i  the particle velocity vector, and

V  the magnitude of the particle velocity.

**EXAMPLES**

DISPERSION for C 5 and 1 meters
DISPERSION for C LONGitudinal coef 5; TRANsverse value = 1 meters for ID=SAND
DISPERSIVITY for C LONGitudinal coef 5 meters ID=SAND
DISPERSION for C TRANsverse value = 1 meters for ID=SAND
MODE 2: Dispersion Coefficient as a General Function

SYNTAX

**DISP** \{Φ \} \{LONG | TRAN \} \{xyz \} \{func[ξ] \} \{N₁, N₂, ..., Nₙ, fname \} \{subrgn \}

Φ

The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are those for thermal and species equations listed in Table 2.7.1. There is no default value; a symbol must be specified.

LONG

The longitudinal dispersion coefficient is specified.

TRAN

The transverse dispersion coefficient is specified.

xyz

One of the character strings: XX, YY, ZZ, XY, YX, XZ, ZX, YZ and YZ. It denotes the component of the dispersion tensor to which the input is applied. The first 3 denote the diagonal components of the tensor while the others denote the off-diagonal components. Since the tensor is symmetric, XY and YX, XZ and ZX, and YZ and ZY are equivalent.

func

One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the value of the appropriate distribution coefficient for the corresponding Φ variable. In this mode a function must be specified.

ξ

One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname

The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

subrgn

The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

COMMENTS

The implementation proceeds in the manner above except that if the xyz modifier is present, then the corresponding component of the \( D_{ij} \) in Equation 2 above is directly set to the values computed from the specified function.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (DISP) must replace the keyword used in these examples.
MODE 3: Dispersion Coefficient for Vertically Stratified Anisotropic Soils

SYNTAX

\[ \text{DISP} \{ \Phi \} \{ \text{STRA} \} \{ \alpha_{\text{LH}}, \alpha_{\text{TH}}, \alpha_{\text{LV}}, \alpha_{\text{TV}} \} \{ \text{subrgn} \} \]

\( \Phi \) The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are those for thermal and species equations listed in Table 2.7.1. There is no default value; a symbol must be specified.

\( \text{STRA} \) The input is being specified for a stratified anisotropic media where the dispersion contribution will be computed as given by Equation 3 below. This modifier is effective only for 3D problems. For 2D problems this formulation collapses to that given by Equation (2); in this case \( \alpha_{\text{LH}} = \alpha_{\text{L}}; \alpha_{\text{TH}} = \alpha_{\text{T}} \) and \( \alpha_{\text{LV}} \) and \( \alpha_{\text{TV}} \) are ignored.

\( \alpha_{\text{LH}} \) The horizontal longitudinal dispersion coefficient. The default value is 0.

\( \alpha_{\text{TH}} \) The horizontal transverse dispersion coefficient. The default value is 0.

\( \alpha_{\text{LV}} \) The vertical longitudinal dispersion coefficient. The default value is 0.

\( \alpha_{\text{TV}} \) The vertical transverse dispersion coefficient. The default value is 0.

\( \text{subrgn} \) The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

COMMENTS

The general formulation for anisotropic porous media requires 5 empirical coefficients (see, e.g., Bear and Bachmat, 1986). The mode described here is based upon the work of Burnett and Frind (1987) and employs 4 constants. It is suitable for vertically stratified (such a layered) porous media. The individual components of the \( D_{ij} \) tensor, assuming that the vertical direction is \( z \), are then given by:

\[
D_{xx} = \alpha_{\text{LH}} \frac{V_x^2}{V} + \alpha_{\text{TH}} \frac{V_y^2}{V} + \alpha_{\text{TV}} \frac{V_z^2}{V}, \quad (3a)
\]

\[
D_{yy} = \alpha_{\text{TH}} \frac{V_x^2}{V} + \alpha_{\text{LH}} \frac{V_y^2}{V} + \alpha_{\text{TV}} \frac{V_z^2}{V}, \quad (3b)
\]

\[
D_{zz} = \alpha_{\text{TV}} \frac{V_x^2}{V} + \alpha_{\text{TV}} \frac{V_y^2}{V} + \alpha_{\text{LV}} \frac{V_z^2}{V}, \quad (3c)
\]

\[
D_{xy} = D_{yx} = (\alpha_{\text{LH}} - \alpha_{\text{TH}}) \frac{V_x V_y}{V}, \quad (3d)
\]

\[
D_{xz} = D_{zx} = \left\{ 0.5 (\alpha_{\text{LH}} + \alpha_{\text{LV}}) - \alpha_{\text{TV}} \right\} \frac{V_x V_z}{V}, \quad (3e)
\]

\[
D_{yz} = D_{zy} = \left\{ 0.5 (\alpha_{\text{LH}} + \alpha_{\text{LV}}) - \alpha_{\text{TV}} \right\} \frac{V_y V_z}{V}, \quad (3f)
\]

This equation becomes identical to Equation (2) when:

\( \alpha_{\text{LH}} = \alpha_{\text{LV}} = \alpha_{\text{L}} \) and \( \alpha_{\text{TH}} = \alpha_{\text{TV}} = \alpha_{\text{T}} \)

EXAMPLES

DISPERSION for C STRATIFIED option: 5, 1, 3 and 0.5 meters for ID=SAND
COMMAND  DISTRIBUTION COEFFICIENT

PURPOSE  To specify the distribution coefficient for the governing differential equations. This command is effective only for the PORFLOW™ Software Tool.

MODE 1:  Distribution Coefficient as a General Linear Function

SYNTAX  DIST  {Φ}  {func[ξ]}  {N_1}  {N_2 ... N_n  fname}  [subrgn]  [TOTA]

Φ  The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

func  One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the value of the appropriate distribution coefficient for the corresponding Φ variable. If no function is specified then the value is assumed to be constant.

ξ  One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N_1,...,N_n  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  The name of the file containing the numerical values N_2 through N_n. This option is available only for selected functions. See Section 3.3 for additional information.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

TOTA  By default any chemical species is assumed to adsorb only in the wetted part to the solid:

\[ Q_s = \rho_s \, S \, (1 - \Theta_E) \, C_s , \]

where, \( Q_s \) is the mass of species C in solid, \( \rho_s \) is the density of solid, \( S \) is the fluid phase saturation, \( \Theta_E \) is the effective porosity and \( C_s \) is the concentration of species C in solid.

If linear equilibrium of the species in the primary (usually liquid) and the solid phases is assumed then, with \( k_d \) as the distribution coefficient and \( R_d \), retardation coefficient:

\[ C_s = \rho_s \, k_d \, C \]

\[ R_d = 1 + \frac{1 - \Theta_E}{\Theta_E} \, k_d . \]

However if the TOTA modifier is present, then the species is assumed to be stored in the total solid and the above relations are replaced by:

\[ Q_s = \rho_s \, (1 - \Theta_E) \, C_s , \]

\[ R_d = 1 + \frac{1 - \Theta_E}{S \, \Theta_E} \, k_d . \]

COMMENTS

PORFLOW™ also provides for non-linear relations between the solid and liquid concentrations as well as separate computations of partitioning between solid and liquid phases. These options are implemented by other modes of the DISTRIBUTION command.

The term “distribution coefficient” is normally applied only to the transport of chemical species. However, this command may be used to specify the “storage coefficient” for any of the governing transport equations.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (DIST) must replace the keyword used in these examples.
MODE 2: Distribution Coefficient as a Special Function

SYNTAX

DIST {Φ} {FREU|LANG} [subrgn] [N1] [N2] [TOTA]

Φ

The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

FREU

The concentration of the species in the solid phase, $C_s$, is given by the Freundlich Isotherm:

$$C_s = \frac{\rho_s k_d C^n}{\rho_s C^k + \rho_s},$$

where $\rho_s$ is the density of solid, $k_d$ is a distribution coefficient, $C$ is the concentration in the liquid phase and $n$ is an empirical exponent.

LANG

The concentration of the species in the solid phase, $C_s$, is given by the Langmuir equation

$$C_s = \frac{c_{s\text{max}} C}{C_{\text{lang}} + C},$$

where $c_{s\text{max}}$ is the maximum concentration per unit mass in the solid phase and $C_{\text{lang}}$ is the Langmuir constant. It is seen that when $C \ll C_{\text{lang}}$, the relation become equivalent to a linear isotherm with $k_d = c_{s\text{max}} / C_{\text{lang}}$.

subrgn

See Mode 1 specification.

N1

The distribution coefficient, $k_d$, for the Freundlich Isotherm or the $c_{s\text{max}}$ for the Langmuir equation.

N2

The power exponent, $n$, for the Freundlich Isotherm or the Langmuir constant, $C_{\text{lang}}$, for the Langmuir equation.

TOTA

See Mode 1 specification.

COMMENT

This command mode is available only with the PORFLOW™ Simulation Tool for all the species equations and for the first phase pressure equation. It is one of the means available in PORFLOW™ to incorporate non-linear isotherms with geochemistry. Non-linear kinetics can also be implemented by functional forms of the distribution or retardation coefficients (see Mode 1 of DISTRIBUTION and RETARDATION commands) and by the REACTION command.

For the first phase pressure equation in PORFLOW™, the variable the species concentration, $C$, is replaced by $P$, the pressure. The units of $k_d$ and $c_{s\text{max}}$ are such that the units of $C_s$ are those of volumetric unit of adsorbed gas in the solid phase divided by the mass density of solid. $C_{\text{lang}}$ has units of pressure, $P$.

EXAMPLES

DISTribute C as FREUndlich Isotherm with $k_d=0.22$, $n = 0.8$ for ID=CLAY
DISTribute C as LANGmuir equation with $C_{s\text{max}}=1.89$, $C_{\text{lang}}=0.2$ for ID=CLAY
**MODE 3:** Distribution Coefficient from Fluid & Solid Phase Concentrations

**SYNTAX**

```
DIST {CONC} {Φ} {TABL} [subrgn] {N_sets} [N_1, ..., N_n].fname [TOTA]
```

**CONC**

The distribution coefficient is computed from a specified table of concentration in the fluid phase as a function of the concentration in the solid. The total initial property can be specified by the `SET` command with `INVENTORY` modifier. If the initial inventory is not specified, then it is assumed that the initial amount in each element is equal to the initial concentration multiplied by the volume of the fluid in that element. The specified fluid concentration is then modified so that initial amount is distributed between the fluid and solid phases according to the specified tabular function.

**Φ**

The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

**TABL**

The data is specified as a table of two values per data set. The first value is the concentration in the solid phase and the second is that in the liquid phase. A typical set of data is shown plotted below.

![Distribution Coefficient Plot](image)

**subrgn**

See Mode 1 specification.

**N_sets**

Number of sets of data in the table.

**N_1, .., N_n**

The values (2 * N_sets) of solid and liquid concentration of species.

**fname**

The name of the file containing the numerical values N_1 through N_n.

**TOTA**

See Mode 1 specification.

**COMMENT**

This mode of the command is available only with the PORFLOW™ Simulation Tool. It is one of the means available in PORFLOW™ to incorporate non-linear isotherms with geochemistry. Non-linear kinetics can also be implemented by functional forms of the distribution or retardation coefficients (see Mode 1 of DISTRIBUTION and STORAGE commands) and by the REACTION command. More complex geochemistry can be implemented by separately solving the transport equations for the concentration of species in the liquid and solid phases.

**EXAMPLES**

```
DISTribute C as CONCentration TABLe of values: 6 sets
(0., 0.) (1., 0.), (1.0001, 1.), (2., 1) (2.0001, 0.5) (3., 0.2)
DISTribute C2 in CONCentration mode for ID=ZN10 as TABLe of values: with 6 sets:
(0., 0.) (1., 0.), (1.0001, 1.), (2., 1) (2.0001, 0.5) (3., 0.2)
DIST C CONCentration as TABLe of 20 sets from file 'KD_ALL’ for ID=ZN10.
```
MODE 4: Distribution Coefficient from A Chain of Species or RadioNuclides

SYNTAX

```
DIST {CHAIN} {Φ₁, Φ₂, .. Φₖ} {TABL} {STEP|LINE|SECO|CUBI} [subrgn] {N₁,..., Nₙ | fname} [TOTA]
```

CHAIN

The distribution coefficient is computed from a specified table of concentration in the fluid phase as a function of the concentration in the solid for the total mass of all species (or nuclides) in the chain. The total initial property for each species can be specified by the SET commands with INVENTORY modifier for each species. If the initial inventory is not specified, then it is assumed that the initial amount in each element is equal to the initial concentration multiplied by the volume of the fluid in that element. The specified fluid concentration is then modified so that initial amount is distributed between the fluid and solid phases according to the specified tabular function.

To implement this logic, the total solid concentration over all species is determined from the computed values of the species mass and liquid concentration as:

\[
C_s = \sum_k m_k - \sum_k \phi_k \theta S_f \delta V
\]

\[
\rho_s (1 - \theta) S_s \delta V
\]

Where, \(k\) denotes the species, \(m\) and \(\Phi\) are, respectively, the computed mass and liquid concentration, \(\theta\) is the porosity, \(S_f\) is the saturation of the liquid phase, \(\rho_s\) is the particle density of solid and \(\delta V\) is the volume of the element for which the computation is being performed. The quantity \(S_s\) in the denominator if the TOTAL modifier is specified; otherwise it is equal to \(S_f\).

The effective total concentration in the liquid is then determined from the specified tabular function. The distribution coefficient, \(k_d\) is determined from:

\[
k_d = \frac{C_s}{C_l}; \text{ if } C_l > 0, \quad k_d = \frac{\partial C_s}{\partial C_l}; \text{ if } C_l = 0
\]

Finally a new value for each of the species in the chain is computed as:

\[
\phi_k^{corrected} = \frac{m_k}{\theta S_f \delta V + \rho_s k_d (1 - \theta) S_s \delta V}
\]

\(\Phi₁, \Phi₂, .. \Phiₖ\) The symbols for the dependent variable for which the distribution coefficient is specified. Valid symbols are listed in Table 2.7.1. **There is no default value; a symbol must be specified**

TABL

The data is specified as a table of two values per data set. The first value for each set is the sum of concentration in the solid phase and the second value is that in the liquid phase. A typical table is shown below.
LINE  Linear interpolation is used for the tabular function.  This is the default option.
STEP  Table is interpreted in a step wise manner.
SECO  Quadratic interpolation is used to evaluate the tabular function.
CUBI  Cubic interpolation is used for the tabular function.
subrgn See Mode 1 specification.
Nsets  Number of sets of data in the table.
N1, .., Nn The values (2 * Nsets) of solid and liquid concentration of species.
fname  The name of the file containing the numerical values N1 through Nn.
TOTA  See Mode 1 specification.

COMMENT

This mode of the command is available only with the PORFLOW™ Simulation Tool. It is one of the means available in PORFLOW™ to incorporate non-linear isotherms with geochemistry. Non-linear kinetics can also be implemented by functional forms of the distribution or retardation coefficients (see Mode 1 of DISTRIBUTION and STORAGE commands) and by the REACTION command. More complex geochemistry can be implemented by separately solving the transport equations for the concentration of species in the liquid and solid phases.

EXAMPLES

DISTribute for CHAIN of: U233, U234, U235, U236, U238 as TABLE of values: 6 sets
(0., 0.)  (1., 0.), (1.0001, 1.), (2., 1) (2.0001, 0.5) (3., 0.2)
MODE 5: Distribution Coefficient for One Equation Concrete Degradation Model

SYNTAX

\[ \text{DIST} \{ \text{CONCRETE} \} \{ \text{CAL} \} \{ \text{CAS} \} \{ \text{TABL} \} \{ \text{LINE} \} \{ \text{SECO} \} \{ \text{CUBI} \} \{ \text{NSi} \} \{ \text{N1, ..., Nn} \} \{ \text{name} \} \{ \text{S_{as}} \}, \{ \text{subrgn} \} \]

CONCRETE

This modifier triggers the solution of a CEA developed algorithm for degradation of concrete which is incorporated in the governing equation:

\[
\frac{\partial}{\partial t} (\theta \text{Ca} + \text{Ca}_s) + \frac{\partial}{\partial x_i} (V_i \text{Ca}) = \frac{\partial}{\partial x_i} (\Gamma \frac{\partial \text{Ca}}{\partial x_j}) + S_{\text{Ca}} - Y_{\text{ca}}
\]

Where \( \text{Ca} \) and \( \text{Ca}_s \) are the concentrations of Calcium in the liquid and the solid phase respectively (The default symbolic name of \( \text{Ca} \) is \( \text{CAL} \) and that of \( \text{Ca}_s \) is \( \text{CAS} \)). In this equation \((x_i,t)\) denote the space and time, \( V_i \) is the Darcy velocity, \( \theta \) is the porosity, \( \Gamma \) is the diffusivity, \( S \) and \( y \) are the source and sink (reaction) terms and the subscript \( \text{Ca} \) denotes the \( \text{Ca} \) species. The diffusion coefficient for the governing concentration equations is typically an exponential function of porosity:

\[
\Gamma = \Gamma_o \exp\left(\frac{\theta}{\theta_o}\right)
\]

The diffusion coefficient must be specified by an appropriate \text{DIFFUSION} command. Tognazzi (1998) and Torrenti et al. (1999) quote \( \Gamma_o = 2.3 \times 10^{-13} \) and \( \theta_o = 0.100503 \). Alternative diffusion coefficients may also be specified.

The degradation model is based on the assumption that decalciﬁcation of concrete occurs over a period of time due to multiple factors. The major parameters of degradation are leaching of Calcium (\( \text{Ca} \)) from the concrete components from the solid state into solution. During this process solid structure disintegrates with major changes in the volume of its constituents. The CEA model has been simplified so that both porosity and solid calcium concentration (\( \text{Ca}_s \)) are tabulated functions of the calcium concentration in solution (\( \text{Ca} \)) (Please see References 1, 2 and 3 below for fuller details). The typical variation of \( \text{Ca}_s \) and porosity with \( \text{Ca} \) is as shown in the figures below.

- **CAL** The symbol for the dependent variable, \( \text{Ca} \), for which the distribution and porosity functions are specified.
- **CAS** The symbol for the solid phase concentration, \( \text{Ca}_s \).
- **TABL** Specifies that a tabular function for the normalized \( \text{Ca}_s/S_{\text{Si}} \) ratio and porosity as a function of \( \text{Ca} \) is specified. This modifier must be present; there is no default value.
- **LINE** Linear interpolation is used for the tabular function. This is the default option.
- **SECO** Quadratic interpolation is used for the tabular function.
- **CUBI** Cubic interpolation is used for the tabular function.
**N<sub>Set</sub>**

The number of sets of values that are specified for the characteristic function. There is no default value; a valid value (>0) must be specified.

**N<sub>1</sub>, .., N<sub>n</sub>**

N<sub>Set</sub> set of values for the characteristics. Each set consists of 3 values: Ca, normalized Ca/<i>S</i><sub>Si</sub> ratio, and porosity (θ), in that order.

**fname**

See Mode 1 specification. The numerical values will be read from a file.

**S<sub>Si</sub>**

Concentration of Silicium in the concrete paste that was used to normalize the specified Ca/<i>S</i><sub>Si</sub> ratio above. The specified values will be multiplied with this number to obtain the actual Ca<sub>v</sub> value. The default value is 4900.

**subrgn**

See Mode 1 specification.

---

**COMMENT**

This mode of the command is available only with the **PORFLOW™** Simulation Tool. It is one of the means available in **PORFLOW™** to incorporate the concrete degradation. Other models can be incorporated by defining the phase variables (**ALLOCATE**) and appropriate distribution coefficients (see Mode 1 of **DISTRIBUTION** and **STORAGE** commands) and by the **REACTION** command.

**EXAMPLES**

**DISTRIBUTION** characteristics for CONCRETE given by 5 sets of values in a TABLE:

<table>
<thead>
<tr>
<th>CAL</th>
<th>CAS</th>
<th>POR</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.59</td>
</tr>
<tr>
<td>1.5</td>
<td>0.5</td>
<td>0.59</td>
</tr>
<tr>
<td>2.0</td>
<td>1.0</td>
<td>0.59</td>
</tr>
<tr>
<td>21.0</td>
<td>1.65</td>
<td>0.47</td>
</tr>
</tbody>
</table>
| 22.0 | 3.0 | 0.25| **S<sub>Si</sub> = 4900**
MODE 6: Distribution Coefficient for Two Equation Concrete Degradation Model

SYNTAX

DIST {CONCRETE} {CARB} {CAL} {CAS} {TABL} [LINE|SECO|CUBI] {NSEL} {Ni, ..., Nn,IEEE} {fname}, 
{S1}, {k}, {Caeq}, {θlim}, [Vmol_Calcite], [subrn], [INNE], [EXPL], [UNLI]

CONCRETE

Together with the CARB modifier this triggers the solution of a two equation CEA developed algorithm for degradation of concrete which is incorporated is expressed in the governing equations:

\[
\frac{\partial}{\partial t} \left( \theta Ca + Ca_s \right) + \frac{\partial}{\partial x_j} \left( \Gamma Ca \right) = \frac{\partial}{\partial x_j} \left( \Gamma Ca \right) + S_{Ca} - \gamma_{Ca} - R_{Calcite}
\]

\[
\frac{\partial}{\partial t} (\theta CO_3) + \frac{\partial}{\partial x_j} \left( \Gamma CO_3 \right) = \frac{\partial}{\partial x_j} \left( \Gamma CO_3 \right) + S_{CO_3} - \gamma_{CO_3} - R_{Calcite}
\]

The reaction rate of Calcite formation, \( R_{Calcite} \) and the evolution of porosity are given by:

\[
R_{Calcite} = k \left( \theta - \theta_{lim} \right) \max \left( \min \left( Ca - Ca^*, \ (CO_3 - CO_3^*) \right), 0 \right)
\]

\[
\frac{\partial \theta}{\partial t} = \frac{\partial \theta}{\partial t} - R_{Calcite} \frac{\partial \theta}{\partial t}^\text{Vmol_Calcite}
\]

In these equations \( Ca \) and \( CO_3 \) are the concentrations of Calcium and the Carbonates in liquid and \( Ca_s \) is the concentration of Calcium in solid phase (The default symbolic name of \( Ca, Ca_s \) and \( CO_3 \) are CAL, CAS and CO3, respectively.). The constant k is the reaction rate of Calcite formation, \( \theta_{lim} \) is the minimum porosity, \( W_{Ca} \) is the base porosity in the absence of any calcite formation and \( V_{mol_Calcite} \) is the molar volume of Calcite. \( Ca^* \) and \( CO_3^* \) are the corresponding equilibrium concentration of the species. The rest of the notation is the same as in the previous mode of the command.

The diffusion coefficient for the governing concentration equations is typically an exponential function of porosity:

\[
\Gamma = \Gamma_o \exp \left( \frac{\theta}{\theta_o} \right)
\]

The diffusion coefficient must be specified by an appropriate DIFFUSION command. Tognazzi (1998) and Torrenti et al. (1999) quote \( \Gamma_o = 2.3 \times 10^{-13} \) and \( \theta_o = 0.100503 \). Alternative diffusion coefficients may also be specified.

This degradation model is based on the assumption that the major mechanism of degradation is leaching of Calcium (Ca) from the concrete components from the solid state into solution and that the primary calcification reaction is given by:

\[
Ca^{2+} + CO_3^{2-} = CaCO_3
\]

Further details and theoretical background of this model is described by Bary and Bregeon (2003) and, among others, is based on the work by Adenot and Bull (1992), Mainguy et al. (2000) and Richet et al. (2004).

The CEA model has been simplified so that solid calcium concentration, \( Ca_s \), the base porosity, \( W_{Ca} \), and the equilibrium CO3 concentration, \( CO_3^* \), are tabulated functions of the calcium concentration in solution, \( Ca \). The typical variations of these are shown in the figures below.
CARB
The modifier to trigger the 2 equation concrete degradation model described above.

CAL
The symbol for the dependent variable, Ca, for which the distribution and porosity functions are specified.

CAS
The symbol for the solid phase concentration, Cs.

TABL
Specifies that a tabular function for the normalized Ca/Si ratio and porosity as a function of Ca is specified. This modifier must be present; there is no default value.

LINE
Linear interpolation is used for the tabular function. This is the default option.

SECO
Quadratic interpolation is used for the tabular function.

CUBI
Cubic interpolation is used for the tabular function.

N
Set
The number of sets of values that are specified for the characteristic function. There is no default value; a valid value (>0) must be specified.

N₁, ..., Nₙ
\(N_{\text{Set}}\) set of values for the characteristics. Each set consists of 4 values: Ca, normalized Ca/Si ratio, \(W_{\text{Ca}}\) porosity and CO₃\(^*\), in that order.

fname
See Mode 1 specification. The numerical values will be read from a file.

S
Si
Concentration of Silicium in the concrete paste that was used to normalize the specified Ca/Si ratio above. The specified values will be multiplied with this number to obtain the actual Ca value. The default value is 4900.

k
Reaction rate for the Ca and CO₃ reaction. Typical values are in units of \([s^{-1}]\) but any consistent units may be used. The default value is 1

Ca
\(_{\text{eq}}\)
The equilibrium value of Ca. The default value is 0.11
Keyword Commands

\( \theta_{\text{Lim}} \) The minimum value of porosity. The default value is 0.01

\( V_{\text{mol, calcite}} \) The molar volume of Calcite. The default value is \( 3.69 \times 10^{-5} \text{ [m}^3/\text{mol]} \)

subrgn See Mode 1 specification.

INNE By default the carbonation reaction at any time step is computed before the species equations are solved. Once the new values of the species are computed at any time step, the reaction is not updated unless CONVERGENCE COUPLED SPECIES command is present. If the INNER modifier is present then the reaction is updated in the inner loop for the species which is controlled by the CONVERGENCE command. See COMMENTS below.

EXPL By default at every time step, the new value of the CO3 and CAL are computed on the assumptions that the reaction term can be treated implicitly. If the EXPL modifier is present, then the reaction term is treated explicitly. **This option is not recommended unless the reaction rate is very slow.**

UNLI By default it is assumed that the total reaction at any time step is limited by the amount of species present and the rate of diffusion and advection that can take place. If the UNLI modifier is present, then the reaction term is unbounded. **This option is not recommended unless the reaction rate is very slow.**

COMMENTS

This mode of the command is available only with the PORFLOW™ Simulation Tool. It is one of the means available in PORFLOW™ to incorporate concrete degradation. Other models can be incorporated by defining the phase variables (ALLOCATE) and appropriate distribution coefficients (see Mode 1 of DISTRIBUTION and STORAGE commands) and by the REACTION command.

Unless the reaction rate of CO3 and CAL is very slow, one must use one of two different strategies for convergence. Because of the coupling due to the reaction rate, it may be necessary to perform an outer iteration on the species at every time step by specifying the CONVERGENCE COUPLED SPECIES command with appropriate number of outmost iterations. In most situations, it should be sufficient to perform 2 to 3 iterations on the coupled system. It is also important to ensure that each species is fully converged at each step. Because the reaction term in the equation is changing, it is important that a CONVERGENCE command be specified for each of CO3 and CAL with adequate number of iterations. In most situations, it should be sufficient to perform 2 to 5 iterations on each species. Though both the coupled as well as the inner iteration may be required for stiff system of equations, it is generally more economical and sufficient to perform either the outer coupled iterations or the inner iterations.

EXAMPLES

**DISTRIBUTION CONCRETE CARBONATION** given by 8 sets of values in a TABLE:

<table>
<thead>
<tr>
<th>CAL</th>
<th>CAS</th>
<th>POR</th>
<th>CO3*</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0000</td>
<td>0.6210</td>
<td>0.100</td>
</tr>
<tr>
<td>0.11</td>
<td>0.0000</td>
<td>0.6210</td>
<td>0.100</td>
</tr>
<tr>
<td>1.10</td>
<td>0.4000</td>
<td>0.6210</td>
<td>0.066</td>
</tr>
<tr>
<td>3.09</td>
<td>1.5200</td>
<td>0.6210</td>
<td>0.002</td>
</tr>
<tr>
<td>19.08</td>
<td>2.0100</td>
<td>0.4539</td>
<td>0.001</td>
</tr>
<tr>
<td>20.31</td>
<td>2.2100</td>
<td>0.4410</td>
<td>0.001</td>
</tr>
<tr>
<td>21.54</td>
<td>3.4900</td>
<td>0.2480</td>
<td>0.001</td>
</tr>
<tr>
<td>22.00</td>
<td>3.9687</td>
<td>0.1862</td>
<td>0.001</td>
</tr>
</tbody>
</table>

SSI = 4900

Reaction Rate = 1

Equilibrium Ca = 0.11

Limiting Porosity = 0.01

Calcite Molar Volume: \( 3.69 \times 10^{-5} \text{ [m}^3/\text{mol]} \)
MODE 7: Distribution Coefficient for Gas Phase

SYNTAX: DIST {GAS} {Φ} {func[ξ]} {N₁, N₂, .., Nₙ|fname} [subrgn]

GAS: The species is partitioned in equilibrium between the liquid and gas phases. The partitioning concentration, Cₙ, in the gas phase is given by:

\[ Cₙ = \rhoₙ kₙ C \]

Where \( \rhoₙ \) is the gas density, \( kₙ \) is a distribution coefficient and \( C \) is the concentration in the liquid phase. This \( kₙ \) is akin to the more usual Henry’s Law constant except that the coefficient is defined in a manner that is consistent with that used for the solid phase. **In this mode the density of the gas phase must be separately defined by user input.**

Φ: The symbol for the dependent variable for which the distribution coefficient for the gas phase is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

func: One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. The function specifies the value of the appropriate distribution coefficient for the corresponding \( \Phi \) variable. If no function is specified then the value is assumed to be constant.

ξ: One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,..,Nₙ: The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname: The name of the file containing the numerical values \( N₂ \) through \( N_n \). This option is available only for selected functions. See Section 3.3 for additional information.

subrgn: See Mode 1 specification.

COMMENT: This mode of the command is available only with the PORFLOW™ Simulation Tool. It is one of the means available in PORFLOW™ to incorporate the Henry’s Law for equilibrium phase partitioning. Non-linear equilibrium relations can also be implemented by functional forms of the distribution or retardation coefficients (see Mode 1 of DISTRIBUTION and STORAGE commands) and by the REACTION command.

EXAMPLES: Generic examples for this command are given in Section 4.4. The command keyword (DIST) must replace the keyword used in these examples and the modifier GAS must be specified.
MODE 8: Disable Storage or TransientTerm Completely

SYNTAX DIST {Φ}{OFF}

Φ The symbol for the dependent variable for which the distribution coefficient is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified.

OFF The storage term for the variable for whole of the flow field is completely omitted. In essence, the transient term in the governing differential equation is set to zero. A new Mode 1 specification may follow if storage term is to be reactivated.

EXAMPLES

DIST for C variable is now OFF
COMMAND  EBU

PURPOSE Specify the mixing limited rate and parameters for a given reaction using the eddy breakup model. This command is effective only for the ANSWER™ Software Tool.

MODE 1:  EBU Reaction Variables and Parameters

SYNTAX  EBU  {idreac} {Φ} [HARM] [C_EBU, α, β] [γ]

idreac Character string identifying the idreac reaction on the REACTION command that is limited by the eddy breakup (EBU) limit. To activate this limit, the modifier EBU must also appear in the corresponding REACTION command. The EBU reaction rate is computed from:

\[ R_{EBU} = C_{EBU} \frac{\varepsilon}{k} \Phi_{ebu}^{\text{rms}} \]

\[ \Phi_{ebu}^{\text{rms}} = \min(\Phi_1, \alpha \Phi_2, \beta \Phi_3) \].

If \( R_{KIN} \) is the kinetic reaction rate (see REACTION command), then the actual EBU-limited reaction rate for the idreac is defined by one of the following two options:

\[ R_{Actual} = \min(R_{KIN}, R_{EBU}) \], or

\[ R_{Actual} = \frac{R_{KIN} R_{EBU}}{\gamma R_{KIN} + (1 - \gamma) R_{EBU}} \].

The first equation is used for the default mode of the EBU-limiter whereas the second equation is used if the HARMONIC modifier is specified.

Φ One or more of the symbols in Table 2.8.1-3 which identify the EBU limiting species (\( \Phi_1 \), \( \Phi_2 \), or \( \Phi_3 \)). If no symbol is specified then the species participating in the corresponding REACTION command are used as the limiting species.

HARM By default, the actual reaction rate is computed as the smaller of the kinetic and EBU reactions. If this modifier is present then the harmonic limiter is used.

C_EBU The empirical constant, \( C_{EBU} \), in the \( R_{EBU} \) above. The default value is 3.

α, β The constants, \( \alpha \) and \( \beta \), in the EBU relation given above. The default value is unity.

γ The constant \( \gamma \) in the harmonic limiter as described below. It is the 2nd, 3rd or 4th numerical value on the command depending on whether 1, 2 or 3 symbols define the EBU model. The default value is 0.5.

EXAMPLES

EBU for R1 function of FU with constant = 3.0
EBU for R2 function of CH and O2, values = 3.0 and 0.3
EBU for R2 with CH and O2, 3.0, 0.3 with HARMONic limiter 0.75
EBU for R2 with FU CH and O2, 3.0, 0.5, 0.3 with HARMONic limiter 0.75
MODE 2: Global EBU Reaction Constants

SYNTAX EBU [C_{EBU}] [I_{EBU}]

C_{EBU} The global empirical constant, C_{EBU}, for the eddy breakup relations. This value is used if a value is not explicitly specified with a Mode 1 EBU command for a specific idreal reaction. The default value is 3.

I_{EBU} The first step of the solution procedure at which the EBU limit is invoked. Often at the initial stages of a solution process, the flow and turbulence fields are not well developed. In this case, it is preferable to use the kinetic reaction rate (the maximum possible) during the initial stage. The default value is 10.

EXAMPLES

EBU limit global rate constant = 3.2
EBU limit global rate constant is 3.2. Start at step number 20.
COMMAND   ELSE

PURPOSE   To define an IF construct to control which, if any, of one or two blocks of user input statements are executed.

SYNTAX    ELSE

COMMENTS  This command is part of the IF-ELSE-ENDIF construct; please see the IF command.
COMMAND  END

PURPOSE  To signify the end of a problem.

SYNTAX  END

COMMENTS

This command signifies the end of a problem. The input for a new problem may be continued with a new problem specification after this command. For each problem, this command must be employed as the last command. Failure to do so may cause a loss of some or all of the data and output files, depending on the host operating system.

EXAMPLES

END

END of problem number 1
<table>
<thead>
<tr>
<th>COMMAND</th>
<th>ENDIF</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To define an IF construct to control which, if any, of one or two blocks of user input statements are executed.</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>ENDI</td>
</tr>
</tbody>
</table>

**COMMENTS**

This command is part of the IF-ELSE-ENDIF construct; please see the IF command.
Keyword Commands

**COMMAND** FILE

**PURPOSE** To open and close input/output devices.

**SYNTAX** FILE [CLOS|OPEN] [fname] [attribute] [filetype|NUNIT]

- **CLOS** The specified file unit or I/O device is closed.
- **OPEN** The specified file unit or I/O device is opened. If the same file unit was previously open, then it is closed and the new unit with the specified name is opened.
- **fname** The name of the file to be opened or closed. See Section 3.3 for additional information. If **fname** is specified, then the named file, if connected to a unit, will be closed. If **filetype** or **NUNIT** refer to a different file unit, then that unit, if open, will also be closed. If the **OPEN** modifier is present, then a new file with the specified name will be opened and connected to the unit specified by **filetype** or **NUNIT**.
- **attribute** The attributes of the file to be opened. This input is ignored if **CLOSE** modifier is present.

<table>
<thead>
<tr>
<th>attribute</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>FORM</td>
<td>File is opened in the FORMATTED mode. This is the default option.</td>
</tr>
<tr>
<td>UNFO</td>
<td>File is opened in the UNFORMATTED mode.</td>
</tr>
<tr>
<td>UNKN</td>
<td>File status is defined as UNKNOWN. This is the default option.</td>
</tr>
<tr>
<td>NEW</td>
<td>File status is defined as NEW. An error will occur if the file already exists.</td>
</tr>
<tr>
<td>OLD</td>
<td>File status is defined as OLD. An error will occur if the file does not exist.</td>
</tr>
<tr>
<td>BOTH</td>
<td>File is available for both READ &amp; WRITE operations. This is the default option.</td>
</tr>
<tr>
<td>READ</td>
<td>File is available only for READ operations.</td>
</tr>
<tr>
<td>WRIT</td>
<td>File is available only for WRITE operations.</td>
</tr>
</tbody>
</table>

- **filetype** One of the modifiers below that identify the file to be opened or closed.

<table>
<thead>
<tr>
<th>filetype</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEBU</td>
<td>Debug output file (DEBUG), Unit 17, is selected for the operation.</td>
</tr>
<tr>
<td>FLUX</td>
<td>Flux output file (FLUX), Unit 14, is selected for the operation.</td>
</tr>
<tr>
<td>HIST</td>
<td>Time History file (HISTORY), Unit 13, is selected for the operation.</td>
</tr>
<tr>
<td>SAVE</td>
<td>The default Archive file (SAVE), Unit 11, is selected for the operation.</td>
</tr>
<tr>
<td>TRAC</td>
<td>Particle track file (TRACK), Unit 18, is selected for the operation.</td>
</tr>
</tbody>
</table>

- **NUNIT** The file or I/O device unit number for the file for which the operation is performed. The unit number is ignored if one of the **filetype** modifiers is present.

**COMMENTS**

In general FORTRAN language does not differentiate between lower and upper case characters. However that is not true of many operating systems (O/S). It is in fact the O/S that performs all file handling. O/S peculiarities have been reported where, for example, there was no case distinction for read/write operations but the O/S distinguished between upper and lower case for file closing. It is therefore strongly recommended that the user should be consistent in using the same case characters if a previous file is referred to during file operations.

**EXAMPLES**

- FILE OPEN 'mynewfile.now' on 37
- FILE OPEN OLD file 'mydatafile.now' on unit 37 in UNFORMatted READ only mode
- FILE OPEN NEW SAVE file 'mynewsavefile.now' on in FORMatted WRITe only mode
- FILE CLOSE SAVE HISTory file now
- FILE CLOSE file by name 'OLDFILE.TMP'
COMMAND       FIX

PURPOSE        To fix the values or the matrix coefficients of selected variables for a subregion within the domain of calculation.

MODE 1:       Fix Variable Values

SYNTAX        FIX [Φ] [subrgn]

Φ             One or more of symbols that denote the dependent variables for which the values are fixed for the selected subregion. Up to 20 symbols may be specified with one command. The valid symbols are listed in Table 2.7.1. If no symbol is specified, the values are fixed for all variables.

subrgn        The subregion for which the input is specified. If no subregion is specified, the entire computational domain is selected. See Section 3.4.

COMMENTS
This command can be used only to fix the values of a variable inside the domain of computation. The values at the domain boundary cannot be fixed by this command (the boundary values can be fixed by the BOUNDARY command). Multiple commands may be used to fix values in an arbitrary manner. The INITIAL, READ or SET commands may be used to define the variable values. Once specified, these values remain unchanged unless modified by a subsequent INITIAL, READ or SET command.

EXAMPLES
FIX T for active subregion at previously defined value
FIX P for subregion with ID=FREEstream
FIX P, T and C for subregion identified as ID = ID01
FIX values for all variables in ID=BLOCK
MODE 2: Fixed Matrix Coefficients for the Variable

SYNTAX

```plaintext
FIX  [Φ] [subrgn] {N₁, ..., Nₙ}; n=6 for 2D and 8 for 3D input mode
```

Φ
A symbol that denotes the dependent variable for which input is specified. The valid symbols are listed in Table 2.7.1. There is no default value.

subrgn
The subregion for which the input is specified. If no subregion is specified, the entire computational domain is selected. See Section 3.4.

N₁, .., Nₙ
The values of the matrix coefficients for the variable. For 2D simulation, with reference to the below figure, the actual value is computed according to the implicit formula:

\[
Φₚⁿ = N₁ + N₂ Φₚ + N₃ Φₚₚ + N₄ Φₚₚ + N₅ Φₚₕ + N₆ Φₚₕ
\]

where superscript 'o' denotes the existing value and 'n' denotes the new computed value. The subscripts P, W, E, S and N denote the node being computed and the nearest neighboring nodes in the X-, X+, Y- and Y+ directions, respectively.

For 3D simulation, the formula is:

\[
Φₚⁿ = N₁ + N₂ Φₚ + N₃ Φₚₚ + N₄ Φₚₚ + N₅ Φₚₕ + N₆ Φₚₕ + N₇ Φₚₜ + N₈ Φₚₜ
\]

where D and U denote the neighboring nodes in the Z- and Z+ directions, respectively, as shown in the figures below.
MODE 3: Disable Previously Specified Fixed Commands

SYNTAX

```
FIX {OFF} [Φ] [subrgn]
```

**OFF**

Previously specified FIX commands for Φ, for the identified subregion, are deactivated. A new specification for this subregion may follow. This command can only be used for previous FIX commands that appeared with no Φ symbol or only a single Φ symbol.

**Φ**

A symbol that denotes the dependent variable for which the input is specified. The valid symbols are listed in Table 2.7.1. There is no default value.

**subrgn**

The subregion for which the input is specified. If no subregion is specified, the entire computational domain is selected. See Section 3.4.

EXAMPLES

```
FIX T in ID=FIXD OFF
FIX T & P OFF for ID=FIX1
FIX all OFF in ID=FIXAll
```
Keyword Commands

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>FLOW</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To specify the flow rate and other dependent variables at a boundary.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>Flow Injection or Withdrawal with Fixed Variable Values</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>FLOW [TOTA [option] [func(ξ)] {N₁, N₂, .., Nₙ} fname] [Φ₁ = N₁+₁, .., Φₘ = Nₘ] [ρₛ] [subrgn] {dir}</td>
</tr>
<tr>
<td>TOTA</td>
<td>By default, the amount of flow specified, or computed from ( \text{func}(\xi) ), is applied to each element of the subrgn. If this modifier is present then the amount is assumed to be the total amount over whole of the subrgn. In this case, the amount is distributed equally to all the elements of the subrgn unless the VOLUME or AREA modifiers are present.</td>
</tr>
<tr>
<td>option</td>
<td>Options selected for implementation of the source.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>VOLU</td>
<td>In the absence of the TOTAL modifier, the flow for each element is computed as: ( Q = q \delta V ). Here ( q ) is the amount specified by the user and ( \delta V ) is the volume of the element. The ( q ), in turn, is computed from ( \text{func}(\xi) ) and ( N₁ ) through ( Nₙ ). If the TOTAL modifier is present, the amount for each element is computed as: ( Q = q \delta V/V ), where ( V ) is the volume of the total subrgn.</td>
</tr>
<tr>
<td>AREA</td>
<td>In the absence of the TOTAL modifier, the source for each element is computed as: ( Q = q \delta A ), where ( \delta A ) is the area of the element boundary indicated by dir. If the TOTAL modifier is present, the amount for each element is computed as: ( Q = q \delta A/A ), where ( A ) is the total area of the subrgn in the dir direction.</td>
</tr>
<tr>
<td>INTE</td>
<td>By default, if dir points to a wall, then any special treatment for that wall (such as wall function for turbulent flow) is deactivated and the diffusive flux at the wall is set to zero if the INTERNAL modifier is present then the wall treatment and wall diffusive flux are retained.</td>
</tr>
<tr>
<td>NORM</td>
<td>In the absence of the TOTAL modifier, the source, ( Q ), is computed as: ( Q = q \sum_{i} A_i \cdot V_i ) where ( A_i ) is the ( i )-th direction component of the element boundary area specified by dir. ( V_i ) are the values specified by ( Nₙ+₁ ) through ( Nₙ ) (2 for 2D, and 3 for 3D). In the presence of the TOTAL modifier, ( Q ) is computed in a manner identical to that for the AREA modifier.</td>
</tr>
<tr>
<td>DENS</td>
<td>The computed source, ( Q ), is further multiplied by density. The density may be specified as the last value, ( ρₛ ), on the command. The boundary value of density is overwritten by the specified value. If this value is omitted, then the existing boundary value at the node indicated by the dir direction is used.</td>
</tr>
</tbody>
</table>

**func**, One of the modifiers listed in Table 4.2.1 that denotes the functional form of the flow rate. If no function is specified, the value is assumed to be constant.

**ξ**, One of the independent variables listed in Table 4.2.2. If no independent variable is specified, the variable is assumed to be time.

**subrgn**, The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected.

**N₁, .., Nₙ**, The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

**fname**, The name of the file containing the numerical values \( N₁ \) through \( Nₙ \). This option is available only for selected functions. See Section 3.3 for additional information.

**Φ₁, .., Φₘ**, The dependent variables for the properties that are injected along with the flow such as heat(enthalpy or temperature) and concentration of species, etc.

**Nₙ+₁, .., Nₘ**, The corresponding values of \( Φ₁, .., Φₘ \) that are injected with the flow. Each of these values
must follow the symbol for the corresponding $\Phi$.

$\mathbf{N}_{m+1}, \ldots, \mathbf{N}_k$ The normalizing vector components, $V_i$, if the \texttt{NORMAL} modifier is present. These must be the last numerical values on the input command except for the value of the density (see below). Two values must be specified for 2D and 3 for 3D flows.

$\rho_B$ The density value that multiplies the computed source. It can only be specified if the \texttt{DENSITY} modifier is present and then it must be the last value on the command. If no value is specified but the modifier \texttt{DENSITY} is present, then default value is the boundary value at the node indicated by the \texttt{dir} modifier.

\texttt{dir} The orientation index for the element boundary associated with the source. See Section 3.5 for available choices. There is no default value for this input.

**COMMTPMENTS**

The \texttt{FLOW} command is primarily designed to allow injection of fluid through a solid boundary (or blocked region) inside the domain of computation. Its use is most appropriate when the scale of injection is comparable to the grid size. The command is implemented in terms of boundary “fluxes” entering the domain of computations. If the scale of injection is much smaller than the grid size, then the \texttt{SOURCE FLOW} command may be more appropriate. The injection at an exterior domain boundary is more appropriately accounted for by the \texttt{INLET} command.

In implementing this command it is assumed that at the point of injection, the boundary wall has essentially been removed. The computational treatment is akin to that for inflow such as through an \texttt{INLET} boundary. If the injection occurs through a blocked element or at an exterior boundary of the domain, then the injected values are also assumed to be the boundary values of the variables.

If the wall needs to be retained, such as for flow percolating through a solid matrix or through holes much smaller than the boundary area of the inflow element, then the \texttt{INTERNAL} modifier should be used.

**EXAMPLES**

Generic examples for this command are given in Section 4.4. The command keyword (\texttt{FLOW}) must replace the keyword used in these examples. Some additional examples that illustrate the use of the attributes specific to this command are given below.

\begin{verbatim}
FLOW injection: amount = 0.001 with T=50, C=1.
FLOW per unit AREA of X- face: = 0.001 with T=50, C=1.
FLOW withdrawal: amount =-0.001 per second
FLOW \texttt{TABLE} 3 sets \texttt{SELECTed} \texttt{(0, 0), (100, 1), (200, 0) U=1, V=0.1, W=0, T=10, K=0.001, L=1}
FLOW: \texttt{EXPO}nential series with \texttt{TIME} 7 sets from \texttt{‘SOURCE’ T=100, C=0}.
FLOW $q=10$ X- direction $T=100, U=20$. \texttt{NORMALized} velocity 0., 1.5, 2.5 \texttt{ID=VSOURce};
FLOW $q=-10$ in X- dir with \texttt{NORMALized} vel 1., 1.5, 2.5 and \texttt{DENSIty} for \texttt{ID=VSOURce}
FLOW $q=10$ X- dir variable values: $U=10, V=0, W=-20, T=100, K=0.03, L=0.5$ \texttt{INTErnal} with \texttt{NORMALized} vel 1., 1.5, 2.5 and \texttt{DENSIty} for \texttt{ID=VSOURce}:
FLOW $q=10$ per unit \texttt{VOLUme} injected variables: $U=10, V=0, W=-20, T=100, K=0.03, L=0.5$ multiply by \texttt{DENSIty} = 5 for \texttt{SELECTed region}
\end{verbatim}
**MODE 2:** Flow Injection with Fixed Variable Values and Computed Momentum Components

**SYNTAX**

```
FLOW {MOME} [TOTA] [option] [func(ξ)] {N1, N2, .., N_n} [fname] [Φ1=Ns1, .., Φ_m=N_m] [N_{m+1}, N_k] [ρ_B] [subrgn] {dir}
```

**MOME** Velocity components, \( V_j \), of the injected flow are computed from flow rate, \( Q \), for the element:

\[
V_j = \frac{Q}{\rho_B A} n_j,
\]

where \( \rho_B \) is the density, \( A \) is the area of the element boundary specified by the \( \text{dir} \) modifier, and \( n_j \) is a normalizing vector. If the \( \text{NORMAL} \) modifier is present, then \( n_j \) is obtained from the user input, otherwise the area unit vector (\( A_j/A \); where \( A_j \) is the component in the \( j^{th} \) direction) is used as the normalizing vector. By default the density is the fluid density at the boundary, unless the user specifies a value. Any velocity input given by the user is ignored.

**TOTA** See Mode 1 specification

**option** See Mode 1 specification. Unless the \( \text{NORMAL} \) modifier is present, it is assumed that the \( \text{AREA} \) modifier is in effect. Any specification of the \( \text{VOLUME} \) modifier is ignored. All other modifiers can be used as for Mode 1 Specification.

**func** See Mode 1 specification.

**ξ** See Mode 1 specification.

**N_1, .., N_n** See Mode 1 specification.

**fname** See Mode 1 specification.

**Φ_1, .., Φ_m** See Mode 1 specification.

**N_{m+1}, .., N_m** See Mode 1 specification.

**N_{m+1}, .., N_k** See Mode 1 specification.

**ρ_B** See Mode 1 specification.

**subrgn** See Mode 1 specification.

**dir** See Mode 1 specification. This modifier must be present for this mode of command.

**EXAMPLES**

All the examples cited for Mode 2, except those with \( \text{VOLUME} \) modifier, are applicable provided that the modifier \( \text{MOMENTUM} \) is added. Some illustrative examples specific to this mode are given below.

- **FLOW** with \( \text{MOMENTUM q=10 X- direction with ID=VSOURce; T=100, K=0.05, L=0.02} \)
- **FLOW** MOMENTum q=10 X- direction with ID=VSOURce; T=100, K=0.05, L=0.02, DENSity= 5
- **FLOW** MOMENTum q=10 X- direction with ID=VSOURce; T=100, K=0.05, L=0.02, NORMal 1. –1, 0
- **FLOW** MOMENTum q=10 X- ID=VSOURce; T=100, K=0.05, L=0.02, NORMal 1. –1, 0, DENSity=5.
- **FLOW** MOMENTum: TABLe 2 sets SELEct (0, 0), (100, 1) T=10, K=0.001, L=1
- **FLOW** MOMENTum EXPONential SERles TIME 7 sets ‘SOURCE’ T=100, C=0. NORMal 1. –1 SELEcted
- **FLOW** MOMENTum q=10 X- dir INTEmal for ID=VSOURce: injected variables: T=100, K=0.03, L=0.5 NORMalized vel 1., 1.5, -0.7 and DENSity as exists
MODE 3: Flow Injection at Fixed Spherical Angles with Computed Momentum Components

SYNTAX
```
FLOW {ANGL} [TOTA] [func[ξ]] {N1, N2, .., Nn}[fname] [Φ1=Nn+1, .., Φm=Nm] [Nm+1, ..., Nm+5][DENS|SPEE] [ρB|Vs][subrgn] {dir}
```

**ANGL**
Fluid is injected or withdrawn. The amount of the property of the injected (or withdrawn) fluid acts as the source or sink for each of the relevant properties. If the flow is injected, then the velocity component of the injected flow, \( U_i \) in the \( i^{th} \) direction, is either computed from the source flow rate, \( Q \), or determined from a specified injection speed, \( V_S \), as:

\[
U_i = \frac{Q}{\rho_B A} n_i \quad \text{or} \quad U_i = V_S n_i
\]

where \( \rho_B \) is the density at the neighboring element and \( A \) is the area of the element boundary specified by the \( \text{dir} \) modifier. The local direction vector, \( n_i \), for each segment of the surface is obtained from the user input of two spherical angles and a reference axis.

**TOTA**
See Mode 1 specification.

**func**
See Mode 1 specification.

**ξ**
See Mode 1 specification.

**N1, .., Nn**
See Mode 1 specification.

**fname**
See Mode 1 specification.

**Φ1, .., Φm**
See Mode 1 specification.

**Nm+1, .., Nm**
The spherical angle, \( Φ \) in degrees measured as the deflection of the injection vector from the face normal. The magnitude of the angle must be less than 180 degrees.

**Nm+2**
The spherical angle, \( Φ \) in degrees measured as the rotation of the injection vector with respect to the projection of the axis vector onto the face plane.

**Nm+3, ..., Nm+5**
The direction cosines of the axis vector used to measure the angle \( Φ \); 3 values must be specified since this option is only available for 3D flows.

**DENS**
The density, \( ρ_B \), is specified as the last value on the command.

**ρB**
See Mode 1 specification.

**SPEE**
The injection speed, \( V_S \), is specified as the last value on the command.

**Vs**
The value \( V_S \) if the \text{SPEED} modifier is present. There is no default value for this input.

**subrgn**
See Mode 1 specification.

**dir**
See Mode 1 specification.

EXAMPLES

All examples cited for Mode 1 are applicable provided that the modifier \texttt{ANGL} is added and appropriate input for spherical angles is appended. Some illustrative examples of the use of attributes specific to this mode are given below.

```
FLOW q=10, X- direction with ID=VSOURce; T=100, K=0.05, L=0.02, Theta=45, phi=20, axis=1., 0., 0
FLOW q=10, X- ID=VSOURce; T=100, K=0.05, L=0.02, Theta=45, phi=20, axis=1., 0., 0, SPEEd=120
FLOW q=10, X- ID=VSOURce; T=100, K=0.05, L=0.02, Theta=45, phi=20, axis=1., 0., 0, DENsity=2.5
```
**MODE 4:** Flow Injection with Multiple Tabular Functions

**SYNTAX**

\[
\text{FLOW \{Φ\} \{TABL\} \{MULT\} \{option\} \{N_{sets}\} \{N_1,...,N_n\}[fname][subrgn]}
\]

Φ  
One or more of the symbols that denote the dependent variables, which are specified as functions of time. There is no default value; at least one symbol must be specified.

TABL  
The variables are specified as tabular functions of time. This is the only available option in this mode.

MULT  
Multiple variables are tabular functions of time.

**option**  
See Mode 1 specification.

**N_{sets}**  
The number of sets of data for the tabular functions.

**N_1, ..N_n**  
The N_{sets} sets of data for the flow rate and variables as tabular functions of time. Each set must consist of time, flow rate, and one value for each variable specified by the symbol Φ on the command, in that order. Thus if 4 variables are selected, then each data set must consist of 6 values. There is no default value; the correct number of values must be specified. If the flow rate is negative (withdrawal of fluid), then specified value of the property is ignored since it is assumed that the fluid is being withdrawn with an amount of property equal to the local value of that property.

fname  
See Mode 1 specification.

subrgn  
See Mode 1 specification.

**EXAMPLES**

**FLOW with MULTiple TABLe functions: 4 sets**

<table>
<thead>
<tr>
<th>Time</th>
<th>Flow</th>
<th>U</th>
<th>V</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.001</td>
<td>1.00</td>
<td>0.02</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>0.002</td>
<td>0.50</td>
<td>0.01</td>
<td>200</td>
</tr>
<tr>
<td>2</td>
<td>0.004</td>
<td>2.00</td>
<td>0.01</td>
<td>500</td>
</tr>
<tr>
<td>5</td>
<td>0.010</td>
<td>5.00</td>
<td>0.02</td>
<td>600</td>
</tr>
</tbody>
</table>

**FLOW with MULTiple TABLe: 4 sets per unit VOLUme**

<table>
<thead>
<tr>
<th>Time</th>
<th>Flow</th>
<th>U</th>
<th>V</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.001</td>
<td>1.00</td>
<td>0.02</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>0.002</td>
<td>0.50</td>
<td>0.01</td>
<td>200</td>
</tr>
<tr>
<td>2</td>
<td>0.004</td>
<td>2.00</td>
<td>0.01</td>
<td>500</td>
</tr>
<tr>
<td>5</td>
<td>0.010</td>
<td>5.00</td>
<td>0.02</td>
<td>600</td>
</tr>
</tbody>
</table>
MODE 5: Flow Injection or Withdrawal at a Boundary

SYNTAX

FLOW {ONLY} [option] [func[ξ]] {N1, N2, ..., Nn} [fname] [subrgn]

ONLY

By default the injected (or withdrawn) flow is assumed to be accompanied by a specification of all other variables (properties) that are assumed to be automatically injected with it (see Mode 1 specification). If this modifier is present, then it is assumed that only the flow rate is specified by this command. The boundary flux of other variables is computed by a product of the injected flow and the prevailing value of the variable at the boundary node.

option
See Mode 1 specification.

func
See Mode 1 specification.

ξ
See Mode 1 specification.

N1, ..., Nn
See Mode 1 specification.

fname
See Mode 1 specification.

subrgn
See Mode 1 specification.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (FLOW) must replace the keyword used in these examples. Some additional examples that illustrate the use of the attributes specific to this command are given below.

FLOW T is TABLE per unit AREA in X-direction: 3 sets (TIME, value) (0., 0.01), (100., 0.10), (200, -0.20)
FLOW for T 10 per unit AREA in X-direction for SELECTed region
FLOW for T 10 per unit area in X-direction with NORMalized velocity of 0., 1.5, 2.5 ID=VFLOW
FLOW for T 10 in X-dir with NORMalized vel 1., 1.5, 2.5 and DENSity for ID=VFLOW
MODE 6: Disable Previously Specified FLOW commands

SYNTAX

FLOW \{Φ\} \{OFF\} \{subrgn\}

Φ See Mode 1 specification.

OFF Previous FLOW commands for the identified subregion are deactivated. A new specification may follow.

subrgn See Mode 1 specification.

EXAMPLES

FLOW OFF for T for most recently SELECTed region
FLOW OFF for T for ID=MIDDle
COMMAND FLUID

PURPOSE To specify thermal and transport properties of the fluid. This command is effective only for the PORFLOW™ and TIDAL™ Software Tools.

MODE 1: Fluid Compressibility

SYNTAX FLUI {COMP} [phase|SATU] {α}

COMP The compressibility of fluid is specified. The exact interpretation depends on the presence of the phase or SATU modifier. The compressibility is sued to compute the storage term in the continuity equation. This mode of input is applicable only for the PORFLOW™ Software Tool.

phase The fluid phase for which the input is specified. See Section 3.6 for available options. If no phase modifier exists, the input is assumed to be for the 1st phase of the fluid.

\[ \alpha_f = \frac{1}{\rho^n} \left( \frac{\partial \rho^n}{\partial P^n} \right) \]

In this equation, \( \alpha_f \) is the fluid compressibility, \( \rho \) is the density, \( P \) the pressure and superscript \( n \) denotes the phase of the fluid.

SATU This modifier is meaningful only for multi-phase flow simulation in PORFLOW™ Software Tool. However, if this modifier is present, the storage term also accounts for the changes in volume due to compression or expansion of the phase immediately “above” the one being simulated. In this case a term equal to:

\[ \alpha_s = \min \left( \frac{\partial S}{\partial p_c}, \alpha \right) \]

Where \( \alpha \) is user input value to set a minimum threshold for the computed phase saturation compressibility, \( \alpha_s \). \( S \) is the phase saturation and \( p_c \) is the corresponding capillary pressure.

\( \alpha_f \) The compressibility of the fluid; \( \alpha_f \) or the input for the minimum phase compressibility. The default value is zero.

EXAMPLES

FLUId COMPressibility is 5.E-10 for water
FLUId COMPressibility for SECond phase is 1.E-5
FLUId COMP due to SATURATION is 0.001
MODE 2: Fluid Enthalpy or Latent Heat

SYNTAX FLUI {LATE} {L}

LATE Latent heat of freezing option in PORFLOW™ is specified.
L The latent heat of phase change. The default value is 1000.

COMMENTS This mode of input is applicable only for the freezing option in PORFLOW™ Software Tool. For evaporation option, the specific heat-enthalpy relation must be specified. See the SPECIFIC HEAT command.

EXAMPLES FLUID LATENT heat of freezing is 1000
MODE 3: Specific Heat of the Fluid

SYNTAX FLUI {SPEC}

COND The input is for the specific heat of the fluid.

COMMENTS

This mode of the command has been superseded by the SPECIFIC HEAT command. Please refer to that command.
MODE 4: Thermal Conductivity or Mass Diffusivity of the Fluid

SYNTAX FLUI \{COND\}

COND The input is for the conductivity or diffusivity of the fluid.

COMMENTS
This mode of the command has been superseded by the CONDUCTIVITY command. Please refer to that command.
MODE 5: Fluid Density

SYNTAX FLUI {DENS}

DENS Density of the fluid is specified.

COMMENTS

This mode of the command has been superseded by the DENSITY command. Please refer to that command.
COMMAND  FLUX

PURPOSE  To compute and obtain output of the flux balance for a dependent variable for a selected subregion within the flow domain.

MODE 1: Computation and Output of Flux Balance for a Variable

SYNTAX  FLUX  {Φ} [subrgn] [dir] [fname] [TIME] [VFrq-File, VFrq] [NOW] [OLD]

Φ  One or more symbols for the dependent variables for which the flux-balance output is required. The valid symbols are listed in Table 2.7.1. There is no default value.

subrgn  The subregion for computations. If no subregion is specified, the entire domain is selected.

dir  The orientation index for the boundary for which the flux output is required. See Section 3.5 for available choices. There is no default value for this input. In this case the convective and diffusive fluxes at the selected boundary are written to both the flux file and the standard output file in a tabulated form at the end of computations.

fname  The name of the output file. If no name is specified then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by "_FLUX.TMP". For example, if the Standard Output file is "PROBLEM.OUT", then the file is named "PROBLEM_FLUX.TMP". At any time only one flux file can be open. Output from all active commands is directed to this file. If a new file name is given, then the previous file is closed and output from all active FLUX commands is directed to the new file.

TIME  By default, VFrq-File and VFrq are interpreted as the frequency of output in terms of number of steps. If this modifier is present, then VFrq-File and VFrq are interpreted to be the time interval between successive outputs.

VFrq-File  The frequency (step or time interval) at which the fluxes are written to the flux file specified by 'fname'. See Section 3.7 for further details. The default value is 1.

VFrq  The frequency (step or time interval) at which a summary of flux balance is written to the standard output file (file unit 16; see Section 2.4) where is this reference in a manner similar to VFrq-File. The default value is such that a summary of fluxes is obtained only at the end of simulations.

NOW  A flux record is written immediately both to the flux output file and the standard output device.

OLD  The flux record to the flux file is written in the old format which has now been replaced. This modifier affects only the output to the file named by the fname modifier. It does not affect the output of fluxes to the Standard Output Unit. The use of this modifier is not recommended; it is retained only for compatibility with archived data sets and output.

COMMENTS

All fluxes in ACRi Software are defined so that a flux ENTERING the computational domain (or a subregion) is POSITIVE and that LEAVING the domain is NEGATIVE.

The flux for mass is reported under the flux balance for pressure (P) since the continuity equation is solved in terms of pressure.

By default, the flux balance for each relevant dependent variable is automatically computed for the whole domain. This command can be used to obtain fluxes for additional subregions, to control the output, and to deactivate the flux computations in a selective manner. If no FLUX command is specified, then the summary of the flux balances is still directed to the standard output file at the end of computations. The output to the flux file, on the other hand, is generated only if a FLUX command is explicitly specified.
The flux balance output produced by ACRi Software Tools consists of cumulative fluxes for the subdomain and instantaneous fluxes crossing the boundaries. The flux balance for a variable is composed of cumulative changes due to storage ($Q_O$ and $Q_N$), inflow ($Q_{in}$), outflow ($Q_{out}$), and decay ($Q_{decay}$). The flux balance disparity, $Q_d$, is defined as:

$$Q_d = (Q_O - Q_N) + Q_{in} - Q_{out} - Q_{decay} + Q_{move},$$

where $Q_O$ is the amount of property present originally, $Q_N$ is the amount present now, and $Q_{in}$, $Q_{out}$ and $Q_{decay}$ are the cumulative inflow, outflow, decay, respectively. $Q_{move}$ is the net influx due to moving or evolving sub-regions.

The $Q_{in}$ and $Q_{out}$ are, in turn, each composed of three components:

$$Q = Q_{conv} + Q_{diff} + Q_{so}.$$

Here $Q_{conv}$ and $Q_{diff}$ denote the cumulative contributions due to convective and diffusive fluxes, respectively, and $Q_{so}$ denotes the net input due to sources (inflow – outflow).

All ACRi software allows arbitrary user specified units. The actual units for the reported fluxes therefore depend on the units selected by the user. For an arbitrary property, $\Phi$, the units of the cumulative flux are the units of $\Phi$ multiplied by the units of the density ($\rho$) and the units of volume ($L^3$). For PORFLOW the fluxes for mass and transport species (but not heat) are further divided by the density of the fluid; therefore these are in volumetric rather than mass units. The units of the instantaneous fluxes are those of the cumulative fluxes divided by units of time.

A more detailed description of each of the components that are reported in the flux output is given in the table that follows on the next page. In this table:

1. Fluxes in Items 4 through 21 are in cumulative units. For flow (pressure) equation these are in terms of mass units (e.g. kg) for ANSWERTM and TIDAL™, and in terms of volume units (e.g. $m^3$) for PORFLOW™. For thermal transport, the flux is reported in units of heat (e.g. J). For transport equation of a species, if the property is expressed in units of kg/m$^3$, then the flux balance is in terms of kg.
2. The instantaneous fluxes in Item 22 through 24 are in rate units. The units of these are the units of the cumulative flux expressed per unit time. In fact, the cumulative flux is the time integral of the instantaneous flux.

**EXAMPLES**

| FLUX for U for the entire domain |
| FLUX for T for SELECTed region every 20 steps |
| FLUX for V in SELECTed region: file every 20 steps; printer every 4 steps |
| FLUX balance for T for subregion defined by ID=VAULT every 200 steps |
| FLUX for T at XY plane defined by ID=PLN1 print every 10 steps |
| FLUX balance for T NOW for whole of the domain |
| FLUX balance for T for ID=VAULT OFF |
| FLUX for U to ‘FLUX.OUT’ for SELECTed region at TIME interval of 0.4 |
### Terms and Notation Used to Report Flux Balance in Output

<table>
<thead>
<tr>
<th>#</th>
<th>Term and Notation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Active Subdomain:</td>
<td>Particulars of the Sub-domain for which Flux Balance is given</td>
</tr>
<tr>
<td>2</td>
<td>Subdomain ID:</td>
<td>ID assigned to the Sub-domain by the user or the default ID automatically assigned if none given by User</td>
</tr>
<tr>
<td>3</td>
<td>Time:</td>
<td>The simulation Time at which the flux summary is computed</td>
</tr>
<tr>
<td>4</td>
<td>Net flux disparity (Qin-Qout-Qa-Qdecay)</td>
<td>The total “disparity” or “error” in the subregion. It is a sum of the total inflow minus the total outflow for the system</td>
</tr>
<tr>
<td>5</td>
<td>Total inflow (Qin = Qc_in+Qd_in+Qsor)</td>
<td>Total inflow into the subregion by convective flux (Item 11), diffusive flux (Item 12) and incoming (or positive) Sources (Item 13)</td>
</tr>
<tr>
<td>6</td>
<td>Total outflow (Qout = Qc_out+Qd_out+Qsnk):</td>
<td>Total outflow from the subregion by convective flux (Item 14), diffusive flux (Item 15) and Sinks or outgoing (or negative) Sources (Item 16)</td>
</tr>
<tr>
<td>7</td>
<td>Net accumulated gain (Qa = Qn-Qo)</td>
<td>Net increase in the amount of property (storage) in the subregion from the start of simulations.</td>
</tr>
<tr>
<td>8</td>
<td>Decay from start (Qdecay)</td>
<td>Net accumulated decay in the property in the subregion from the start of simulations.</td>
</tr>
<tr>
<td>9</td>
<td>Total initial property in region (Qo)</td>
<td>Initial amount of property present in the subregion at start of simulations.</td>
</tr>
<tr>
<td>10</td>
<td>Total property in region now (Qn)</td>
<td>Amount of property currently present in the subregion.</td>
</tr>
<tr>
<td>11</td>
<td>Convective influx (Qc_in):</td>
<td>Net inflow of property due to convection from all boundaries of the subregion from the start of simulations.</td>
</tr>
<tr>
<td>12</td>
<td>Diffusive influx (Qd_in):</td>
<td>Net inflow of property due to diffusion or dispersion from all boundaries of the subregion from the start of simulations.</td>
</tr>
<tr>
<td>13</td>
<td>Source influx (Qsor):</td>
<td>Net inflow of property due to sources in the subregion from the start of simulations.</td>
</tr>
<tr>
<td>14</td>
<td>Convective outflux (Qc_out)</td>
<td>Net outflow of property due to convection from all boundaries of the subregion from the start of simulations.</td>
</tr>
<tr>
<td>15</td>
<td>Diffusive outflux (Qd_out)</td>
<td>Net outflow of property due to diffusion or dispersion from all boundaries of the subregion from the start of simulations.</td>
</tr>
<tr>
<td>16</td>
<td>Sink outflux (Qsnk):</td>
<td>Net outflow of property due to sources or sinks in the subregion from the start of simulations.</td>
</tr>
<tr>
<td>17</td>
<td>Flux disparity due to mass balance (div*F)</td>
<td>Error in flux balance due to the fact that the flow field itself may not be mass conservative. This is included in the total disparity reported in Item 4 above. The error in flux balance can be both due to the error in the flow and that in the solution of the transport equation.</td>
</tr>
<tr>
<td>18</td>
<td>Convective Influx from Blocks</td>
<td>The inflow from the blocked areas of computational domain that were defined by the BLOCK or LAND command.</td>
</tr>
<tr>
<td>19</td>
<td>Diffusive Loss to Blocks</td>
<td>The diffusive/conductive outflow to the blocked areas of computational domain that were defined by the BLOCK or LAND command.</td>
</tr>
<tr>
<td>20</td>
<td>Influx due to Sub-domain Movement</td>
<td>The inflow due to movement of regions that evolve or move during simulation and change their nature of position.</td>
</tr>
<tr>
<td>21</td>
<td>Change from last time step</td>
<td>Change in the amount for property from the last time step</td>
</tr>
<tr>
<td>22</td>
<td>Instantaneous convective flux (in-out):</td>
<td>The current net inflow of convective flux at all boundaries of the subregion.</td>
</tr>
<tr>
<td>23</td>
<td>Instantaneous diffusive flux (in-out):</td>
<td>The current net inflow of diffusive flux at all boundaries of the subregion.</td>
</tr>
<tr>
<td>24</td>
<td>Instantaneous source-sink:</td>
<td>The current net inflow of property due to sources in the subregion.</td>
</tr>
</tbody>
</table>
MODE 2: Convective Flux and Flux-Average Value of a Variable

SYNTAX  

\[ \text{FLUX} \{ \text{AVER} \} \{ \Phi \} \{ \text{option} \} \{ \text{subrgn} \} \{ \text{dir} \} \{ \text{fname} \} \{ \text{TIME} \} \{ \text{V}_{\text{Frq}} \} \{ \text{NOW} \} \{ \text{OFF} \} \]

**AVER**  
The convective flux and the flux-weighted mean of the variable, its average, minimum and maximum values, the flow rate and, area at the selected boundary (or boundaries) are printed to the output device or file.

**Φ**  
One or more symbols for the dependent variable for which output is required. Up to 10 symbols may be specified per command. The valid symbols are listed in Table 2.8.1-3. If no symbol is specified then output is obtained for each active variable.

**option**  
The boundary type for which output is required. More than one option may be selected. If an option is specified, then the **subrgn** and **dir** modifiers are ignored. If no option is specified, then the averages are computed for the specified **subrgn** and **dir** modifiers.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>INLE</td>
<td>Boundaries specified by the INLET command are selected.</td>
</tr>
<tr>
<td>OUTL</td>
<td>Boundaries specified by the OUTLET command are selected.</td>
</tr>
<tr>
<td>OPEN</td>
<td>Boundaries specified by the OPEN command are selected.</td>
</tr>
<tr>
<td>IO</td>
<td>All boundaries specified by INLET, OUTLET or OPEN command are selected.</td>
</tr>
<tr>
<td>WALL</td>
<td>Walls specified by WALL or BLOCK command are selected.</td>
</tr>
<tr>
<td>EXTE</td>
<td>All external (or outer) boundaries of the computational domain are selected.</td>
</tr>
<tr>
<td>ALL</td>
<td>All of the above boundaries are selected.</td>
</tr>
</tbody>
</table>

**subrgn**  
The subregion for computations. This specification is ignored if any of the **option** modifiers is present. If no subregion is specified, the entire domain is selected.

**dir**  
The orientation index for the boundary for which the output is required See Section 3.5 for available choices. If no input is given, then the output is obtained for all boundaries of the **subrgn**. This specification is ignored if any of the **option** modifiers is present.

**fname**  
The file name for output. If a file name is specified then the output is directed to the named file, otherwise the output is directed to the standard output device. The total number of open files in any simulation cannot exceed 64.

**TIME**  
By default \( V_{\text{Frq}} \) is interpreted as the frequency of output in terms of number of steps. In the presence of **TIME** this is the time intervals between successive outputs.

**V_{Frq}**  
The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the output is obtained only at the end of simulations.

**NOW**  
A record of fluxes is written to the output device at the next time step when the equation for the dependent variable is solved. This is in addition to the output from the \( V_{\text{Frq}} \) specification.

**OFF**  
Any previously specified **FLUX AVERAGE** commands for the specified variables and subregion are disabled. New commands may be subsequently specified.

**EXAMPLES**

- FLUX AVERage for ALL boundaries
- FLUX AVERage for T (temperature) at IO boundaries
- FLUX AVERage for T (temperature) at INLET and OPEN
- FLUX AVERage for T at INLET and BOUNDaries
- FLUX AVERage for T at ALL on file 'FLUX.FIL'
- FLUX AVERage for T at ALL every 5 steps to file 'FLUX.FIL'
- FLUX AVERage for T at ALL at TIME=0.01 to file 'FLUX.FIL'
- FLUX AVERage to file 'FLUX.FIL' every 1 step
MODE 3: Disable Previously Specified Mode 1 Flux Balance Computations

SYNTAX

\[ \text{FLUX \{OFF\} \{Φ\}\{subrgn\}} \]

OFF

Any previously specified flux balance command for the specified variable and subregion is disabled. New FLUX commands may be subsequently specified.

Φ

The symbol for the dependent variable for which the previously specified flux-balance computation is disabled. The valid symbols are listed in Table 2.7.1. One and only one character string must be specified for each command.

subrgn

The subregion for flux computations. If no subregion is specified, the entire domain is selected.

EXAMPLES

- FLUX balance computation OFF for T for whole domain
- FLUX computations OFF for T for the currently active subregion
- FLUX computations OFF for T for the ID=UPPER
MODE 4: Disable Default Flux Balance Computations

SYNTAX FLUX \{OFF\}

OFF By default the flux balance is computed automatically, for the whole of the computational domain, for each variable for which a transport equation is solved. This is in addition to any flux balance computation in response to FLUX commands for that variable. If this modifier is present, then the automatic flux computations are disabled with one exception. The exception is the mass balance equation, for which the flux balance is always computed irrespective of the user input.

EXAMPLES

FLUX balance computation OFF for all variables except mass
FLUX default computations OFF
FLUX OFF
**COMMAND** FOR

**PURPOSE** To select the soil or rock material types or soil/rock zones to which the property information following the FOR specification is applicable.

**SYNTAX** FOR \{N1\}

**N1** The material type number to which the property specification applies. The maximum number of material type is set by default to be 10240.

**COMMENTS**

This command is being retained temporarily only for backward compatibility. Its function has been superseded by the specification of \(\text{ID}=\text{idsub}\) on the input commands. The use of this command is not recommended.

The property information to which this command applies is specified through the HYDRAULIC, MULTIPHASE, ROCK, SOIL, THERMAL and TRANSPORT commands. The input remains effective for subsequent property commands until another FOR command is encountered.

**EXAMPLES**

FOR material type 3 properties are specified by the following commands
COMMAND   FRACTURE

PURPOSE Define embedded fractures in the porous matrix. This command is effective only for the PORFLOW™ Software Tool.

MODE 1: Specification of a Fracture with Arbitrary Orientation

SYNTAX   FRAC {ID=subrgn} {Wfrac} [func[ξ]] [N1, N2, .., Nn] [fname] [ADJU] [DETA]

FRAC The material type designation is for a fracture. This feature is only available with the structured grid mode of PORFLOW™.

ID The modifier to indicate that the input is for a previously defined subregion.

subrgn The subregion in which the fracture is located. The subregion must be previously specified by a LOCATE FRACTURE command.

Wfrac Nominal width of the fracture which may be replaced by a computed value if the function is specified on the command. There is no default value; a value > 0 must be specified.

func One of the modifiers listed in Table 3.4 that denotes the functional form for fracture width. If no function is specified, the value is assumed to be constant.

ξ One of the independent variables listed in Table 4.2.2.

N1,...,Nn The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname The name of the file containing the numerical values N2 through Nn. This option is available only for selected functions. See Section 3.3 for additional information.

ADJU If this modifier is present, and a functional form for the width is specified, then the hydraulic conductivity of the fracture is modified as a cubic function of the width.

DETA If this modifier is present, then a detailed table of the elements and faces that form the fracture is printed out to the Standard Output Device.

COMMENTS This mode of the command allows the specification of a fracture with arbitrary orientation. See the LOCATE FRAC command for further details. This type of fracture can evolve with time in its own plane if the MOVE modifier is present on the corresponding LOCATE FRAC command and one or more MOVE commands are specified for the evolution of the fracture with time.

The fracture properties must be specified with the POROSITY, HYDRAULIC, THERMAL, TRANSPORT and DENSITY SOLID commands. Functional options for corresponding properties that apply to the porous matrix are not available for fractures. Specification of solid density is optional; other input must be specified if the corresponding transport equation is solved. If solid density is not specified, it is set equal to the porous matrix density at the 1st fracture element.

EXAMPLES

FRACTURE ID=FRACTURE_01 width = 0.1; print DETAIL
FRACTURE ID=UPPER_FRAC width = 0.1; varies LINEARLY 0.1 + 0.0001 * P; ADJUST K_hydraulic
Keyword Commands

MODE 2: Specification of a Fracture Aligned with Principal Axis

SYNTAX

FRAC {ID=subrgn} \{W_{frac}\} \{func[\xi]\} \{N_1, N_2, ..., N_n, fname\} \{INCL \{dir\{ALL|NONE\}\}\{ADJU\}\{DETA\]

FRAC

The material type designation is for a fracture. This feature is only available with the structured grid mode of PORFLOW™.

ID

The modifier to indicate that the input is for a previously defined subregion.

subrgn

The subregion in which the fracture is located. The subregion must be previously specified by a suitable LOCATE command without the FRAC modifier. The subregion must be such that a continuous path exists for the flow. It is best to use a index (LOCATE IJK) or coordinate (LOCATE COOR) based window for this subregion.

W_{frac}

Nominal width of the fracture which may be replaced by a computed value if the function is specified on the command. There is no default value; a value > 0 must be specified.

func

One of the modifiers listed in Table 4.2.1 that denotes the functional form for fracture width. If no function is specified, the value is assumed to be constant.

\xi

One of the independent variables listed in Table 4.2.2.

N_1, ..., N_n

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname

The name of the file containing the numerical values N_2 through N_n. This option is available only for selected functions. See Section 3.3 for additional information.

INCL

BY default only the boundary faces in the principal direction (determined from the LOCATE command) are included in the definition of the fracture faces. If this modifier is present, together then the boundary faces specified are included based on the dir, ALL or NONE modifier.

dir

One of the direction modifiers (X-, X+, Y-, Y+, Z-, Z+) which indicates the face to be included if the INCL modifier is present.

ALL

All boundary faces in the sub domain are included if the INCL modifier is present.

NONE

No boundary faces in the sub domain are included if the INCL modifier is present.

ADJU

See Mode 1.

DETA

See Mode 1.

COMMENTS

This is an older mode of specifying fracture which is retained for backward compatibility. **Mode 1 should be used which allows arbitrary orientation.** This type of fracture can evolve with time in its own plane if the MOVE modifier is present on the corresponding LOCATE command and one or more MOVE commands are specified for the evolution of the fracture with time.

EXAMPLES

FRACture ID=FRACTURE_X width = 0.1
FRACture ID=FRACTURE_X width = 0.1; varies LINEARLY 0.1 + 0.0001 * P; ADJUST K_hydraulic
COMMAND  FRICTION

PURPOSE  To specify the bottom friction or wind stress coefficients. This command is effective only for the TIDAL™ Software Tool.

MODE 1:  Bottom Friction Coefficients

SYNTAX  FRIC [MANN|CHEZ], {Cf1}, [Cf2]

MANN  By default the bottom friction coefficient is assumed to be constant. If this modifier is present then the bottom friction is calculated according to Manning's formula.

\[
C_f = g \left( \frac{C_{f1}}{C_{f2}} \right)^{2} \frac{1}{H^{1/3}}
\]

In the above relation, \( g \) is the constant of gravitational acceleration and \( H \) is the total depth of water.

CHEZ  If this modifier is present then the bottom friction is calculated according to Chezy's formula.

\[
C_f = \frac{g}{C_{f1}^{2}} \left( C_{f2} + \frac{1}{\sqrt{H}} \right)^2
\]

\( C_{f1} \)  When no modifier is present then this value is equal to the bottom friction coefficient that appears in the momentum equations. When either MANN or CHEZ is present it is equal to \( C_{f1} \) of the respective formula. The default value is 0.02.

\( C_{f2} \)  When no modifier is present this input is ignored. When either MANN or CHEZ is present it is equal to \( C_{f2} \) of the respective formula. The default value is 1.0.

COMMENTS  This command is implemented only for the TIDAL™ Software Tool.

EXAMPLES

FRICtion coefficient on the bottom: 0.003
FRICtion coefficient on the bottom: 0.003
FRICtion coefficient CHEZy's formula: cf1=0.001, cf2 =1.
FRICtion coefficient MANNing's formula: cf1=0.01, cf2 = 1.5.
**MODE 2:** Specification of Wind Stress Coefficients and Reference Wind Speed

**SYNTAX**

FRIC (WIND) \( [C_{w1}, C_{w2}, w_0] \)

**WIND**

The input is for the wind stress coefficients at a given wind speed, \( W \), according to the formula given below.

\[
C_w = C_{w1} + C_{w2} \{ \max [0, (1 - \frac{w_0}{W})^2] \},
\]

- **\( C_{w1} \)**: Linear component of wind stress coefficient, \( C_{w1} \), in the equation given above. The default value is \( 1.0E-6 \).
- **\( C_{w2} \)**: Non-linear component of wind stress coefficient, \( C_{w2} \) in the equation given above. The default value is \( 1.4E-6 \).
- **\( w_0 \)**: Reference wind speed, \( w_0 \) in the equation given above. The default value is \( 7.0 \).

**EXAMPLES**

FRICtion parameters for WIND:\( C_{W1} = 2.4E-6, C_{W2} = 0.00, w_0 = 0 \) m/s

FRICtion - WIND parameters: all values are set to zero
COMMAND  FUEL

PURPOSE  To specify the amount of carbon and hydrogen in the fuel, and the fuel enthalpy. This command is effective only for the ANSWER™ Software Tool.

SYNTAX  FUEL  \{N_C, N_H\} [H_C]

N_C  The fuel for a combustion process is assumed to have a chemical formula of the type C_nH_m. The N1 (>0) specifies the number of carbon atoms n. The default value is 10.

N_H  The number of hydrogen atoms (>0), the m in the fuel formula. The default value is 19.

H_C  The lower heat of combustion (>0), energy per unit mass; for fuel in J/kg. The default value is 4.50E7.

EXAMPLES

FUEL formula C=8 H=18
FUEL formula C=8 H=18: heat of combustion 5.788E7
FUEL is equivalent to C=10.25, H=20.5
Keyword Commands

COMMAND  GAS

PURPOSE To specify composition and properties of the gas phase. This command is effective only for the ANSWER™ and PORFLOW™ Software Tools.

MODE 1: Gas Molecular Weights for Gas Constituents

SYNTAX  GAS  \{ [\Phi_1=N_1, \Phi_2=N_2, ..., \Phi_n=N_n] \}

\Phi_n One or more of the symbols for gas constituents for which the molecular weights are specified. The valid symbols are problem dependent and may be selected by the user from the list of default dependent variables or those defined by the user. The user may define up to 64 gas constituents.

N1, .., Nn Molecular weights (> 0) for the variables in the order of the symbols. There are no default values; appropriate values must be specified. If a single numerical value is specified without any symbol then it is assumed that the value specifies the molecular weight of the default gas, which is assumed to be the 1st defined transport variable.

COMMENTS

If this mode of the command is missing then by default the gas is defined to be single species gas with a molecular weight of 29. The one exception to this rule is the ANSWER™ Software Tool if a REACTION command is given with default chemical reactions. In this case 8 gas species are automatically defined; these are FU, CH, O2, CO, CO2, H2, H2O and N2.

EXAMPLES

GAS molecular weights: H2O=18, CO2=44, N2 = 28, O2=32
GAS molecular weight is 18! Gas species by default
MODE 2: Gas Datum and Reference Pressure

SYNTAX GAS {PRES|P} {V1} [V2]

PRES The reference datum gas pressure, $p^*$, is specified.

P Same as the modifier PRES above.

V1 The datum pressure for the fluid. All pressure values, including the initial and boundary values, are relative to this pressure. This pressure will be added to the gas pressure to compute the absolute gas pressure if the gas density law is invoked. The default value for the datum pressure is 101325 for incompressible mode of computations but 0 for compressible mode of computations.

V2 This value is read only if the compressible mode of computations is invoked. In this case, it is interpreted as the reference value of the gas pressure which is required for some of the computations (such as the droplet evaporation correlations) where the ratio of the gas pressure to the atmospheric pressure is required. If this value is not specified, then the reference gas pressure is computed as the average of the specified initial pressure.

For incompressible flow, the reference gas pressure is set equal to the datum pressure.

EXAMPLES

GAS datum PRESSure is 2.5E5
GAS datum P is 2.5E5
GAS P = 0, Datum=0., reference value = 1.E6
Keyword Commands

MODE 3: Gas Sonic Speed and Specific Heat Ratio

SYNTAX GAS {SONI|GAMM} {V1}

SONI The sonic speed for the gas is specified. This may be used to compute the Mach number of the flow (see the OPTION command).

GAMM \( \gamma \), the ratio of specific heat at constant pressure to that at constant volume is specified. This constant may be used to compute the Mach number of the flow (see the OPTION command).

V1 The reference sonic speed or \( \gamma \) for the gas. The default value is 300 for the sonic speed and 1.4 for the ratio of specific heats (\( \gamma \)).

EXAMPLES

GAS SONIC speed is 275 m/s
GAS GAMMA is 1.2
MODE 4: Universal Gas Constant

SYNTAX GAS {CONS} [func[ξ]] [N₁, N₂, ..., Nₙ] fname

CONS The universal gas constant, R, used to compute fluid density and other gas properties.
func One of the modifiers listed in Table 4.2.1 which denotes the functional form of the gas constant. If no function is specified, then the gas constant is assumed to be fixed.
ξ One of the independent variables listed in Table 4.2.2. If no variable is specified, the independent variable is assumed to be time.
N₁,...,Nₙ The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.
fname The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (GAS) must replace the keyword used in these examples. Some additional examples are given below.

GAS CONStant is 1545!!! ft lbf/lb-mole R
GAS CONStant is LINEar function: 30. -0.015 * P
GAS CONStant POLynomial in P: (10., 0.5, 0., -0.1, 0.)
GAS CONStant is a TABLe in P: 3 sets: (0., 0.01), (100., 0.10 ), (200, -0.20)
**COMMAND**  
GEOMETRY

**PURPOSE**  
To modify or specify the geometry for the computational domain.

**MODE 1:**  
Exchange Previously Specified Coordinates

**SYNTAX**  
GEOM {EXCH} \{dir\1} \{dir\2}

**EXCH**  
The coordinates in the two directions specified by dir\1 and dir\2 are exchanged with each other. For example, with x and y as the specified directions, the new x and y coordinates at a point will be equal to the old y and x coordinates, respectively, at that point. For an orthogonal grid this effectively results in a rotation of the coordinate system by 90 degrees.

**dir\1, dir\2**  
Two of the X, Y, Z, R or THETA modifiers that, respectively, denote the x, y, z, r or \(\zeta\) coordinates to be exchanged with each other.

**EXAMPLES**

- GEOMETRY EXCHANGE X and Y
- GEOMETRY EXCHANGE X and R
- GEOMETRY EXCHANGE X and Z
MODE 2: Rotate Previously Specified Coordinates

SYNTAX

GEOM {ROTA} {dir1} {dir2} [φ₁, φ₂]

ROTA

The coordinates in the two directions specified by dir₁ and dir₂ are rotated in the plane defined by dir₁ and dir₂ by φ₁ and φ₂ degrees, respectively, according to the following equations:

\[
X_{\text{New}} = X_{\text{Old}} \cos φ₁ + Y_{\text{Old}} \cos φ₂
\]

\[
Y_{\text{New}} = X_{\text{Old}} \sin φ₁ + Y_{\text{Old}} \sin φ₂
\]

dir₁, dir₂

Two of the X, Y, Z, R or THETA modifiers that, respectively, denote the x, y, z, r or θ coordinates to be rotated in the plane defined by dir₁ and dir₂.

φ₁

The angle φ₁ (in degrees) for the transformation defined above. For a rectangular system, it represents the angle between the old and the new x-direction coordinates. The default value is 0 degrees.

φ₂

The angle φ₂ (in degrees) for the transformation defined above. For a rectangular system, it represents the angle between the old x-direction and new y-direction coordinates. If no value is specified then N₂ = N₁ + 90 degrees.

EXAMPLES

GEOMetry ROTAt e X and Y by 45 degrees
GEOMetry ROTAt e X by 45 and Y by 135 degrees!! same as above
GEOMetry ROTAt e X and Y by -45 deg.
GEOMetry ROTAt e X and Y 30 and Z by 115 degrees from old x-axis
MODE 3: Scale Previously Specified Coordinates

SYNTAX

GEOM {SCAL} {dir} { VMult } [ VAdd ]

SCAL

The coordinates in the direction(s) specified by dir are scaled according to the following equation:

\[ X_{\text{New}} = X_{\text{Old}} \times V_{\text{Scale}} + V_{\text{Add}} \]

dir

One or more of the X, Y, Z, R or THETA modifiers that, respectively, denote the x, y, z, r or \( \zeta \) coordinates each of which is scaled according to the equation given above.

VMult

The multiplication factor for the transformation defined above. There is no default value; a value must be specified.

VAdd

The offset for the coordinate. The default value is 0.

EXAMPLES

GEOMetry SCALe X by 0.3048
GEOMetry SCALe X by 0.3048 add 1.00
GEOMetry SCALe X and R by 0.3048 add 1.00
GEOMetry SCALe X, Y and Z by 0.3048 add 1.00
MODE 4: Generate Cylindrical Geometry in r-θ Plane

SYNTAX

GEOM {CYLI|CIRC} (R) [Θ₁, Θ₀]

CYLI

Generates a cylindrical grid for the computational domain in the r-θ plane.

CIRC

Same as CYLI modifier.

R

The radius of the cylinder. There is no default value; a value must be specified.

Θ₁

The angle of the cylinder circumference in degrees. The default value is 180 degrees.

Θ₀

The starting angle from the origin for the cylinder in degrees. The default value is 0 degrees.

COMMENTS

This command is available only if the computational domain is located in the 1st or 2nd quadrant.

EXAMPLES

GEOMetry is CYLIndrical with radius = 1.
GEOMetry is CIRCular with r = 1, theta = 90
GEOMetry is CYLIndrical with radius = 1., theta = 90
GEOMetry is CYLIndrical with r = 1., theta = 90, alpha=90
MODE 5: Generate Annular Geometry in \( r - \theta \) Plane

SYNTAX

\[
\text{GEOM} \{\text{ANNU}\} \{R_o\} \{R_i, e, \theta_1, \theta_0\}
\]

ANNU

Generates an annular geometry for the computational domain in the \( r - \theta \) plane.

\( R_o \)

The outer radius of the annulus. \textit{There is no default value; a value must be specified.}

\( R_i \)

The inner radius of the annulus. \textit{The default value is 0.}

\( e \)

The eccentricity of the annulus. The inner cylinder of the annulus is displaced to the left of the outer cylinder by this value. \textit{The default value is 0.}

\( \theta_1 \)

The total angle for the outer arc of the cylinder in degrees. \textit{The default value is 180 degrees.}

\( \theta_0 \)

The starting angle from the origin for the cylinder in degrees. \textit{The default value is 0 degrees.}

COMMENTS

Currently this command is available only if the computational domain is located in the 1\textsuperscript{st} or 2\textsuperscript{nd} quadrant.

EXAMPLES

\[
\text{GEOM} \textit{etry is ANNUlar with radius = 1.}
\]

\[
\text{GEOM} \textit{etry is ANNUlar with rin=1, rout=0.5}
\]

\[
\text{GEOM} \textit{etry is ANNUlar with rin=1, rout=0.5, epsilon=0.1}
\]

\[
\text{GEOM} \textit{etry is ANNUlar with rin=1, rout=0.5, epsilon=0.1, theta = 90}
\]

\[
\text{GEOM} \textit{etry is ANNUlar: rin=1, rout=0.5, epsilon=0.1, theta = 90, alpha=90}
\]
MODE 6: Transform from Cartesian to Cylindrical Geometry, or vice versa

SYNTAX  
GEOM \{CART \| RADI\} \{dir_1\} \{dir_2\}

CART  
Convert existing cylindrical radial coordinates to Cartesian coordinates according to the transformation:

\[ x_1 = r \cos \theta \]
\[ x_2 = r \sin \theta \]

RADI  
Convert existing Cartesian coordinates to cylindrical radial coordinates according to the transformation:

\[ r = \sqrt{x_1^2 + x_2^2} \]
\[ \theta = \tan^{-1}\left(\frac{x_2}{x_1}\right) \]

\textit{dir_1, dir_2}  
Two of the \textit{X, Y, Z, R or THETA} modifiers that, respectively, denote the \textit{x_1} and \textit{x_2} directions in the Cartesian framework to be transformed to or from the \textit{r} and \textit{\theta} directions of the cylindrical coordinate system. By default \textit{r} direction is assumed to be aligned with the \textit{y} direction and the \textit{\theta} with the \textit{z} direction.

COMMENTS  
Transformation from Cartesian to radial framework is possible only for a 3-dimensional grid since in the 2-dimensional mode only \textit{(x, r)} coordinate system is available. For the transformation to a cylindrical system the resulting \textit{r} is stored at the same location as \textit{x_1} and \textit{\theta} at \textit{x_2}. For transformation to a Cartesian system the resulting \textit{x_1} is stored at the same location as \textit{r} and \textit{x_2} at \textit{\theta}.

EXAMPLES  
GEOMetry converts R and THETA to CARTesian
GEOMetry convert Y and Z to RADial! Only with a 3D grid system
GEOMetry convert X and Y to RADial! Only with a 3D grid system
**Keyword Commands**

**COMMAND**  GRAVITY

**PURPOSE**  To specify the gravitational acceleration vector and its components.

**SYNTAX**  GRAV {g_x, g_y, g_z}, [g] [ ABSO|RELA|PASS]

- **g_x, g_y, g_z**  The components of the gravitational acceleration vector, \( g_j \), in the three principal directions. A positive value implies that the acceleration vector is directed in the principal direction; a negative value implies that it is directed opposite to the principal direction.

For **ANSWER™** and **TIDAL™** Software Tools, the default values are all set to 0.

For **PORFLOW™** Software Tool, only the ratio \( g_j / g \) appears in the equations, therefore normalized values may be specified for this input. The default values are set so that, for multiphase or free-surface flow, \( g_y = -9.81 \) for 2D flow and \( g_z = -9.81 \) for 3D flow; otherwise, the values are 0.

- **g**  The absolute value of the gravitational constant, \( g \). If no value is specified, then the value is computed as the square root of the sum of squares of the 3 components. If no GRAVITY command is specified then the default value is set to 9.81.

For **PORFLOW™** Software Tool, \( g \) is used for computing pressure head, \( P \), from thermodynamic pressure, \( p \), or vice versa. This input is necessary only if \( g_x, g_y, g_z \) are specified in a normalized mode.

- **ABSO**  For the **ANSWER™** Software Tool, the gravitational body force term, \( B_i \), in the \( i \)th direction momentum equation is given by:

\[
B_i = \rho g_i
\]

In this case the computed pressure represents the thermodynamic pressure, \( p \). This is the default option for the **ANSWER™** Software Tool.

For the **PORFLOW™** Software Tool the pressure equation is solved for the thermodynamic pressure head, \( P^n \). In this case the gravitational body force, \( B_i^n \), for the \( n \)th phase in the \( i \)th direction momentum equation is given by:

\[
b_i^n = \frac{\rho^n}{\rho^*} g_i
\]

- **RELA**  For the **ANSWER™** Software Tool, the gravitational body force term, \( F_i \), in the \( i \)th direction momentum equation is modified and defined as:

\[
F_i = (\rho - \rho^*) g_i
\]

Where \( \rho^* \) is the reference density. However, the computed pressure, \( P \), is no longer equal to the thermodynamic pressure, \( p \), but is related to it by:

\[
P = p - \rho^* \{g_x x + g_y y + g_z z\}
\]

For the **PORFLOW™** Software Tool the gravitational body force, \( B_i^n \), in the \( i \)th direction of the momentum equation is modified as:

\[
b_i^n = \frac{\rho^n - \rho^*}{\rho^*} g_i
\]

The pressure equation is solved for the Total head, \( H^n \). This is the default option for the **PORFLOW™** Software Tool.

This RELATIVE mode improves the stability of computations by decreasing the magnitude of the body force and hence the round-off errors. This should be the preferred mode of computations for most problems.

- **PASS**  The body force in the equations is ignored.
APPLICABILITY NOTES

For the ANSWER™ Software Tool the absolute value \((g)\) is used only if the PROBLEM ATMOSpheric or REFERENCE HYDRAulic command is present. In this case, this value is used to compute the hydrostatic pressure head from the thermodynamic pressure. Otherwise only the individual components in each direction appear in the momentum equations.

For the PORFLOW™ Software Tool the GRAVITY ABSOLUTE command is specified, then the governing pressure equation is solved in terms of pressure head, \(P\); otherwise the governing equation is solved in terms of the total head, \(H\). The boundary and initial conditions may be specified in terms of either \(P\) or \(H\). For unsaturated (multi-phase, Vadose or free surface) flow, the gravitational force is always included (GRAVITY RELATIVE) by default. For saturated flow, if no GRAVITY command is specified, then the body force is neglected and the \(P\) and \(H\) are equivalent.

For the TIDAL™ Software Tool, only the absolute value appears in the governing equations since the equations are integrated in the vertical direction (assumed to be opposed to the direction of the gravity vector). Therefore only a single value \((g_x)\) may be specified; the absolute value \((g)\) will be set equal to this value since the other values are assumed to be zero.

COMMENTS

For the ANSWER™ Software Tool, this command triggers the inclusion of the gravitational body force in computations. As such, it must be present for computations where this body force is present. The most common example is that of natural convection. Of course for natural convection to occur, the density of the fluid must vary due to thermal and/or other effects. Otherwise a uniform body force merely acts to alter the datum for pressure.

For the PORFLOW™ Software Tool, if flow is single-phase and the density is uniform, then the buoyancy term, \(B_j\), is uniform and constant. The net buoyancy contribution is then zero because it is the gradient of the buoyancy term that appears in the pressure equation. In this instance, the gravitational components may be set equal to zero. It should be noted that these conditions lead to the pressure head, \(P\), being identical to the total head, \(H\).

EXAMPLES

- GRAVity constants: \(0., -9.81\) RELATIVE mode  
  Orientation against y-axis
- GRAVity constants: \(-6.937, -6.937, 0.\)  
  ABSOLUTE mode  
  45 deg to x & y
- GRAVity constants: \(0., 0., -9.81\)  
  Orientation against z-axis
- GRAVity constants: \(0., 0., -32.2, 32.2\)  
  Orientation against z-axis
- GRAVity constant is 9.81
Keyword Commands

COMMAND GRID

PURPOSE To specify the number of elements or grid nodes and the dimension of the problem.

MODE 1: Structured Grid Specification

SYNTAX GRID [NODE|ELEM] [Nx] [Ny, Nz]

NODE The number of nodes is specified. For a structured grid the number of nodes in each direction is equal to the number of elements plus two additional nodes, one at each external boundary. This is the default option.

ELEM Nx, Ny and Nz specify the number of elements in each direction. The number of elements in each direction is 2 less than the number of grid nodes since there is one grid node per element and one boundary node at each end. The use of this modifier is not recommended; it is being retained for compatibility with old legacy input file. Some of the new LOCATE commands are not compatible with this input mode.

If this modifier is specified then all subregion input specification must be consistent with the indices in terms of elements rather than in terms of nodes. The element indices are numbered one less than the grid node indices. For example, for a 2D problem, the element grid index set (1,1) is equivalent to specifying the grid node (2,2) and so on. The boundary nodes cannot be explicitly specified in this mode; they are automatically captured by a LOCATE command if the element next to the boundary is specified.

Nx The number of grid elements or grid nodes in the x direction. The number of nodes is denoted by IMAX in this document. The default value is 1 element or 3 nodes.

Ny The number of grid elements or nodes in the y or r direction. The number of nodes is denoted by JMAX. The default value is 1 element.

Nz The number of grid elements or nodes in the z or θ direction. The specified value is denoted by KMAX. If the specified number of elements is 1 or more, then the 3D mode is activated. If a 0 or negative value is explicitly specified, then the 2D solution mode is invoked but it is assumed that all subregion input specification is in the 3D mode. If Nz is not specified, then the 2D solution mode is invoked and it is assumed that all subregion input specification is also in the 2D mode. There is no default value for this input.

EXAMPLES

GRID is 32! 1D problem: JMAX automatically set to 3
GRID is 32 by 27 by 1 NODEs! 2D problem: grid related input in 3D mode
GRID is 32 by 27 by 12 NODEs! 3D problem: grid related input in 3D mode
MODE 2: Unstructured Grid Specification

SYNTAX
GRID {UNST} [THRE] {N_Elem} [NODE] {N_Node}

UNST
Grid is specified in an unstructured mode. In this mode, the user must specify a list of vertices and the connectivity of those vertices to the grid elements. The coordinates of the vertices must be specified on a file through the COORDINATE command. The connectivity of the vertices to the elements is specified on a file through the CONNECTIVITY command.

THRE
By default the problem is assumed to be a 2D problem. This modifier must be used to specify a 3D problem.

N_Elem
The number of grid elements for the unstructured problem. There is no default value for this input.

NODE
By default the total number of nodes (one for each element plus one for each external boundary segment) are computed from the given connectivity information. If this modifier is present, then N_Node is interpreted to be the total number of nodes for the problems.

N_Node
The total number of grid nodes (sum of number of elements and number of external boundary segments) for the problem. This information is generated by most unstructured grid generators. If specified, this number helps in optimizing the use of the required memory arrays. By default this number is automatically generated by ACRi Software Tools from the connectivity information.

COMMENTS
All subregion input specification must be in terms of grid element numbers.

EXAMPLES
GRID is UNST with 100 elements ! 2D problem
GRID is UNSTructured with 1000 elements in THREE-dimensional mode
GRID is UNSTructured with 1000 elements and 1256 NODES in THREE-dimensional mode
MODE 3: Grid Less Computations

SYNTAX GRID {NONE} {fname}

NONE The computations are performed in ACRi’s revolutionary Virtual Finite Volume (VFM) method which consists of computation from a collection of arbitrary points in the computational domain. No grid is necessary.

fname The name of the file that contains the locations of node points and other pertinent information. This file format is internal to ACRi and the file is generated by software provided by ACRi.

EXAMPLES

GRID NONE the data is on file “GRIDLESS.FIL’
MODE 4: Unstructured Grid Directly from Connectivity File

SYNTAX

GRID {CONN} {VERTEX|HYBRID} {fname} [THRE]

CONN
Grid and connectivity is specified in an unstructured mode. In this mode, the connectivity data is read from the specified file and the number of field elements is automatically determined from the input. A separate CONNECTIVITY command is not required. The coordinates of the vertices must be specified on a file through the COORDINATE command.

VERTEX
The VERTEX mode of the CONNECTIVITY command is invoked. Please see the CONNECTIVITY command for further details. This is the default option.

HYBRID
The HYBRID mode of the CONNECTIVITY command is invoked. Please see the CONNECTIVITY command for further details.

fname
The name of the file containing the numerical input for the connectivity. There is no default value; a file name must be specified.

THRE
By default the problem is assumed to be a 2D problem. This modifier must be used to specify a 3D problem.

EXAMPLES

GRID CONNnectivity of VERTices to elements on file "VERT2ELM.CNC"
GRID CONNnectivity for HYBRID elements on file "MIXED_ELEMENTS.CNC" THREE D problem
Keyword Commands

**HISTORY**

**PURPOSE**
To obtain output of the time history for dependent variables at selected nodes.

**MODE 1:**
Specification of Time History For a Set of Variables in a Subregion

**SYNTAX**

```
HIST {subrgn} [Φ] {fname} [TABL] [PLOT] [NOW | OFF | ON] [COMP] [VFrq] [TIME]
```

- **subrgn**: The subregion for which the time history is required. See Section 3.4. For this mode to be invoked a subregion previously defined by a LOCATE command must be specified with an ID=subrgn or a SELECT/LOCATE modifier. There is no default value.
- **Φ**: One or more symbols that denote the variables for which the time history output is required. The valid symbols are listed in Table 2.8.1-3. By default, the output is obtained for all variables for which the equations are solved plus other variables that are of interest to the problem being solved. The variables can be specified only once for each time history command; a new command must be specified if a different set of variables is to be selected.
- **fname**: The file name for time history output. See Section 3.3 for additional information. Except for the 1st command, a file name must be specified with each command. The default file name, for the 1st command, is “acr_HISTORY.TMP”. To avoid confusion, it is recommended that a file name be specified with each command.
- **TABL**: The time history data are printed in a tabular form at the end of simulations.
- **PLOT**: A printer plot of time history of variables is generated at the end of simulations.
- **NOW**: One record of time history output is produced immediately.
- **OFF**: Time history output is discontinued.
- **ON**: Time history output is resumed if it was previously suppressed.
- **COMP**: By default the time history output file contains the project tile and information about grid. If this modifier is specified then this information is omitted.
- **VFrq**: The output frequency (step or time interval) for writing to the output device. See Section 3.7 for further details. By default the time history is generated at every step.
- **TIME**: By default, VFrq is interpreted as the frequency of output in terms of number of steps. If this modifier is present, then VFrq is interpreted as the time interval between successive outputs.

**COMMENTS**

Multiple Mode 1 commands may be specified. Each command can have its own set of variables and other modifiers and frequency. This command mode is strongly recommended over the Mode 2 and 3 of the HISTORY command.

**EXAMPLES**

- HISTORY for U, V, W only for ID=HIS region on “UVW.HIS” file.
- HISTORY for region ID=HISTORY every 20 steps on file ‘ALL.HIS’
- HISTORY ID=HISTORY at TIME interval of 1.75 hours output to file ‘ALL.HIS’
- HISTORY ID=HISTORY for U, P, T, K on file ‘HISTORY.OUT’ every 20 steps
- HISTORY ID=HISTORY for U, P on file ‘HISTORY.OUT’ TIME=2.50 hrs; print TABLes also
- HISTORY ID=HISTORY for U, P, T, K at TIME interval 0.23: print TABLes also ‘UPTK_HIS.TMP’
- HISTORY ID=HISTORY U & T on ‘HIS.NEW’ at every 20 steps; print TABLes and PLOTs
MODE 2: Specification of Location of Time History Nodes

SYNTAX

HIST \{N_1, \ldots, N_n\} \ [fname]

N=m in unstructured mode, = 2m in 2D and =3m in 3D mode

N_1, \ldots, N_n 

The grid index locations for the elements for which the time history output is obtained. For unstructured grids, the input is that of the element numbers. For structured grids the input consists of the grid indices (I, J, K) in the 3D or (I, J) in the 2D mode. If the grid is unstructured, then at least two elements must be specified; a single number will be interpreted as the frequency (See Mode 3 of command). If history at a single element is desired in the unstructured mode, then it must be specified through Mode 1 of the command.

fname

See Mode 1 Specification.

COMMENTS

This mode of the command works in conjunction with Mode 3. This mode of HISTORY command is now obsolete and has been superseded by Mode 1 of the command, which provides the combined functionality of both Mode 2 and Mode 3. It is being retained only temporarily to maintain compatibility with legacy files. It is strongly recommended that Mode 1 be used in preference to this mode of the command.

If this mode of the HISTORY command is used, then it must precede any Mode 1 command.

EXAMPLES

HISTORY at (2, 2), (2, 5), (5, 2), (11, 17) and (17, 11)! Input in 2D mode
HISTORY at elements 57, 33, 165 and 915! Unstructured mode
HISTORY output OFF at (2, 2) and (2, 5)
HISTORY at node (7, 11) and (7, 15) to be added to previous ones
HISTORY at (2, 2, 2), (2, 5, 7), (5, 2, 7), (11, 17, 19) & (17, 11, 12)! Input in 3D mode
HISTORY OFF at (2, 2, 2) and (2, 5, 7)
HISTORY output again at (2, 2, 2) and (2, 5, 7)
MODE 3: Specification of Variables and Output Options for Mode 2

SYNTAX

HIST [Φ] [fname] [TABL] [PLOT] [NOW|OFF|ON] [COMP] [VFrq] [TIME]

Φ See Mode 1 Specification.
fname See Mode 1 Specification.
TABL See Mode 1 Specification.
PLOT See Mode 1 Specification.
NOW See Mode 1 Specification.
OFF See Mode 1 Specification.
ON See Mode 1 Specification.
COMP See Mode 1 Specification.
VFrq See Mode 1 Specification.
TIME See Mode 1 Specification.

COMMENTS

This mode of the command works in conjunction with Mode 2. This mode of HISTORY command is now obsolete and has been superceded by Mode 1 of the command, which provides the combined functionality of both Mode 2 and Mode 3. It is being retained only temporarily to maintain compatibility with legacy files. It is strongly recommended that Mode 1 be used in preference to this mode of the command.

If this mode of the HISTORY command is used, then it must precede any Mode 1 command.

EXAMPLES

HISTory on file 'HISTORY.TIM'
HISTory for U, V, W only
HISTory every 20 steps
HISTory at TIME interval of 1.75 hours
HISTory for U, P, T, K on file 'HISTORY.OUT' every 20 steps
HISTory for U, P on file 'HISTORY.OUT' TIME=2.50 hrs; print TABLEs also
HISTory for U, P, T, K at TIME interval 0.23; print TABLEs also
HISTory U & T on 'HIS.NEW' at every 20 steps; print TABLEs
HISTory U & T on 'HIS.NEW' at every 20 steps; print TABLEs and PLOTs
MODE 4: History at an Arbitrary Point in Space

SYNTAX

HIST  {COOR}  { Φ } {fname} [TABL] [SQUA] [N1,..Nn] [VFreq] [TIME]

COOR

History is required at an arbitrary point in space specified by its (x, y, z) coordinates.

Φ

One or more symbols for the variables for which the history is required. No more than 10 symbols can be specified on one command. The valid symbols are listed in Table 2.7.1. There is no default value.

fname

The file name for output. A different output file may be specified for each command. If no file name is specified then the output is directed to the most recent previously specified file. If no previous file was specified, then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by "_HISTORY_XYZ.TMP". For example, if the Standard Output file is "PROBLEM.OUT", then the file is named "PROBLEM_HISTORY_XYZ.TMP". A summary of output is also printed to the standard output device at the end of simulations.

TABL

The time history data are printed in a tabular form at the end of simulations.

LINE

The values at the specified (x, y, z) location are computed by linear interpolation from its nearest neighbors. This option is active by default.

SQUA

The values at the specified (x, y, z) location are computed by inverse distance squared interpolation from its nearest neighbors.

N1, .., Nn

The grid coordinates (x, y, z) of the point. Two numerical values for 2D and three for 3D input modes must be provided. There is no default value for this input; the required number of numerical values must be specified.

VFreq

The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. If present, this must be last value on the command. By default the time history is generated at every step.

TIME

By default, VFreq is interpreted to be the frequency in terms of number of steps. If this modifier is present, then VFreq is interpreted to be the time interval between successive outputs.

COMMENTS

This command generates output of history of values at an arbitrary location in space, which may or may not coincide with the computational nodes. The history of values at computational nodes can be obtained by Mode 1 specification.

EXAMPLES

HISTORY of U at point with COORDinate x=1.35, y=0.796 every 3 steps
HISTORY of U at point with COORDinate x=1.35, y=0.796 every 20 steps with inverse SQUAare interpolation
HISTORY of U, V, W, T at COORDinate x=1.35, y=0.796, z=0.0975 at TIME interval of 1.75 units
HISTORY of U, T, C at COORDinates (1.35, 0.796, 0.0975) TIME interval 0.235 on ‘HISTORY.XYZ’
HISTORY U, T, C COORD (1.35, 0.796, 0.0975) TIME interval 0.235; SQUARe method ‘HISTORY.XYZ’
MODE 5: History of Source for a Variable

SYNTAX  
\[ \text{HIST} \{\text{SOUR}\} \{\Phi\} \{\text{subrgn}\} \{\text{name}\} \{\text{TABL}\} \{\text{OFF}\} \{\text{VFrq}\} \{\text{TIME}\} \]

SOUR Output for the source term for \( \Phi \) is required.

\( \Phi \) The symbol for the variable for which the source inventory is required. Only those symbols may be specified for which a differential equation is solved. The valid symbols are listed in Table 2.7.1. There is no default value.

subrgn The subregion for computations. If no subregion is specified, the entire domain is selected.

fname The file name for output. A different output file may be specified for each command. If no file name is specified then the output is directed to the file with the same name as the Standard Output file but with the extension removed and replaced by ".SOURCE.TMP". For example, if the Standard Output file is "PROBLEM.OUT", then the file is named "PROBLEM_SOURCE.TMP". A summary of output is also printed to the standard output device at the end of simulations.

TABL The time history data are printed in a tabular form at the end of simulations.

OFF Any previously specified command for the specified \( \Phi \) and subrgn is deactivated.

VFrq The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the time history is generated at every step.

TIME By default, VFrq is interpreted to be the frequency in terms of number of steps. If this modifier is present, then VFrq is interpreted to be the time interval between successive outputs.

COMMENTS

This command generates output of the history of "source" term for the variable. This includes all source (or sink) terms for the variable including the terms originally present in the governing equation (e.g. pressure gradient terms for momentum equations for ANSWER™) and those specified by the user through the various SOURce, DECAY and REAction commands. The output is the integral of the source for the variable \( \Phi \) over the volume of the subrgn.

The output is printed to the file specified by fname. In addition, at the end of simulations, tables of output are printed to the standard output file. These tables are sorted by variable and subregion.

EXAMPLES

- HISTory SOUR or C for the entire domain
- HISTory for SOURce of C for the entire domain
- HISTory of SOURCE for T for SELECTed region every 20 steps
- HISTory of SOURCE for T for subregion defined by ID=VAULT every 200 steps
- HISTory of SOURCE for T for ID=VAULT OFF
- HISTory of SOURCE for Ton 'SOURCE.OUT' for SELECTed region at TIME interval of 0.4
MODE 6: History of Mass or Property Inventory for a Variable

SYNTAX

HIST {STOR} {Φ} [subrgn] [fname] [TABL] [OFF] [V_Freq] [TIME]

STOR
Output for the storage or accumulation term for Φ is required.

Φ
The symbol for the variable for which the inventory is required. Only those symbols may be specified for which a differential equation is solved. The valid symbols are listed in Table 2.7.1. There is no default value.

subrgn
The subregion for computations. If no subregion is specified, the entire domain is selected.

fname
The file name for output. A different output file may be specified for each command. If no file name is specified, then the output is directed to the most recently previously specified file. If no previous file was specified, then the output is directed to a file with the same name as the Standard Output file with the extension replaced by “_STORAGE_TMP”. For example, if the Standard Output file is “PROBLEM.OUT”, then the file is named “PROBLEM__STORAGE_TMP”. A summary of output is also printed to the standard output device at the end of simulations.

TABL
The time history data are printed in a tabular form at the end of simulations.

OFF
Any previously specified command for the specified Φ and subrgn is deactivated.

V_Freq
The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the time history is generated at every step.

TIME
By default, V_Freq is interpreted to be the frequency in terms of number of steps. If this modifier is present, then V_Freq is interpreted to be the time interval between successive outputs.

COMMENTS

This command generates output of the history of “accumulation” or “storage” term for the variable. The output is the integral of the property represented by the variable Φ over the volume of the subrgn.

The output is printed to the file specified by fname. In addition, at the end of simulations, tables of output are printed to the standard output file. These tables are sorted by variable and subregion.

EXAMPLES

HIST STOR for C for the entire domain
HISTORY of STORage for T for SELECTed region every 20 steps
HISTORY of STORage for T for subregion defined by ID=VAULt every 200 steps
HISTORY of STORage balance for T for ID=VAULt OFF
HISTORY of STORage for T on “STORAGE.OUT” for ID=REGION1 at TIME interval of 0.4
Keyword Commands

**COMMAND** HYDRAULIC

**PURPOSE** To specify the reference hydraulic properties of the host porous matrix or of the planar or linear features. This command is effective only for the PORFLOW™ Software Tool.

**SYNTAX** HYDR \{α_s [K_x, K_y, K_z] [subrgn]\}

- **α_s** The matrix compressibility (≥ 0) with a default value of 0. This input is used to compute the effective storativity, S_e as defined by:

\[
S_e^n = R^n S^n \alpha_s + R^n \theta_E \left( S^n \alpha_f^n + \alpha_{Sat}^n \right)
\]

- **K_x, K_y, K_z** The reference values (≥ 0) of the three diagonal components of the hydraulic conductivity tensor, K_{ij} in the three principal directions, (x, y, z) or (x, r, θ), respectively. All off-diagonal components (i ≠ j) are assumed to be zero. The default value is 0.

\[
K_{ij} = k_{ij} \rho^* g / \mu^*
\]

In this relation, k is the relative permeability, and K_i are the reference values of the hydraulic conductivity tensor for a reference fluid (usually water) of density ρ* and viscosity μ*. The K_{ij} is specified from field data for a given soil or rock formation.

- **subrgn** The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

**COMMENTS**

More complex functional relations for storativity can be specified by the STORAGE or DISTRIBUTION commands and those for hydraulic conductivity can be specified by the CONDUCTIVITY command.

**EXAMPLES**

- HYDRAULIC properties: ss = 0.2, K_{x*} = 2, K_{y*} = 0.2, K_{z*} = 0.2 ft per day
- HYDRAULIC properties: ss = 0.2, K_{x*} = 2, K_{y*} = 0.2, K_{z*} = 0.2 ft per day for ID=Clayey_Sand
COMMAND  
IF-ELSE-ENDIF

PURPOSE  
To define an IF construct to control which, if any, of one or two blocks of user input statements are executed.

SYNTAX  
IF  \{variable\} = \{Ψ|V\} then

1\text{st} block of FREEFORM statements

[ELSE

2\text{nd} block of FREEFORM statements]

ENDIF

\textbf{variable}  
A symbolic variable that at run-time is compared to the value assigned to Ψ or V. The 'variable' must be the 1st modifier following the IF command. Only the first 8 characters are meaningful; any subsequent characters are ignored. The DEFINE command provides a powerful way to define such variables and may be used to control the IF-construct. The input for the variable must be symbolic if Ψ is specified and numeric if V is specified.

\textbf{Ψ}  
The character string that is compared to the ‘variable’ to determine the status of the IF construct as true or false. If the status is true then the 1\text{st} block of statements is executed and the 2\text{nd} block, if present, is ignored. If the status is false then the 1\text{st} block of statements is ignored and the 2\text{nd} block, if present, is executed. This modifier, if it exists, must immediately follow the modifier ‘variable’ without any other intervening character strings. Only the first 8 characters are significant; any subsequent characters are ignored.

\textbf{V}  
The numerical value that is compared to the ‘variable’ to determine if the status of the IF construct is true or false. If the status is true then the 1\text{st} block of statements is executed and the 2\text{nd} block, if present, is ignored. If the status is false then the 1\text{st} block of statements is ignored and the 2\text{nd} block, if present, is executed. If both V and Ψ are specified, then V input takes precedence.

COMMENTS  
This command provides a powerful means of performing conditional branching with ACRi FREEFORM™ commands. The IF construct can be used to consolidate input data sets. This construct, together with the DEFINE commands can be used for creating 'prototype' data input files for parametric or multivariate studies.

Each block of FREEFORM™ statement is composed of zero or more statements. The presence of the 2\text{nd} block is optional. However, if the 2\text{nd} block is present, then it must be preceded by an ELSE command. If the ELSE statement is present, then exactly one of the two blocks is executed. The IF construct must be completed by an ENDIF command otherwise unforeseen consequences may arise. The ENDIF statement must appear as stated. For example, the statement END IF will be misinterpreted as an END statement.
EXAMPLES

DEFINE GEOM_3D = 3! This statement defines a numerical value for variable GEOM_3D
IF (GEOM_3D = 2) THEN
GRID = 20 BY 20 BY 20! This block will be ignored because the IF status is false
ELSE
GRID = 20 BY 20! This block will be executed
ENDIF

DEFINE YESNO = OUTPUT
IF (OUTPUT = YESNO) THEN
OUTPUT U, V, W and T! This block will be executed because the IF status is true
ELSE
OUTPUT OFF! This block will be ignored
ENDIF

DEFINE YESNO = NOOUTPUT
IF (OUTPUT = YESNO) THEN
OUTPUT OF U, V, W and T
ENDIF
**COMMAND**  
INCLUDE

**PURPOSE**  
To include a file at run time in the input data stream.

**SYNTAX**  
INCL  [fname]

**fname**  
The name of the file which is to be included in the current input data file. The specified file must be compatible with the FREEFORM™ language. It must consist of valid keyword commands and input data only. The INCLUDE command provides for unlimited nesting in that the file being incorporated may itself contain embedded INCLUDE commands. For this particular command the file name need not be included in single or double quotes.

If the user wants to specify a file name on-the-fly at run time, then a question mark (“?”) can be inserted anywhere on the command line. In this case, the user will be prompted for the file name at run time.

**COMMENTS**

In one important aspect, the INCLUDE keyword is treated differently than other FREEFORM™ keywords commands. This keyword does not have to start in the 1st column (character) of a command line. That is INCLUDE command can be indented, if desired. INCL must, of course, be the 1st four non-blank characters on the command. This is different from all other keyword commands, which must start with the 1st character (column) unless an INDENT command was previously given.

**EXAMPLES**

INCLUDE file 'INCLUDE.NOW'
INCLUDE commands from file INCLUDE.NOW
INCLUDE! User will be prompted
INCLUDE?! User will be prompted
Keyword Commands

COMMAND        INDENT

PURPOSE        To allow FREEFORM™ commands to be indented.

SYNTAX         INDE [ON|OFF]

ON             Ordinarily, the FREEFORM™ input commands are assumed to start with the 1st character of the input command even if it is a blank character. Any leading blanks are considered to be significant in processing the input (please see Appendix B for a general description of the FREEFORM™ command syntax). If the ON modifier is present, then any leading blanks are ignored and the meaningful input is assumed to start with the 1st non-blank character of the input. This is the default option; i.e. if no modifier is specified, then the ON modifier is assumed.

OFF            Any previous INDENT command is deactivated; new INDENT commands may follow.

COMMENTS
When INDENT is ON care should be exercised in specifying commands with continuation lines. In this case, a continuation line can not start with the first non-blank character as an alphabetic character (A through Z, in upper or lower case) otherwise the leading blanks will be ignored and the “continuation” command will be interpreted as a “Keyword” command. It is a safe practice to start the continuation lines with numeric or special non-alpha characters. A recommended practice is to always start a continuation command with an ampersand (&) character. For example, consider the sequence of commands:

    INDENT ON from now
    LOCATE ID=ZONE1 COORDinate from (0.0, 0.0, 0.0)
    &
    3.0, 2.0
    INDENT OFF

Here, the “&” character in the 3rd line ensures that this input will be treated as a continuation line. If the “&” is removed, then the string “to” will be incorrectly interpreted as the keyword command “TO”. Since this keyword is invalid, the execution will be terminated.

EXAMPLES

    INDENT from now on ! Any leading blanks in commands will be ignored
    IF (GEOM_3D = 2) THEN
        GRID = 20 BY 20 BY 20
    ELSE
        GRID = 20 BY 20
    ENDIF
    INDENT OFF starting with next command ! Any leading blanks will not be ignored from now on
**COMMAND**  INITIAL

**PURPOSE**  To specify the initial conditions for dependent variables for structured grids

**SYNTAX**  INIT \( \{ \Phi = \Phi_o \} \ [N_1, ..., N_n] \)

*\( \Phi \)*  The symbol that denotes the field variable for which input is provided. The valid symbols are listed in Table 2.8.1-3. **One, and only one, symbol must be specified.** There is no default value.

*\( \Phi_o \)*  The initial value for the variable.

*\( N_1, ..., N_n \)*  These values define the subregion to which the input is applied. In the default mode, the subregion is defined by 4 values for the 2D and 6 for the 3D input mode. **If only one value, that is** \( N_1 \), **is specified, then it is assumed that** \( N_1 \) **is the material or zone number to which the input applies.** If this input is completely omitted, then the subregion is defined to be the entire domain.

**COMMENT**

This command is available only for structured grids. **SET command is a much more powerful option for setting field values of the variables for structured or unstructured grids.**

**EXAMPLES**

\begin{verbatim}
INITial U is 0.1 everywhere
INITial T is 1.E-3 from (2, 2) to (7, 9)  ! 2D input mode
INITial T is 1.E-3 from (2, 2, 2) to (7, 9, 4)  ! 3D input mode
INITial T is 1.E-3 for zone 5
\end{verbatim}
COMMAND: INJECTION

PURPOSE: To specify properties and parameters relating to injection of water films, curtains, or to condensation. This command is effective only for the ANSWER™ Software Tool.

MODE 1: Location and Properties for Water Films

SYNTAX:

INJE {[FILM] [subrgn] {TINJ=V_{Tinj}} {QINJ=V_{Qinj}} {TIME} {TEMP} {COOR=V_X V_Y V_Z} [STAR=V_{Start} STAR NOW] [STOP=V_{Stop} STOP NOW] [ELAP=V_{Elap}] [HIST=V_{Hist} [fname]]

subrgn: The subregion for which the input is specified. This subregion must be defined with LOCATE INJECTION command. If this subregion is a boundary of the domain, then the temperature must be fixed or the boundary must be adiabatic. If this subregion is a boundary of a solid body, then conduction heat exchange may be taken into account. See Section 3.4 for additional details.

TINJ: Introduces water film temperature.

V_{Tinj}: Water film temperature (in Kelvin). There is no default value.

QINJ: Introduces the mass rate of water in the film.

V_{Qinj}: Mass rate of water in the film. There is no default value; a positive value must be specified.

TIME: By default, values of V_{Start}, V_{Elap}, V_{Stop} and V_{Hist} (see below) are in time step number. If this modifier is present, then values are in time units.

TEMP: By default, the value of V_{Start} (see below) is a step or a time value. If this modifier is present, V_{Start} is a temperature for which the water film starts to be active.

COOR: If modifier TEMP is present then this keyword must be added to define coordinates of the point at which film temperature monitored.

NOW: By default, keywords START and STOP must be followed by values. If NOW is set with START/STOP, the water film is activated/stopped at the current step.

START: Introduces the start time of the film. By default, this is defined by INJE FREQ for all injections.

V_{Start}: Step, Time (modifier TIME) or Temperature (modifier TEMPERATURE) value.

ELAP: Introduces the film duration. By default, this is defined by INJE FREQ for all injections.

V_{Elap}: Step or Time (if modifier TIME is present) value.

STOP: Introduces the film end time. By default, this is defined by INJE FREQ for all injections.

V_{Stop}: Step or Time (if modifier TIME is present) value.

V_X, V_Y, V_Z: Coordinate values at which temperature is monitored. There is no default value.

HIST: By default, no history file of the water film is written. In the presence of this keyword, an history file is computed.

V_{Hist}: Step or Time (if modifier TIME is present) frequency of history computation.

fname: The file name for history output. A different output file may be specified for each command. If no file name is specified then the output is directed to the most recent previously specified file. If no previous file was specified, then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by "_FILM.TMP". For example, if the Standard Output file is "PROBLEM.OUT", then the file is named "PROBLEM_FILM.TMP".

EXAMPLES:

INJEction FILM ID=FILM, TINJection=280. Kelvin, QINJ=10 kg/s, HISTory every 1 step, ‘FILM.HIS’

INJEction FILM ID=FILM STARt TEMP is 340 Kelvin with COORinates (2.00,3.00,2.00) ELAPS maximum TIME is 180 seconds
MODE 2  Location and Properties for Water Curtains

SYNTAX  

\[
\text{INJE} \{\text{CURTAIN} \{ID=\text{subrgn}\} \{\text{QINJ}V_{\text{Qinj}}\} \{\text{DIAM}V_{\text{Diam}}\} \{\text{TIME}\} \{\text{TEMP}\} \{\text{STAR}V_{\text{Start}}\} \{\text{STAR NOW}\} \{\text{STOP}V_{\text{Stop}}\} \{\text{STOP NOW}\} \{\text{ELAP}V_{\text{Elaps}}\} \{\text{HIST}V_{\text{Hist}}\} [\text{fname}]\]
\]

\text{subrgn}  
The subregion for which the input is specified. This subregion must be defined with \text{LOCATE INJECTION} command. See Section 3.4 for additional details.

\text{QINJ}  
Introduces the mass rate of water in the film. There is no default value; a positive value must be specified.

\text{V}_{\text{Qinj}}  
Mass rate of water in the film

\text{DIAM}  
Introduces droplet diameter of water curtain

\text{V}_{\text{Diam}}  
Droplet diameter. There is no default value; a positive value must be specified.

\text{TIME}  
By defaults, values of \text{V}_{\text{Start}}, \text{V}_{\text{Elaps}}, \text{V}_{\text{Stop}} and \text{V}_{\text{Hist}} (see below) are in time step number. If this modifier is present, then values are in time units.

\text{TEMP}  
By default, the value of \text{V}_{\text{Start}}, (see below) is a step or a time value. If this modifier is present, \text{V}_{\text{Start}} is a temperature for which the water film starts to be active.

\text{STAR}  
Introduces the start time of the film. By default this is defined by \text{INJE FREQ} for all injections.

\text{V}_{\text{Start}}  
Step or Time (if modifier \text{TIME} is present) or Temperature (if modifier \text{TEMP} is present) value.

\text{ELAP}  
Introduces the film duration. By default this is defined by \text{INJE FREQ} for all injections

\text{V}_{\text{Elaps}}  
Step or Time (if modifier \text{TIME} is present) value.

\text{STOP}  
Introduces the film end time. By default this is defined by \text{INJE FREQ} for all injections

\text{V}_{\text{Stop}}  
Step or Time (if modifier \text{TIME} is present) value.

\text{COOR}  
If modifier \text{TEMP} is present then this keyword must be added to define coordinates of the point at which film temperature monitored.

\text{V}_{X}, \text{V}_{Y}, \text{V}_{Z}  
Coordinate values at which temperature is monitored. There is no default value.

\text{HIST}  
By default no history file of the water film is written. In the presence of this keyword, a history file is written.

\text{V}_{\text{Hist}}  
Step or Time (if modifier \text{TIME} is present) frequency of history computation.

\text{fname}  
The file name for history output. A different output file may be specified for each command. If no file name is specified then the output is directed to the most recent previously specified file. If no previous file was specified, then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by "\_CURTAIN.TMP". For example, if the Standard Output file is "\text{PROBLEM.OUT}" , then the file is named "\text{PROBLEM\_CURTAIN.TMP}".

EXAMPLES

\text{INJE CURTain} \text{ID}=\text{ZCURT} \text{ QINJection}=10. \text{ kg/s} \text{ DIAMeter}=0.001 \text{ m}

\text{START NOw and STOP at TIME 180 seconds}

\text{HISTory every 0 second, file is 'CURTain.his'"}
MODE 3  Location and Properties for Condensation

SYNTAX  INJE {COND} {subrgn} [dir] [option] [TIME] [HIST=VHist] [fname]

subrgn  The subregion for which the input is specified. See Section 3.4.

dir    The orientation index for the boundary associated with the film. See Section 3.5 for available choices.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>DROP</td>
<td>The droplet condensation model is activated. This is the default option.</td>
</tr>
<tr>
<td>FILM</td>
<td>The film condensation model is activated.</td>
</tr>
</tbody>
</table>

TIME    By default, values of VHist (see below) is a time step frequency. If this modifier is present, then the value is in time units.

HIST    By default no history file of the water film is given. In the presence of this keyword, a history file is computed.

VHist   Step or Time (if modifier TIME is present) frequency of history computation.

fname   The file name for history output. A different output file may be specified for each command. If no file name is specified then the output is directed to the most recent previously specified file. If no previous file was specified, then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by "_CONDENSE.TMP". For example, if the Standard Output file is "PROBLEM.OUT", then the file is named "PROBLEMCONDENSE.TMP".

COMMENTS

If FILM model is activated, the water film falling direction is defined the GRAVITY direction. By default this is the Z-axis in the decreasing order of Z.

EXAMPLES

INJEction CONDensation ID=NORD HISTory every 1 step, file is ‘COND_NORD.his’
INJEction COND ID=NORD HISTory TIME every 0.1 second, file is ‘COND_NORD.his’
MODE 4: Injection Computations Parameters

SYNTAX

```
INJE {FREQ} {N₁} [N₂, N₃]
```

**FREQ**  The spray computation frequency parameters are specified.

**N₁**  The frequency of droplet computations in terms of computational steps. The default value is 10.

**N₂**  The first computational step at which the droplet computations are performed. The default value is 1.

**N₃**  The last computational step at which droplet computations are performed. The default frequency is set to 9999999.

**COMMENTS**  
Injection computations are automatically triggered if a INJECTION command in Mode 1 through 3 is encountered. This input is required only if the user wants to modify the default values.

This command will be modified if the NOZZLE FREQuency command is also active. Nozzles and water injections will be computed at the same frequency.

**EXAMPLES**

```
INJEction FREQuency of calculations: 1 start at step number 10
INJEction FREQuency of calculations: 10 start at step number 10 and stop at step 500
```
Keyword Commands

COMMAND  INLET

PURPOSE  To specify an inflow boundary for the domain of computation. This command is effective only for the ANSWER™ Software Tools.

SYNTAX  INLE  {dir} [subrgn] [DIAG] [OFF]

dir  The orientation index for the inlet boundary. See Section 3.5 for available choices. There is no default value, a value must be specified.

subrgn  The subregion to be identified as an inlet. If no subregion is specified, the outermost "dir" oriented boundary of the entire computational domain is selected.

DIAG  By default only summary statistics of total boundary area, average density and velocity, and flow rate are printed to the standard output device. If this modifier is present then a complete detail of area, velocity components, density and flow rate for each segment of the boundary is printed.

OFF  Previously specified inlet boundary for the identified subregion is deactivated. A new specification for this subregion may follow.

COMMENTS

An inlet boundary, by definition, is assumed to be a boundary where the values of all dependent variables are known. This command provides a compact way to specify fixed boundary conditions for all variables at a given boundary. The actual values at the inlet boundary may be specified by INITIAL, READ or SET commands. These values may be changed by a subsequent command during simulations. The only effect of this command is to keep the values at the inlet boundary fixed at the value set by the user.

EXAMPLES

INLE at X- boundary at left (minimum x)
INLE at Y- boundary for the most recently SELECTed subregion
INLE at X+ boundary for subregion ID = INFLow
INLE OFF at X+ boundary for subregion ID = INFLow
COMMAND   INTEGRATION

PURPOSE Choice of discretization scheme for integration of flow, heat and mass transport equations.

SYNTAX \[ \text{INTE} \left[ \Phi \right] \{ \text{HYBR} | \text{BOUN} | \text{CENT} | \text{QUIC} | \text{ACRI} | \text{UPWI} \} \]

\( \Phi \) One or more of the symbols that denote the heat or mass transport variables for which the profile specification is effective. The valid symbols are listed in Table 2.7.1. If no symbol is specified, the input is assumed to be effective for all variables.

HYBR The hybrid scheme (Runchal, 1972) is used for integration. This is the default option.

BOUN A bounded NVD central difference scheme is used.

CENT The \(2^{\text{nd}}\) order central-difference scheme is used for integration. The scheme may generate over- and under-shoots if the local grid Peclet number exceeds 2. It is known to be unstable in the linear sense if the local grid Peclet number exceeds 2.

QUIC A generalized flux-conservative form of the QUICK scheme (Leonard, 1979) is used for integration. This scheme is recommended for use only with hex grids; it should not be used for general polyhedral grids.

ACRI The stabilized \(2^{\text{nd}}\) order central-difference scheme is used for integration. The scheme uses \(2^{\text{nd}}\) order central differences for fluxes but the matrix coefficients are controlled to ensure positive-definite property. The scheme may still show over- and under-shoots if the local grid Peclet number is greater than 2; however it generally extends the range of applicability of the central difference scheme.

UPWI The \(1^{\text{st}}\) order upwind scheme is used computing convective fluxes whereas the diffusive fluxes are still computed by the \(2^{\text{nd}}\) order central differences. The scheme is unconditionally stable in the linear sense but may increase numerical diffusion under certain conditions.

COMMENTS

The default option should be adequate for most applications. However, if the local grid Peclet number as given below is significantly larger than 10 and the direction of flow is not (approximately) aligned with any of the coordinate directions, one of the other schemes, except UPWIND, may be desirable. If robustness is required, then UPWIND is the most robust scheme.

\[ \text{Pe} = \frac{U \delta L}{\Gamma} \]

where \(U\) is the flow speed, \(\delta L\) is the grid interval and \(\Gamma\) is the diffusivity

EXAMPLES

INTEGRation for U by BOUNDED second order scheme
INTEGRation for T by HYBRid profile (same as default)
INTEGRation for T by modified QUICK scheme
INTEGRation for T, C, C2 by CENTral Difference scheme
Keyword Commands

**COMMAND**  LAGRANGIAN TRANSPORT

**PURPOSE**  To select the Lagrangian Random-Walk algorithm for transport of species.

**MODE 1:** Specification of Maximum Number of Particles

**SYNTAX**  LAGR (PART) {NPart} [qPart] [MASS][[LOCA][DENS=ρ][RADI=β]] [OFF]

**PART**  The number of Lagrangian particles to be tracked for transport of a species.

NPart  The maximum number of Lagrangian particles that can be present in the computational domain at any given time. During computations, new particles can be released, the particles can move out of the computational domain, and can be eliminated and consolidated based on specified criteria. *There is no default value.*

qPart  The mass of the Lagrangian particle at time of release into the computational domain. *The default value is 0.001.*

**MASS**  The species concentration at a grid cell is computed by assuming that the mass of a particle is distributed in the immediate neighborhood of the particle according to the inverse of square distance of the particle from the element node. *See Section C.2 in Appendix C for further details. This is the default option.*

**LOCA**  The species concentration is computed by assuming that the mass of a particle is totally contained in the element of its location. *See Section C.2 in Appendix C for further details. The default value is 2.*

**DENS**  The species concentration is computed by assuming that a particle has a volume that is computed from its density. The mass of the particle is then distributed in the immediate neighborhood of the particle according to the intersection of the particle volume with the cell volume. *See Section C.2 in Appendix C for further details. The default value is 2.*

ρ  The mass density of the particles if DENS modifier is present. *The default value is 1.*

**RADI**  The species concentration is computed by assuming that a particle has a radius of influence. The mass of the particle is then distributed in the immediate neighborhood according to the ratio of the distance of the particle to its radius of influence. The radius of influence is set equal to β times the characteristic half length of the element in which the particle is located. *See Section C.2 in Appendix C for further details.*

β  A factor that multiplies the cell characteristic half length to compute the radius of influence of the particle. *The default value is 1.*

**OFF**  By default the concentration of species is computed at every time step. If this modifier is present, then the concentration is computed only in response to an OUTPUT or SAVE command specified with the symbol for the species. The computing time spent in concentration calculations can be saved if the concentration is not required except for purposes of output. *This modifier must not be used if the species concentration is used as an active variable for other purposes.*

**COMMENTS**

A LAGRANGIAN PARTICLE command must be present to initiate the solution of the transport equation by the stochastic RADM (Random Walk Dispersion Method) algorithm. Details of the algorithm and its applications and verification are given in a number of publications by Runchal(1980), Goodin et al. (1980), Goodin et al. (1982), and others. A brief description of RADM is given in Appendix C.

For each computational element (or cell) the concentration of the species is equal to the sum of the mass of particles in the cell divided by the volume of the cell. However in the macro scale simulations, each particle represents a large collection of “molecules” that are distributed around the mean computed position of the particle. Different methods are available for computing the concentration for any element; these are described in Section C.2 in Appendix C.

**EXAMPLES**

LAGRANGIAN transport with 10000 PARTICLES.
LAGRANGIAN transport with 10000 PARTICLES and mass of each as 0.002 kg with RADlus factor as 10.
LAGRANGIAN transport with 10000 PARTICLES and mass of each as 0.002 kg concentration OFF.
MODE 2: Specification of Particle Release Rate

SYNTAX

LAGR {RELE} {Φ} {func{ξ}} {N₁, N₂, ..., Nₙ} [fname] [NUMB=NPart] [INIT|INST] [subrgn]

RELE  A source for release of particles into the computational domain is specified.

Φ  One and only one symbol for the dependent variable for which the Lagrangian transport is computed. Valid symbols are those for the species equations listed in Table 2.7.1. There is no default value; a symbol must be specified.

func  One of the modifiers listed in Table 4.2.1 that denotes the functional form for computing the mass rate of release of particles. The rate of release has units of [M t⁻¹] such as [kg/s].

ξ  One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

NUMB  By default the mass of each particle is assumed to be that specified as qPart with mode 1 of this command. If this modifier is present, then it is assumed that the total number of particles for the release rate are given as NPart and the mass of each is equal to the total release mass divided by the number of particles. If the mass release rate is function of time, then the actual mass of each released particle will vary with time.

NPart  The number of particles to be released at each time step, if the modifier NUMB is present.

INIT|INST  By default the release is assume to be continuous and the specified mass is released at every time step. If either of these modifiers is present, then the source is instantaneous and only once.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

COMMENTS

A number of LAGRANGIAN RELEASE commands may be given for a simulation to accommodate the diversity of sources. However currently only one variable may be selected for Lagrangian transport.

EXAMPLES

LAGRANGIAN transport with 20000 RANDOM numbers.
MODE 3: Specification of a Receptor for Concentration Computations

SYNTAX: LAGR {TABL} [TIME] [Vfrq] [NOW|ONLY|OFF]

RECE: A receptor location is given to compute concentration at the specified subdomain. The default option is to compute the concentration throughout the computational domain at the end of simulations.

TABL: If this modifier is present, then a table of output is produced that includes the complete detail of the current location, mass and status of each particle. As the number of particles increases, this output can become very large especially if the frequency of output is not judiciously chosen.

TIME: By default, Vfrq is the frequency of output in terms of number of steps. If this modifier is present, then Vfrq is interpreted to be time interval between successive outputs.

Vfrq: The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. The specified value is ignored if it is zero or negative. The default value is set so that output is obtained only at the end of simulations.

NOW: The output is produced immediately after the command is encountered.

ONLY: If this modifier is specified then the output is produced only once in response to a NOW modifier or at the frequency determined by Vfrq.

OFF: Output for any previous command(s) for the same subrgn and type is subsequently suppressed.

COMMENTS: This command only results in the computation of the species concentrations for the specified subdomain. A separate OUTPUT command must be given to obtain the output of the concentration field.

EXAMPLES:

LAGRANGIAN RECEPTOR at ID=STATION1 at end of simulations.
LAGRANGIAN RECEPTOR at ID=STATION1 at every TIME=100 units.
MODE 4: Specification of Size of The Random Number Distribution

SYNTAX  LAGR {RAND} {N_{random}}

RAND  The number of random numbers are being specified.

N_{random}  The number of random numbers that comprise a uniform random number distribution with a mean value of zero and a range of unity that is used to simulate the diffusive and dispersive transport of a species. The default value is 10,007.

COMMENTS

These random numbers are sampled during diffusive transport of each Lagrangian particle. The sampling occurs sequentially during transport of these particles. For most applications, 10000 random numbers provide a sufficiently large sample. However the diffusive resolution improves as the number is increased.

EXAMPLES

LAGRANGIAN transport with 20000 RANDOM numbers.
COMMAND     LAMINAR

PURPOSE     To select laminar flow option. This command is effective only for the ANSWER™ Software Tool.

SYNTAX      LAMI

COMMENTS     By default the ANSWER™ Software Tool selects the laminar or turbulent mode of computations automatically. If any of the turbulence related quantities (k, ε, or l) are specified then the turbulence mode is initiated, otherwise flow is assumed to be laminar. This command may be employed to force laminar flow computations. This command is not available with PORFLOW™ and TIDAL™ Software Tools.

EXAMPLES     LAMINAR flow for this problem.
             LAMINAR flow! By default
<table>
<thead>
<tr>
<th>COMMAND</th>
<th>LAND</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To define a land or solid object within the flow domain. This command is effective only for the ANSWER™ and TIDAL™ Software Tools.</td>
</tr>
<tr>
<td>COMMENTS</td>
<td>This command is identical to the BLOCK command. Please see the BLOCK command for details.</td>
</tr>
</tbody>
</table>
**COMMAND**  
LIMIT

**PURPOSE**  
To specify the limiting values for field variables

**SYNTAX**  
LIMIT \{ \Phi \} \{ \Phi_{\text{Min}} , \Phi_{\text{Max}} | \text{OFF} \} [\text{MATR}]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>\Phi</td>
<td>A symbol that denotes the variable for which the limits are being set.</td>
</tr>
<tr>
<td>OFF</td>
<td>All previously set limits for the selected variable are deactivated.</td>
</tr>
<tr>
<td>\Phi_{\text{Min}}</td>
<td>The minimum permissible value for the variable. Any computed value that is less than ( \Phi_{\text{Min}} ) is set to ( \Phi_{\text{Min}} ).</td>
</tr>
<tr>
<td>\Phi_{\text{Max}}</td>
<td>The maximum permissible value for the variable. Any computed value that is greater than ( \Phi_{\text{Max}} ) is set to ( \Phi_{\text{Max}} ).</td>
</tr>
<tr>
<td>MATR</td>
<td>By default when the limit for a variable is specified, the solution computed by the matrix solver is bounded and truncated by the specified bounds. The matrix itself is not modified in any manner to prevent the variable from exceeding the specified limits. If this modifier is present, then the forcing function of the matrix is modified to ensure that the matrix is unlikely to generate values below the specified minimum value. This option can only be used if transient mode of the SOLVE command is invoked.</td>
</tr>
</tbody>
</table>

**COMMENTS**

The default values for all field variables are set to \(-10^{30}\) as the minimum and \(10^{30}\) as the maximum. However, these values may be internally revised for some of the variables (such as mass concentration) based on the nature of the problem and that of the variable. This command may be used to override the internally set values, if so desired.

**EXAMPLES**

LIMIT for \( T \) minimum = 300  
LIMIT for \( T \) minimum = 0 maximum = 100  
LIMIT for \( T \) OFF! Disable any previously specified or internally set limits
COMMAND LOCATE

PURPOSE To locate and identify a subregion in the domain of computation for later reference by other input commands.

MODE 1: Subregion Specification by Grid Indices for a Structured Grid

SYNTAX LOCA [ID=idsub] [FIEL] [FLUI|SOLI] [ILO,JLO,KLO] [IHI,JHI,KHI] [ISK,JSK,KSK] [fname]

idsub A unique identifier for the subregion consisting of up to 32 characters. If there are more than 32 characters, then the subsequent characters are ignored. The 1st character must be an alphabetic (A-Z) character. No distinction is made between the lower and upper case characters. The allowable set of characters includes the alphabetic (A-Z), the numeric (0-9), the underscore (_), the minus (-), the plus (+) and the period (.) characters. The identifier is terminated by the 1st separator character. A list of separator characters is given in Chapter 1. This identifier may be subsequently used in an input command to provide selective input for that subregion. If the identifier is omitted, then the modifier LOCATE or SELECT on the command can make a generic reference to the specified subregion until the next LOCATE or SELECT command. See Section 3.4 for additional details.

FIEL If the LOCATE command identifies an element right next to an exterior boundary of the computational domain, then the node that defines the boundary is included by default in the definition of the subregion. If the FIELD modifier is present, then the subregion comprises only the interior field nodes (or elements) and the exterior boundary nodes are not included in the subregion. However, the FIELD modifier is ignored if the grid indices refer only to an exterior boundary or if any of the skip indices has a value greater than 1. In these cases, only the elements defined by the grid indices are included.

FLUI If this modifier is present then only the fluid elements are retained; any elements that are solid or blocked (BLOCK command) are excluded from the selected set of elements.

SOLI If this modifier is present then only the solid or blocked (BLOCK command) elements are included in the selected set of elements.

ILO, JLO, KLO The grid indices (I,J,K) of the lower left corner of the window.. KLO must be specified only for the 3D geometry. If the values specified lie outside this range then the input values are clipped to lie in the valid range specified by the GRID command. There is no default value; a valid set of values must be specified. See Section 4.4 for additional information.

IHI, JHI, KHI The grid indices (I,J,K) of the upper right corner of the window.. KHI must be specified only for the 3D geometry. If the values specified lie outside this range then the input values are clipped to lie in the valid range specified by the GRID command. If no values are specified, then these values are assumed to be those for the lower corner corner of the window.

ISK The x-direction node interval for the window subregion. Only those nodes occurring at this interval, starting with N1 specification are considered to be part of the subregion. For example, a specification of 3 results in the nodes located at I=ILO+1, ILO+4, ILO+7, etc. to be included in the selected subregion; the intermediate nodes are excluded. The default value is 1.

JSK, KSK The y and z direction node intervals in the manner described above. The default value is 1.

fname If a valid file name is present (see Section 3.3) then an ordered list of element numbers selected by the command is written to the file. For structured grids a list of corresponding (I,J,K) grid indices is also written to the file.

EXAMPLES

LOCATE subregion from (6,10) to (31,10)
LOCATE subregion (6,10) to (31,10) with ID=DMN1
LOCATE region ID=DMN2 as: (6,10,1) to (31,10,15) with interval (2,3,1)
LOCATE region (6,10) to (31,10) with interval (2,3)
LOCATE subregion (1,1) to (22,22) only FIELD nodes as ID=INNR
LOCATE subregion (1,1,3) to (22,22,7) only FIELD nodes as ID=INNR output on file 'INNR.IJK'
MODE 2: Subregion Specification by Grid Coordinates of Rectangular Windows

SYNTAX

```
LOCA {COOR} [ID=idsub] [INTE] [NOT] [EXCL] [FIEL|BOUN] [FLUI|SOLI] {N1, ..., Nn} [fname]
```

COOR One or more “windows” (with a maximum of 1000) are specified by their grid (x, y, z) coordinates. Each window is defined by 2 sets of coordinates. The 1st set defines the “lower-left” and the 2nd set the “upper-right” corner of the window. The subsequent windows are defined in an identical manner. There is no restriction on the coordinate values. But each window must be specified by 4 numerical values for 2D and 6 for 3D geometry.

The elements are selected based on the coordinate value of the element node. All elements with the node located inside or on the boundary of the window are selected by this command. An element is considered either in or out. No account is taken of the fact that the selected elements may be partially in or out. The elements selected are further affected by the presence or absence of FIELD and BOUNDARY modifiers.

idsub See Mode 1 Specification.

INTE If multiple windows are defined, then by default the union (elements that belong to either) is selected. If this modifier is present, then the intersection (elements that belong to more than one window) are selected.

NOT This modifier is effective only if the INTERSECTION modifier is also specified. It selects the union of multiple windows minus their intersection (elements that belong to only one and not more than one window)

EXCL If the modifier is present, then the specified elements are excluded and the complimentary set in the computational domain is selected. For example, if the union is selected, and this modifier is present, then all the elements that belong in the union are excluded and rest of the computational domain is selected.

FIEL See Mode 1 Specification.

FLUI See Mode 1 Specification.

SOLI See Mode 1 Specification.

BOUN If the BOUNDary modifier is present, then only the external boundary nodes are selected. Any elements interior to the computational domain are excluded.

N1, .., Nn The grid coordinates (x,y,z) for the “lower-left” and “upper-right” corners of the window (s). The number of values specified must be in sets of 4 for 2D and 6 for 3D for each window. See Section 4.4for additional information. There is no default value; a valid set of values must be specified.

fname See Mode 1 Specification.

REMARKS

If a SCALE command is specified immediately preceding this command, then the input coordinate values are scaled as described in the SCALE command.

EXAMPLES

```
LOCAte region with COORDinates (0., -20.) to (11571.5, 80.)
LOCAte subregion ID = DMN2 for grid COORDinates (0., 0.) to (100, 1500)
LOCAte subregion ID = DMN2 for COORDinates (0., 0.) to (100, 1500) EXCLUDe selection
LOCAte ID = DMN2 for grid COORDinates (0., 0.) to (2.5,1.5) and (3.25,1.0) to (5.0,5.2)
LOCAte grid COORDinates (0., 0.) to (2.5,1.5) and (3.25,1.0) to (5.0,5.2) and EXCLUDe selected
LOCAte COORDinates (0., 0.) to (2.5,1.5) and (3.25,1.0) to (5.0,5.2) select INTERsection & EXCLUDe
LOCAte COORDinates (0., 0.) to (2.5,1.5) and (3.25,1.0) to (5.0,5.2) select NOT INTERsection & EXCLUDe
LOCAte COORDinates (0., 0.) to (2.5,1.5) and (3.25,1.0) to (5.0,5.2) select output on “DMN2.LOC”
LOCAte COORDinates (0., 0.) to (2.5,1.5) and (3.25,1.0) to (5.0,5.2) select only BOUNDary
```
MODE 3: Subregion Specification by a Polygonal Window

SYNTAX

```
LOCA {POLY} [ID=idsub] [EXCL] [FIEL|BOUN] [FLUI|SOLI] {N₁, ..., Nₙ} [fname]
```

**POLY**

A polygonal region is specified by the coordinates of its vertices. **The polygon must be convex; concave polygons may lead to inaccurate selection.**

For 2D geometry, the pairs of (x, y) coordinates for vertices of the polygon must be specified in a counterclockwise sense.

For 3D geometry, current formulation only allows for the specification of 8-vertex hexahedral windows. First the base of the hex must be defined by 4 sets of (x, y, z) coordinates of its vertices in a counterclockwise sense. The last 4 sets of (x, y, z) coordinates define the top surface of the hex in a counterclockwise sense.

The elements are selected based on the coordinate value of the element node. All elements with the node located inside or on the boundary of the polygon are selected by this command. An element is considered either in or out. No account is taken of the fact that the selected elements may be partially in or out. The elements selected are further affected by the presence or absence of **FIELD** and **BOUNDARY** modifiers.

**idsub**

See Mode 1 Specification.

**EXCL**

If the modifier is present, then the specified elements are excluded and the complimentary set in the computational domain is selected.

**FIEL**

See Mode 1 Specification.

**BOUN**

If the **BOUNDARY** modifier is present, then only the external boundary nodes are selected. Any elements interior to the computational domain are excluded.

**FLUI**

See Mode 1 Specification.

**SOLI**

See Mode 1 Specification.

**N₁, .., Nₙ**

The grid coordinates (x, y) or (x, y, z) for the vertices of the polygon. The number of values must equal N₂₃D * NₙVert where N₂₃D is 2 for 2D and 3 for 3D geometry and * NVert is the number of vertices. **There is no default value; a valid set of values must be specified.**

**fname**

See Mode 1 Specification.

**REMARKS**

If a **SCALE** command is specified immediately preceding this command, then the input coordinate values are scaled as described in the **SCALE** command.

**EXAMPLES**

```
LOCA te POLYgonal region (x, y) coordinates are: (0, 0) (1,0) (1,1) (0,1)  !2D rectangle
LOCA te POLYgon (x, y) coordinates are: (0, 0) (1,-1) (2,0) (1,1)  !Diamond shaped region
LOCA te POLYgon (x, y): (0, 0) (0.5,-0.866), (1.5,-0.866) (2,0) (1.5,0.866) (0.5,0.866)  !Hexagon
LOCA te POLYgon (x, y, z): Base: (0, 0,0) (1,-1,0) (2,0,0) (1,1,0)  
         Top: (0, 0,1) (1,-1,1) (2,0,1) (1,1,1)  !Hexahedral with diamond base
LOCA te region ID=DIAMOND POLYgon (0, 0) (1,-1) (2,0) (1,1) output on “FILE.LOC”
LOCA te ID=NOT_DIAMOND EXCLUDE POLYgon (0, 0) (1,-1) (2,0) (1,1) output on “FILE.LOC”
```
MODE 4: Specification of a Circular or Cylindrical Subregion

SYNTAX
LOCA {CYLI|CIRC} [ID=idsub] [FIEL|BOUN] [FLUI|SOLI] {d_cyl} [N1,... Nn] [IJK|ELEM] [Nn+1,...Nm], [Nm+1] [fname]

CYLI | CIRC A cylindrical (circular in 2D) subregion is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the FIELD modifier is present.

idsub See Mode 1 specification.

FIEL See Mode 1 Specification.

BOUN If the BOUNDARY modifier is present, then only the external boundary nodes are selected. Any elements interior to the computational domain are excluded.

FLUI See Mode 1 Specification.

SOLI See Mode 1 Specification.

d_cyl The diameter of the cylinder of the identified subregion.

N1,...Nn In the absence of the IJK or ELEM modifier, these specify the (x,y) or the (x,y,z) coordinates of the center of the cylinder. In the presence of IJK or ELEM modifier these are interpreted as given below.

IJK The numerical input [N1, . Nn] specifies the grid indices (I,J) or (I,J,K) of the element. The center of the circle or cylinder is assumed to coincide with the center (node) of the element. 2 values must be specified for 2D and 3 for 3D geometry.

ELEM The numerical input [Nn] specifies the element which is at the center of the cylinder. Only 1 value must be specified.

Nm+1 The components of a vector (2 values in 2D and 3 in 3D) normal to the plane in which the center of the cylinder is located. An elliptic region can be selected by appropriate choice of the normal vector. The values may be in arbitrary units and are internally converted to unit normals. At least one value must be specified.

Nm+1 The half-length of the cylinder or the tolerance in the direction normal to the plane of the circle. The logic employed computes the normal and tangential distance of the existing element centers (nodes) from the center of circle in reference to the specified plane. If the tangential distance is ≤ the radius of the cylinder, then the element is included provided its normal distance from the plane is less than the tolerance. By default the tolerance is set to a large number (1.E+30) so that all elements in the projected plane of the circle are captured. This input may be used to specify a different tolerance to capture only elements within a certain distance from the plane. If specified, the intervening values for all components of the unit normal (even if zero) must be specified.

fname See Mode 1 Specification.

EXAMPLES
LOCAte CIRCle dia=0.4, center coordinates (2., 0.5) !2D
LOCAte CIRCle dia=0.4, center coordinates (2., 0.5) external BOUNdary only !2D
LOCAte CIRCle dia=0.4, center coordinates (2., 0.5, 0.5 )
LOCAte CIRCle dia=0.4, center coordinates (2., 0.5, 0.5 ) normals (1.,1.0.) ! 45 degree in xy
LOCAte CYLInder dia=0.4, center coordinates (2., 0.5, 0.5 ) normals (1.,1.0.) half length=0.5
LOCAte CYLInder dia=0.4, center (2., 0.5, 0.5 ) normals (1.,1.0.) half length=0.5 file 'Cylinder.loc'
LOCAte CYLInder dia=0.4, center IJK at (11,5,7 ) normals (1.,1.0.) half length=0.5
LOCAte CYLInder dia=0.4, center ELEMent at (147 ) normals (1.,1.0.) half length=0.5
MODE 5: Specification of a Spherical Subregion

SYNTAX

\texttt{LOCA \{SPHE\} [ID=idsub] [FIEL] [FLUI|SOLI] \{R_{sphere}\} [N_{1}, \ldots, N_{n}] \{fname\}}

SPHE

A spherical (circular in 2D) subregion is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the FIELD modifier is present.

idsub

See Mode 1 specification.

FIEL

See Mode 1 Specification.

FLUI

See Mode 1 Specification.

SOLI

See Mode 1 Specification.

R_{sphere}

The radius of the sphere for the identified subregion.

N_{1}, \ldots, N_{n}

The (x,y) or the (x,y,z) coordinates of the center of the sphere.

fname

See Mode 1 Specification.

EXAMPLES

\texttt{LOCAte SPHEre radius=0.4, center coordinates (2., 0.5)} \quad \text{!2D}

\texttt{LOCAte SPHEre radius=0.4, center coordinates (2., 0.5, 0.5 )}

\texttt{LOCAte SPHEre radius =0.4, center coordinates (2., 0.5, 0.5 ) FIEL node only}

\texttt{LOCAte SPHEre radius =0.4, center coordinates (2., 0.5, 0.5 ) output to file ‘SPHERE.LOC’}
MODE 6: Specification of an Annular Subregion

SYNTAX

LOCA {ANNU} [ID=idsub] [FIEL] [FLUI|SOLI] {} [D_o, D_i] [N_1, N_n] [IJK|ELEM] [N_{n+1},..N_m], [N_{m+1}] [fname]

ANNU
An annular subregion is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the FIELD modifier is present.

idsub
See Mode 1 specification.

FIEL
See Mode 1 Specification.

FLUI
See Mode 1 Specification.

SOLI
See Mode 1 Specification.

D_o
The outer diameter of the annulus (circular or cylindrical) of the identified subregion.

D_i
The inner diameter of the annulus (circular or cylindrical) of the identified subregion.

N_1, N_n
In the absence of the IJK or ELEM modifier, these specify the (x,y) or the (x,y,z) coordinates of the center of the circle or the cylinder. In the presence of IJK or ELEM modifier these are interpreted as given below.

IJK
The numerical input [N_1, ..., N_n] specifies the grid indices (I,J) or (I,J,K) of the element. The center of the circle or cylinder is assumed to coincide with the center (node) of the element. 2 values must be specified for 2D and 3 for 3D geometry.

ELEM
The numerical input N_i specifies the element which is at the center of the cylinder. Only 1 value must be specified.

N_{n+1}, ..., N_m
See Mode 4 Specification.

N_{m+1}
See Mode 4 Specification.

fname
See Mode 1 Specification.

EXAMPLES

LOCAte ANNUlus outer dia=0.4, inner dia = 0.2 center coordinates (2., 0.5) !2D
LOCAte ANNUlar Cylinder dia=0.4, d_inner=0.2 center (2., 0.5, 0.5 ) normal (1.,1.0.) half length=0.5

All Examples from Mode 4 apply except that the inner diameter must follow as the second numerical value. All subsequent input is in the same order.
MODE 7: Subregion Specification by Material Type

SYNTAX

LOCA {MATE|ZONE} [ID=ids]ub [Nmat] {FIEL} [FLUI|SOLI] [fname] 

MATE

The subregion is identified by a Material type of Zone number.

ZONE

Same as MATE modifier.

idsub

See Mode 1 specification.

Nmat

The material type or zone number that previously appeared in a MATERIAL (or an equivalent) command. The material type may denote a non-contiguous and non-rectangular subregion.

FIEL

See Mode 1 Specification.

FLUI

See Mode 1 Specification.

SOLI

See Mode 1 Specification.

fname

See Mode 1 Specification.

COMMENTS

This mode of the LOCA command is currently implemented in a limited manner; please consult ACRi before its use.

EXAMPLES

LOCAte MATErial type 3 as the active subregion
LOCAte ZONE number 5 as subregion with ID=TYP5
LOCAte ZONE number 5 as subregion with ID=TYP5 FIELd nodes only
MODE 8: Subregion Specification by a Random List of Coordinates

SYNTAX

```
LOCA  {COOR} {LIST} [ID=idsub] [FIEL] [FLUI] [SOLI] [fname] {N1, N1, ..., Nn}
```

**COOR**

Explicit list of coordinates that specify a number of points are specified. For each point, the nearest element (by location of its node) is selected and included in the subdomain. Only the internal elements are selected. If a point is located at or outside the domain boundary, then the nearest element inside the domain is selected. Associated boundary nodes are automatically included unless the **FIELD** modifier is present.

**LIST**

This modifier denotes that the **COOR** modifier applies to a random list. It must be present to invoke this mode of the command.

**idsub**

See Mode 1 specification.

**FIEL**

See Mode 1 Specification.

**FLUI**

See Mode 1 Specification.

**SOLI**

See Mode 1 Specification.

**fname**

If a file name is present then the file may be used for input or output. The **input mode** is activated if a file name is specified with only one numerical value (N1). The file may contain a header field with up to 100 lines (records) of information. The header field, if present, must end with the record “END HEADER” and the numerical values must immediately follow this record. In the **output mode**, a file is generated that lists the element and surface number pairs and, for structured grids, a list of (I,J,K) grid indices. In the file input or output mode, a valid name (see Section 3.3) must be specified.

**N1**

If the file input mode with a valid **fname** is activated, then N1 denotes the number of elements to be read from the file. If the file input mode is not activated, then N1, ..., Nn are described below.

**N1, ..., Nn**

The (x, y) or (x, y, z) coordinates for the points that comprise the list. For each point, 2 values must be specified for the 2D and 3 for 3D geometry. There is no default value.

**REMARKS**

If a **SCALE** command is specified immediately preceding this command, then the input coordinate values are scaled as described in the **SCALE** command.

**EXAMPLES**

```
LOCAte COORDinate LIST:  (0.,0.), (2,2), (1.53,1.37), (23.1,27.2)  ! List for 4 points in 2D
LOCAte COORDinate LIST:  (0.,0,0), (2,2,2), (1.53,1.37,1), (23.1,27.2,2)  ! List for 4 points in 3D
LOCAte COORDinate LIST of 500 elements as ID=BIG from file ‘XYZ.LST’  ! Read from file
LOCAte COORD LIST 500 as ID=BIG from file ‘XYZ.LST’ only FIELD  ! Read file; only field
LOCAte COORD LIST:  (0.,0), (2,2), (1.53,1.37), (23.1,27.2) output to ‘FILE.rgn’  ! List with output file
```
MODE 9: Subregion Specification by Grid Indices for Structured Grid

SYNTAX

LOCA {IJK|IJ} [EXTE] [ID=idsub] [FIEL] [FLUI|SOLI] [fname] {N_1|N_1, ..., N_n}

IJK
An explicit list of grid indices of elements (I,J) for 2D or (I,J,K) for 3D geometry is specified. This option can be used only for structured grids. Unless the modifier EXTERIOR is present, only the internal elements of the computational domain can be specified.

IJ
Same as IJK.

EXTE
By default only the internal elements of the domain of computations can be included in the list. If this modifier is present, then the list may include the grid indices for the corners, edges and boundaries of the domain of computations.

idsub
See Mode 1 specification.

FIEL
See Mode 1 Specification.

FLUI
See Mode 1 Specification.

SOLI
See Mode 1 Specification.

fname
If a file name is present then the file may be used for input or output. The input mode is activated if a file name is specified with only one numerical value (N_1). The file may contain a header field with up to 100 lines (records) of information. The header field, if present, must end with the record “END HEADER” and the numerical values must immediately follow this record. In the output mode, a file is generated that lists the element and surface number pairs and, for structured grids, a list of (I,J,K) grid indices. In the file input or output mode, a valid name (see Section 3.3) must be specified.

N_1
If the file input mode with a valid fname is activated, then N_1 denotes the number of elements to be read from the file. If the file input mode is not activated, then N_1, ..., N_n are described below.

N_1, ..., N_n
These specify the grid indices for the list of elements. For each element, 2 values must be specified for the 2D and 3 for 3D geometry.

EXAMPLES

LOCAte ID=LISTIJK by IJK indices: (2,5), (3,3), (5,7), (9,2), (3,4) for a two-dimensional structured grid
LOCAte ID=LIST by IJ indices: (2,5), (3,3), (5,7), (9,2), (3,4) only FIELD elements
LOCAte IJK indices: (2,5,2), (3,3,5), (5,7,2), (9,2,3), (3,4,5) for three-dimensional structured grid
LOCAte IJK indices: (1,1), (1,22), (22,1), (22,22), EXTERIOR corner points of the grid
LOCAte IJK indices: 50 values from the file ‘GETLIST.IJK’
MODE 10: Subregion Specification by a List of Elements

SYNTAX

```
LOCA {LIST} [ID=idsub] [FIEL] [FLUI|SOLI] [fname] {N₁|N₁,...,Nₙ}
```

**LIST**

Explicit list of element numbers is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the **FIEL** modifier is present. For unstructured grids this is the default mode of the command; however the modifier must be specified for a structured grid.

**idsub**

See Mode 1 specification.

**FIEL**

See Mode 1 Specification.

**FLUI**

See Mode 1 Specification.

**SOLI**

See Mode 1 Specification.

**fname**

If a file name is present then the file may be used for input or output. The **input mode** is activated if a file name is specified with only one numerical value (N₁). The file may contain a header field with up to 100 lines (records) of information. The header field, if present, must end with the record “END HEADER” and the numerical values must immediately follow this record. In the **output mode**, a file is generated that lists the element and surface number pairs and, for structured grids, a list of (I,J,K) grid indices. In the file input or output mode, a valid name (see Section 3.3) must be specified.

**N₁**

If the file input mode with a valid **fname** is activated, then N₁ denotes the number of elements to be read from the file. If the file input mode is not activated, then N₁, ..., Nₙ are described below.

**N₁,..,Nₙ**

The element numbers that define the subregion.

**EXAMPLES**

```
LOCAte element numbers LIST:  1, 2, 3, 7, 17, 29           ! Structured Grid
LOCAte element numbers:  1, 2, 3, 7, 17, 29                ! Default for Unstructured Grid
LOCAte LIST of  500 elements from file ‘ZONE.BIG’          ! Read from file
LOCAte  5000 elements from file ‘ZONE.BIG’                  ! Read from file for Unstructured Grid
LOCAte LIST 79, 33, 34, 89, 2, 7 with ID=LST1 and output on file “LST1.LOC” ! Write to file
```
MODE 11: Subregion Specification Defined by Sequential Elements

SYNTAX

LOCA {SEQU} [ID=idsub] [FIEL] [FLUI|SOLI] {N1, N2} [N3]

SEQU

A sequence of elements is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the FIELD modifier is present. For unstructured grids this is the default mode of the command; however the modifier must be specified for a structured grid.

idsub

See Mode 1 specification.

FIEL

See Mode 1 Specification.

FLUI

See Mode 1 Specification.

SOLI

See Mode 1 Specification.

N1, N2, N3

These three numbers specify the starting, the ending and the interval index for the element numbers in the sense of a FORTRAN DO loop. If N3 is not specified, it is assumed to be 1.

EXAMPLES

LOCAte ID=ILISTSEQ of SEQUential elements from 1 through 51 interval=10
LOCAte SEQUence from 31 to 51 ! All elements from 31 to 51, inclusive
MODE 12: Subregion Specification Defined by Sequential Elements

SYNTAX

LOCA {RANG} {Φ} {Φ_min, Φ_max} [ID=idsub] [FIEL] [FLUI|SOLI]

RANG
A sequence of elements that have a value of the variable that satisfies the given constraints is included in the specified subdomain identified with ID=idsub.

Φ
A symbol for the variable the value of which is used as the criterion for selecting the elements that fall within the specified range. The valid symbols are listed in Table 2.8.1-3.

Φ_min, Φ_max
All elements that satisfy the criterion Φ_min ≤ Φ ≤ Φ_max are selected to be included in the subdomain.

idsub
See Mode 1 specification.

FIEL
See Mode 1 Specification.

FLUI
See Mode 1 Specification.

SOLI
See Mode 1 Specification.

EXAMPLES

LOCAte RANGE of P between 10 and 100 as ID=P_RANGE
LOCAte RANGE of P between 10 and 100 for FLUID elements as ID=P_FLUID
MODE 13: Specification of a Given Location as a Station

SYNTAX

LOCA {STAT} {ID=idsub} {N, ..., N} [fname]

STAT

A single location is identified as a station for subsequent input. The field values are then obtained by interpolation of values at the specified stations.

idsub

See Mode 1 specification. In this mode, the identifier must be specified.

N1, .., Nn

The grid coordinates (x,y,z) for the station. Two numerical values for 2D and three for 3D input modes must be provided. There is no default value for this input; the required number of numerical values must be specified.

fname

See Mode 1 Specification.

EXAMPLES

LOCAte STAT ID=LOC2 at (0., -20.)
LOCAte STATion ID=LOC2 at coordinates (x=50., y=0., z=0.20)
LOCAte STATion ID=LOC2 at coordinates (x=50., y=0., z=0.20) output on file ‘Station.Loc’
MODE 14: Subregion of Matched Elements

SYNTAX  LOCA {CORR} {ID=idsub1} {ID=idsub2} [ID=idsub] [fname]

CORR  A subregion of correlated elements is defined for special purposes. The subregion consists of two sets of elements which are paired with each other. The pairing takes place in a parallel sequential mode where the 1st element in the 1st subregion is paired with the 1st element of the 2nd subregion, and so on. This type of subregion can only be used with certain commands (e.g. CORRLEATION) where the values at the elements in the 1st set are paired with, or dependent on, the values of the elements in the 2nd set.

idsub1  The name of the 1st subregion to be operated upon. There is no default value; a valid name of a previously specified subdomain with the ID modifier must be specified.

idsub2  The name of the 2nd subregion to be operated upon. There is no default value; a valid name of a previously specified subdomain with the ID modifier must be specified.

idsub  A unique identifier for the subregion. Only the first 8 characters are meaningful; any subsequent characters are ignored. This identifier may be subsequently used in an input command to provide selective input for that subregion. If the identifier is omitted, then the modifier LOCATE or SELECT on the command can make a generic reference to the specified subregion until the next LOCATE or SELECT command. See Section 3.4 for additional details.

fname  If a file name is present then a file is generated that lists the elements and, for structured grids, a list of (I,J,K) grid indices. A valid name (see Section 3.3) must be specified.

EXAMPLES

LOCAte CORRelated Elements from ID=REGION1 and ID=REGION2
LOCAte CORRelated Elements from ID=REGION1 and ID=REGION2 as ID=MATCHED on file='match.fil'
MODE 15: Boundary Specification by Paired Element and Surface Numbers

SYNTAX

LOCA {PAIR} [ID=idsub] [fname] [N1, N2, N3, ..., Nn]

PAIR

Explicit paired list of element and surface numbers is specified.

idsub

See Mode 1 specification.

fname

If a file name is present then the file may be used for input or output. The input mode is activated if a file name is specified with only one numerical value (N1). The file may contain a header field with up to 100 lines (records) of information. The header field, if present, must end with the record "END HEADER" and the numerical values must immediately follow this record. In the output mode, a file is generated that lists the element and surface number pairs and, for structured grids, a list of (I,J,K) grid indices. In the file input or output mode, a valid name (see Section 3.3) must be specified.

N1

If the file input mode is activated, then, N1 denotes the number of pairs of element and surface numbers to be read from the file. Each pair must specify an element number and a surface number as explained in N1, N2 below. If the file input mode is not activated, then N1 is interpreted as given below.

N1, N2

N1 is the element number and N2 is the surface number for the 1st element and surface pair that comprise the subregion. The surfaces of the element are numbered from 1 to 4 in the 2D and 1 to 6 in the 3D mode. See Section 3.4 for further details of the manner in which these surface numbers are assigned.

N3, ..., Nn

The element number and a surface number for the rest of the elements which comprise current subregion in the manner N1 and N2.

EXAMPLES

LOCAe (element, surface) PAIRs: (35,1), (53,3), (77,2), (13,4)
LOCAe PAIR : (35,1), (53,3), (77,2), (13,4) as boundary ID=BNDRy
LOCAe PAIR : 500 sets as ID=BNDRy from file ‘BOUNDARY.BIG’
LOCAe PAIR : (35,1), (53,3), (77,2), (13,4) as boundary ID=BNDRy
LOCAe PAIR : (35,1), (53,3), (77,2), (13,4) as boundary ID=BNDRy
LOCAe PAIR : (35,1), (53,3), (77,2), (13,4), (28,5), (33,3), (35,6) output on file “Boundary.LOC”
**MODE 16:** Boundary Specification by List of Vertices

**SYNTAX**

\`\`LOCA \{VERT\} \{ID=idsub \} \{fname\} \{EXCL\} \{SEQU\} \{option\} \{N_1, N_2, ..., N_n\}\`

**VERT**
The boundary region defined by the specified sets of vertices is selected.

**idsub**
See Mode 1 specification.

**fname**
If a file name is present then the file may be used for input or output. The input mode is activated if a file name is specified with only one numerical value (N_1). The file may contain a header field with up to 100 lines (records) of information. The header field, if present, must end with the record “END HEADER” and the numerical values must immediately follow this record. In the output mode, a file is generated that lists the element and surface number pairs and, for structured grids, a list of (I,J,K) grid indices. In the file input or output mode, a valid name (see Section 3.3) must be specified.

**EXCL**
If the modifier is present, then the boundary specified by the vertices is excluded and the complimentary set of the domain boundary is selected.

**SEQU**
The numerical input specifies a sequence of element numbers.

**option**

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANY</td>
<td>By default a boundary element (or node) is included in the selection only if all its vertices are included in the list of vertices. If ANY modifier is specified then a boundary element is included if any of its vertices is included in the list.</td>
</tr>
<tr>
<td>ONE</td>
<td>A boundary element is included if at least one of its vertices is included.</td>
</tr>
<tr>
<td>TWO</td>
<td>A boundary element is included if at least two of its vertices are included.</td>
</tr>
<tr>
<td>THRE</td>
<td>A boundary element is included if at least three of its vertices are included.</td>
</tr>
<tr>
<td>FOUR</td>
<td>A boundary element is included if at least four of its vertices are included.</td>
</tr>
</tbody>
</table>

**N_1**
If the file input mode is activated, then, N_1 denotes the number of vertices to be read from the file. If the file input mode is not activated, then N_1, ..., N_n are described below.

**N_1,...,N_n**
In the absence of the SEQUENCE modifier, these numbers identify the vertices that define the boundary of interest. In the presence of the SEQUENCE modifier only N_1, N_2 and N_3 are meaningful. In this case, these three numbers specify the starting, the ending and the interval index for the vertices in the sense of a FORTRAN DO loop.

**REMARKS**
The complementary operation cannot be performed on regions that are defined by MATCHED PAIR or CORRELATED type of element sub-domains or on previous LOCATE commands defined with a FIELD modifier.

**EXAMPLES**

- `LOCAt: VERTices 1,3,7,8,10,20,55,99,203,105,77`
- `LOCAt VERTices: in SEQUence from 23 through 231 in steps of 3 as boundary ID=BNDRy`
- `LOCAt VERTices: 500 values as ID=BNDRy from file ‘BOUNDARY.BIG’`
- `LOCAt VERTices: in SEQUence 23 to 231 in steps of 3 ID=BNDRy output file: ‘Boundary.LOC’`
MODE 17: Boundary Specification by Exclusion of Previously Specified Boundary

SYNTAX LOCA \{BOUN\} \{UNSP\} [ID=idsub]

BOUN A boundary subregion is selected from the total external boundary of the domain by excluding the surfaces defined by all the previous LOCATE commands which identify a boundary (LOCATE PAIR, LOCATE VERTex, LOCATE COORDINATE BOUNDARY and LOCATE POLYGON BOUNDARY commands). This modifier must be present to activate this mode of the command.

UNSP Selects the previously unspecified boundary. This modifier must be present to activate this mode of the command.

idsub See Mode 1 specification.

EXAMPLES

LOCAte previously UNSpecified BOUNdary
LOCAte previously UNSpecified BOUNdary as ID=BND_UNSpecified
MODE 18: Boundary Specification as a Complimentary Surface of a Previous Subregion

SYNTAX

LOCA {COMP} {ID=idsub1} {dir1} [ID=idsub] [fname]

COMP
A new sub region is created that represents the complimentary side of the surface of a previous sub region. Each surface that connects two elements can be viewed from the side of either element. This command can be used to select the complimentary side. It can not be used for the exterior surface of the domain or on regions that are defined by MATCHED PAIR or CORRELATED type of element sub domains or on previous LOCATE commands defined with a FIELD modifier.

Idsub1
The identification or name of the previous subregion to be operated upon. There is no default value; a valid name must be specified.

dir1
The orientation index of the subregion idsub1 that points to the surface to be matched with the complimentary surface. See Section 3.5 for available choices. This input is not required if idsub1 was defined by a LOCATE PAIR command.

Idsub
See Mode 1 Specification.

fname
If a file name is present then a file is generated that lists the elements and, for structured grids, a list of (I,J,K) grid indices. A valid name (see Section 3.3) must be specified.

EXAMPLES

LOCAte COMPlimentary ID=DMN1 as ID=DMN2
LOCAte COMPlimentary of X- direction of ID=DMN1 ID=DMN2
Keyword Commands

MODE 19: Specification of a General Second Order Surface

SYNTAX

```
LOCA  { SURF } { BOUN } { N1, N2, ... Nn } [ TOLE = (ε) ] [ ID=idsub ] [ fname ]
```

**SURF**

All boundaries of the elements in the vicinity of a general second order surface are selected. The 2D and 3D surfaces are specified, respectively, as:

\[
C_0 = C_1 x + C_2 y + C_3 x^2 + C_4 y^2 + C_5 x y
\]

\[
C_0 = C_1 x + C_2 y + C_3 z + C_4 x^2 + C_5 y^2 + C_6 z^2 + C_7 x y + C_8 y z + C_9 z x
\]

This specification results in the location of a boundary Pair type of subregion that consists of the element nearest to the surface and the element boundary in the vicinity of the surface.

**BOUN**

If this modifier is present then only the external boundary nodes are searched to satisfy the surface constraint. Otherwise all the element boundaries are searched.

**N1,..,Nn**

These specify the coefficients \( C_0 \) through \( C_5 \) (for 2D) or \( C_0 \) through \( C_9 \) (for 3D). Any trailing coefficients not specified are assumed to be zero. At a minimum \( C_0 \) through \( C_2 \) (for 2D) or \( C_0 \) through \( C_3 \) (for 3D) must be specified.

**TOLE**

If this modifier is present then the last value on the command is assumed to be the tolerance for judging the proximity to the specified surface.

\( \varepsilon \)

The tolerance for judging the proximity to the surface. This numerical value must be present if the modifier **TOLERANCE** is specified. The default value is \( 10^{-7} \).

**idsub**

See Mode 1 specification.

**fname**

If a file name is present then a file is generated that lists the element boundary pairs, and, for structured grids, a list of (I,J,K) grid indices. A valid name (see Section 3.3) must be specified.

**EXAMPLES**

```
LOCAte SURFACE 2 = 1. *x + 1. * y \\
    ! 2D mode
LOCAte external BOUNdary SURFACE 2 = 1. *x + 1. * y + 0. * z \\
    ! 3D mode
LOCAte SURFACE 1 = -1. x -1. y -1. z + 1. xx + 1. yy +1. zz +0. xy -1. yz
LOCAte SURFACE 1 = -1. x -1. y -1. z + 1. xx + 1. yy +1. zz +0. xy -1. yz ID=SURF2 file="SURF2.LOC"
LOCAte BOUNdary SURFACE 1 = -1. -1. -1. +1. +1. TOLERance=1.1.E-9 ID=SURF2
```
MODE 20: Matched Surface Subregion from Specified List

SYNTAX

LOCA \{MATC\} \[ ID=idsub \] \{fname\} \{ N_1|N_1,…,N_4, N_5, … , N_n \}

MATC

A matched surface type of subregion is defined which is a special type of subregion consisting of two matched surfaces. It can only be used with the TRANSFER command that transports fluid flux along with specified fluid properties from one surface to another with or without transformation.

idsub

See Mode 1 Specification.

fname

If a file name is present then the file may be used for input or output. The input mode is activated if a file name is specified with only one numerical value (N_1). The file may contain a header field with up to 100 lines (records) of information. The header field, if present, must end with the record “END HEADER” and the numerical values must immediately follow this record. In the output mode, a file is generated that lists the element and surface number pairs and, for structured grids, a list of (I,J,K) grid indices. In the file input or output mode, a valid name (see Section 3.3) must be specified.

N_1

If the file input mode is activated, then, N_1 denotes the number of matched sets of pairs of element and surface numbers to be read from the file. Each set of pairs must specify 4 values as explained in N_1,…,N_4 below. If the file input mode is not activated, then N_1 is interpreted as defined in N_1,…,N_4 below.

N_1,…,N_4

A set consisting of 2 element and surface number pairs which define the 1st and 2nd surfaces to be matched. N1 and N2 define the 1st surface whereas N3 and N4 define the 2nd surface. The surfaces of the element are numbered from 1 to 4 in the 2D and 1 to 6 in the 3D mode. See Section 3.4 for further details of the manner in which these surface numbers are assigned.

N_5,…,N_n

The matched sets of element and surface number pairs in the manner of N_1,…,N_4 above.

EXAMPLES

LOCAte MATCH LIST of values: (23,1) & (57,2); (25,3) & (67,4); (27,3) & (69,5) ID=MATCHED
LOCAte MATCH LIST (23,1) & (57,2); (25,3) & (67,4); (27,3) & (69,5) ID=MATCHED on file='match.fil'
LOCAte MATCH LIST 3 sets from file 'match.loc'
MODE 21: Matched Surface Subregion from Two Previously Defined Subregions.

SYNTAX

```
LOCA {MATC} {ID=idsub1} {dir1} {ID=idsub2} {dir2} [INTE] [ID=idsub] [fname]
```

MATC

A matched surface type of subregion is defined which is a special type of subregion consisting of two matched surfaces. It can only be used with the TRANSFER command that transports fluid flux along with specified fluid properties from one surface to another with or without transformation.

idsub1

The name of the 1st subregion to be operated upon. There is no default value; a valid name must be specified.

dir1

The orientation index of the subregion idsub1 that points to the surface to be matched with a similar surface of subregion idsub2. See Section 3.5 for available choices. This input is not required if idsub1 was defined by a LOCATE PAIR command.

idsub2

The name of the 2nd subregion to be operated upon. There is no default value; a valid name must be specified. However idsub2 may be identical to idsub1, if required.

dir2

The orientation index of the subregion idsub2 that points to the surface to be matched with a similar surface of subregion idsub1. See Section 3.5 for available choices. This input is not required if idsub2 was defined by a LOCATE PAIR command.

INTE

By default the faces that are matched are the outward directed surfaces (dir1 and dir2 with normal pointing out of the body) of the subregions idsub1 and idsub2. If the INTERIOR modifier is present, then the interior surfaces of the idsub1 and idsub2 are matched with each other.

idsub

See Mode 1 Specification.

fname

If a valid file name is present, then an ordered list of elements and surface numbers selected by the command are written to the file. For a structured grid, the grid indices (I,J,K) are also written to the file.

EXAMPLES

```
LOCAte MATCH X- direction of ID=DMN1 and X+ direction of ID=DMN1 as ID=MATCHED
LOCAte MATCH X- direction of ID=DMN1 and X- of ID=DMN2 INTERnal surfaces as ID=MATCH2
LOCAte MATCH X- direction of ID=DMN1 and X- of ID=DMN2 as ID=MATCH2 also file='MATCH.FIL'
```
MODE 22: Subregion by Union or Intersection of Two Previous Subregions

SYNTAX

\[ \text{LOCA} \{ \text{UNIO} | \text{INTE} \} \{ \text{ID}=\text{id1} \} \{ \text{ID}=\text{id2} \} \cdots \{ \text{ID}=\text{idn} \} \{ \text{NOT} \} \{ \text{EXCL} \} \{ \text{ID}=\text{idsub} \} \{ \text{FIEL} \} \{ \text{fname} \} \]

UNIO

The new subregion is created from the union (elements that belong to either) of two or more previously specified subregions. There is no default value. Either UNIO or the INTERSECTION modifier must be present to invoke this mode of the command.

INTE

The new subregion is created from the intersection (elements that belong to more than one subregion) of previously specified subregions.

id1, id2,...idn

The identification or name of the 1st through the n\textsuperscript{th} subregion to be operated upon. There is no default value; a set of valid names for previously specified subregions must be given. If one subdomain is of the surface or boundary type (see, e.g., LIST PAIR), then all subdomains must be of the same type. **No more than 256 subregions may be specified on one command.**

NOT

This modifier selects the union of multiple subregions minus their intersection (elements that belong to one and not more than one subdomain). This modifier is effective only if the INTERSECTION modifier is also specified.

EXCL

If the modifier is present, then the specified elements are excluded and the complimentary set in the computational domain is selected. For example, if the union is selected, and this modifier is present, then all the elements that belong in the union are excluded and rest of the computational domain is selected. **This modifier can not be used if the any of the specified subdomains is of the surface (e.g., LIST PAIR) type.**

idsub

See Mode 1 Specification.

FIEL

See Mode 1 Specification.

fname

If a valid file name is present, then an ordered list of elements and/or surface numbers selected by the command are written to the file. For a structured grid, the grid indices (I,J,K) are also written to the file.

REMARKS

The union and intersection operations cannot be performed on subregions that were previously defined by a LOCATE command with MATCHED PAIR, CORRELATED or INJECTION modifiers.

EXAMPLES

- \text{LOCA}te UNIO\text{n} of ID=DMN1 and ID=DMN2
- \text{LOCA}te UNIO\text{n} of ID=DMN1 and ID=DMN2 as ID=DMN3
- \text{LOCA}te INTER\text{section} ID=DMN1 and ID=DMN2
- \text{LOCA}te UNIO\text{n} of subregions ID = DMN1 and ID=DMN2 EXCLude selection only FIELd elements
- \text{LOCA}te UNIO\text{n} of ID=DMN1 and ID=DMN2; EXCLude selected and name ID=DMNM12
- \text{LOCA}te ID=DMN1 plus ID=DMN2 select INTER\text{section} & EXCLude
- \text{LOCA}te ID=DMN1 plus ID=DMN2 select NOT INTER\text{section} & EXCLude output on file ‘DMN12.LOC’
MODE 23: Subregion Contiguous to a Boundary or Surface

SYNTAX

```
LOCA {CONT} {ID=idsub1} {ID=idsub2} {x0, y0, [z0]} {ID=idsub} [FIEL] [fname]
```

**CONT**
This modifier selects that part of the subregion **idsub1** that is bifurcated by the 2nd subregion (**idsub2**) that contains the coordinate specified by **x0, y0, [z0]**. The new subregion is created from the elements that belong to the 1st subregion and are contiguous to the 2nd subregion but only on the side of the 2nd subregion where the point specified by the **x0, y0, z0** coordinates is located. The nodes contained in the 2nd subregion will also be excluded. The 2nd subregion must bifurcate the 1st region completely into 2 parts for this command to be effective. If bifurcation is incomplete then all points minus the 2nd subregion will be selected. There is no default value.

**idsub1**
The identification or name of the 1st subregion to be operated upon. This subregion must not be a boundary or surface type (such as LOCATE PAIR) of region. There is no default value; a valid name must be specified.

**idsub2**
The identification or name of the 2nd subregion that divides the 1st subregion into two parts. It can be a region or a boundary or surface. There is no default value; a valid name must be specified.

**x0, y0, [z0]**
The coordinates of the point that decides which part of the bifurcated region is to be selected. The elements selected will contain the node nearest to specified point and all nodes that are connected to it up to, but not including, the nodes in the 2nd subregion or nodes on the other side of the 1st subregion. The coordinates must lie within the boundaries of the 1st subregion. Two values must be specified for 2D and three for 3D geometry. There is no default value.

**idsub**
See Mode 1 Specification.

**FIEL**
See Mode 1 Specification.

**fname**
If a valid file name is present, then an ordered list of elements and/or surface numbers selected by the command are written to the file. For a structured grid, the grid indices (I,J,K) are also written to the file.

**EXAMPLES**

```
LOCAte CONTiguous part of ID=DMN1 bifurcated by ID=DMN2 and containing point (2.02, 1.002) !2D
LOCAte CONTiguous section of ID=DMN1 bifurcated by ID=DMN2 with point (2.02, 1.002, 3.46) !3D
```
MODE 24: Subregion by Reassignment of a Previous Subregion

SYNTAX

\[ \text{LOCA} \{ \text{ID}=\text{idsub1} \} \{ \text{EXCL} \} \{ \text{ID}=\text{idsub} \} \{ \text{FIEL} \} \{ \text{fname} \} \]

**idsub1**

The identification or name of the subregion to be operated upon. There is no default value; a valid name must be specified.

**EXCL**

By default a new subregion is defined which is identical to the previously specified subregion identified by id=idsub1. If this modifier is present, then the specified elements are excluded and the complimentary set in the computational domain is selected.

**idsub**

See Mode 1 Specification.

**FIEL**

See Mode 1 Specification.

**EXAMPLES**

\[ \text{LOCA} \text{te ID}=\text{DMN1} \text{ as new subdomain called ID}=\text{DMN2} \]
\[ \text{LOCA} \text{te EXCLude ID}=\text{DMN1} \text{ and define new complimentary set as ID}=\text{COMPDMN1} \]
\[ \text{LOCA} \text{te EXCLude ID}=\text{DMN1} \text{ and define new complimentary FIELd only set as ID}=\text{COMPDMN1} \]
\[ \text{LOCA} \text{te EXCLude ID}=\text{DMN1} \text{ and define new complimentary FIELd only set as active subregion} \]
## MODE 25: Modified Subregion with Post-Processing for Special Features

### SYNTAX

```
LOCA {FLUI|SOLI|UNIQ} { ID=idsub1 } [ID=idsub2] [FIEL] [fname]
```

### FLUI
To modify or define a subregion so that only the fluid side elements are retained; any elements that are solid or blocked are eliminated. If the command defines a boundary surface, then only the surface numbers looking from the fluid side are retained; those that are defined by surface number for blocked or solid elements are eliminated.

### SOLI
To modify or define a subregion so that only the solid side elements are retained; any elements that are located in the fluid or unblocked region are eliminated. If the command defines a boundary surface, then only the surface numbers looking from the solid side are retained; those that are defined by elements and surface number pairs where the element is located in the fluid are eliminated.

### UNIQ
Any duplicate specifications of an element or boundary are removed; only the 1st occurrence is retained. If the subregion refers to a boundary segment, then this boundary is shared by two adjoining elements unless it is an exterior boundary of the domain. Any interior boundary can therefore be specified by two alternative pairs – each referring to one of the two elements that share that boundary. Mathematically this is equivalent to specifying a surface and its direction normal pointing in one or the other opposite directions that are 180 degrees apart. Such duplicate specifications are also removed if this modifier is present.

#### idsub1
The identification or name of the subregion to be operated upon. If idsub2 is not present, then the existing idsub1 sub domain will be modified. If idsub2 name is present, the original idsub1 domain is retained and modified sub-domain is defined with the new idsub2 name. There is no default value; a valid name must be specified.

#### idsub2
The identification name of the new subregion. If this modifier is present, then the original subdomain stays unmodified and a new subdomain is created with the modified features.

#### FIEL
See Mode 1 Specification.

#### fname
If a valid file name is present, then an ordered list of elements and/or surface numbers selected by the command are written to the file. For a structured grid, the grid indices (I,J,K) are also written to the file.

### COMMENTS
This command can operate on either the element type of sub-domains (such as LOCATE LIST command) or boundary type of sub-domains (such as LOCATE LIST PAIR). If the idsub1 specifies a set of elements, and idsub2 is not present, then any boundary definition that was originally present is still retained. This implies that if a reference is made to a boundary of modified idsub1 (e.g. a BOUNDARY command with the dir modifier), then the boundary of the original idsub1 will be selected. If however idsub2 is specified, then it will contain the definition of the modified boundary of the sub-domain unless the FIELD modifier is also specified on the command.

### EXAMPLES

```
LOCAtE SOLId elements ID=DMN1
LOCAtE FLUId elements of ID=DMN1 as ID=DMN2
LOCAtE UNIQue elements ID=DMN1
LOCAtE UNIQue boundary segments of ID=BOUN1 as ID=BOUN2
```
MODE 26: Specification of Location of Injected Films and Curtains

**SYNTAX**

```
LOCA {INJE} [ID=idsub1] [dir] {N1, ..., Nn} [ID=idsub] [fname]
```

**idsub1**
The identification or name of the subregion to be operated upon. See Section 3.4. If no subregion is specified, the entire computational domain is selected. If idsub1 identify is a surface subregion or if a "dir" is specified then the type of injection is automatically set in "FILM mode” else type is “CURTAIN mode” (see INJECTION FILM and INJECTION CURTAIN commands).

**dir**
The orientation index for the boundary of the subregion to be selected. See Section 3.5 for available choices. If no "dir" is specified, all available “dir” for idsub1 are selected.

**N1, ..., Nn**
N1 through Nn are the grid coordinates (x, y, z) for extremities of injection segment. A total of 4 numerical values for 2D and 6 for 3D input must be provided. See Section 3.4 for additional information. There is no default value; a valid set of values must be specified.

**idsub**
See Mode 1 Specification.

**fname**
See Mode 1 Specification.

**COMMENTS**

The direction of the falling water film is defined by the direction of gravity. By default this is directed against the Z-axis of the domain.

The coordinates N1, ..., Nn define two geometric points A and B. The segment AB must match points A and B that belong to the idsub1 [dir] surface. If this surface is not a plane then the segment AB may be a curve defined by the intersection between the idsub1 [dir] surface and the plane containing A and B with the normal vector: \[ \text{g} \times (\text{AB} \times \text{g}) \].

**EXAMPLES**

```
LOCAtE INJECTION on entire X- face and define ID=ZFILM
    with injection from (0.0, 0.0, 1.8) to (0.0,5.0,2.0)
LOCAtE INJECTION on ID=BLOCK1 Y+ and define ID=ZFILM
    with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
LOCAtE INJECTION on entire domain and define ID=W CURTAIN
    with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
LOCAtE INJECTION on ID=WALLRIGHt and define ID=W FILM
    with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
LOCAtE INJECTION on SELECTed surface and define ID=W FILM
    with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
LOCAtE INJECTION on SELECTed surface and define a automatically named subregion
    with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
```
MODE 27: Moving or Evolving Rectangular Subregion by Grid Coordinates

SYNTAX

```
LOCA {MOVE | MOVI} {COOR} [ID=idsub] {N1, ..., Nn} [STOR = Nadd] [fname]
```

MOVE

A rectangular window is specified by grid (x, y, z) coordinates that can evolve or move in time.

MOVI

Same as MOVE modifier.

COOR

The window is specified by its grid (x, y, z) coordinates. Each window is defined by 2 sets of coordinates. The 1st set defines the “lower-left” corner and the 2nd set the “upper-right” corner of the window. The window is specified by 4 numerical values for 2D and 6 for 3D geometry. There is no restriction on the coordinate values except that the “upper” values must be greater than the “lower” values.

The elements are selected based on the coordinate value of the element node. All elements with the node located inside or on the boundary of the window are selected by this command. An element is considered either in or out. No account is taken of the fact that the selected elements may be partially in or out.

idsub

See Mode 1 Specification.

N1, .., Nn

N1 through Nn are the grid coordinates (x,y,z) for the “lower-left” and “upper-right” corners of the window (s). A total of 4 numerical values for 2D and 6 for 3D input must be provided. See Section 4.4 for additional information. There is no default value; a valid set of values must be specified.

STOR

The moving window may evolve with time (see MOVE command). During this process elements may be added or removed from the window. At any given time, the set of elements that form the window and the immediate boundary nodes of the window (unless FIELD modifier is specified) are stored in memory. If the number of elements in the window grows, then additional memory is required to store new elements and boundary nodes. By default the amount of additional memory allocated is set equal to the initial number of elements. If the moving window is expected to increase beyond that, then this modifier along with the maximum additional memory must be specified.

Nadd

The additional memory for the moving window over and above that originally allocated for the window. If the specified number is larger than the number of elements in the entire computational domain, then the allocated amount is truncated to the number of total elements.

fname

See Mode 1 Specification.

EXAMPLES

```
LOCAte MOVING region ID=MOVE_FRAC with initial COORDinates (0.,40.0,4.4) to (45.,60.0,4.70)
LOCAte MOVING ID=MOVE_FRAC COORDinates (0.,40.0,4.4) to (45.,60.0,4.70) STOR=1000
```
MODE 28: Stationary or Evolving Embedded Planar Fracture

SYNTAX

LOCA {FRAC} [MOVE] [MOVI] {ID=idsub} {N₁, ..., Nₙ}

FRAC

A subregion of connected elements, through which a fracture passes is specified by (x, y, z) coordinates. The region can evolve or move in time if the MOVE modifier is present. A FRACTURE command must be specified to activate the fracture. In addition one or more MOVE commands need to be specified if the fracture evolves in time.

The fracture is defined by the fracture plane specified by its coordinates. In 2D, the fracture plane is specified by exactly 2 sets of (x,y) points with a total of 4 numerical values. In 3D, the fracture plane can be any arbitrary simply connected planar polygon with non-intersecting edges. A minimum of 3 sets of (x,y,z) points with a total of 9 numerical values must be specified. The points have to be specified in order around the polygon and must form a plane. If the specified points are non-planar, the results are unpredictable.

The elements through which the fracture passes are selected based on the intersection of the fracture plane and the element faces. Elements are selected to create a contiguous path for flow within the fracture. An element is considered either in or out. No account is taken of the fact that the selected elements may be partially in or out.

MOVE

This modifier designates a fracture that can move or evolve in time.

MOVI

Same as MOVE modifier.

idsub

See Mode 1 Specification.

N₁, ..., Nₙ

The coordinates (x,y) or (x,y,z) for the points defining the fracture plane. For 2D geometry 4 numerical values must be specified. For 3D, a minimum of 9 values are required. There is no default value; a valid set of values must be specified.

COMMENTS

Currently this command is fully operational only in the 2D geometry mode. The 3D option is under development. Please contact ACRI for implementation of the 3D option.

EXAMPLES

LOCAte FRACTURE ID=FRAC2D from (20,20) to (80,80)! 2D fracture
LOCAte MOVing FRACTURE ID=FRAC3D from (15,15,25), (35,15,25), (35,35,25), (15,35,25) !3D fracture
Keyword Commands

COMMAND MATERIAL

PURPOSE Define material properties. This command is effective only for the PORFLOW™ Software Tool.

MODE 1: Specification of Material Density

SYNTAX MATE {DENS}

DENS The solid or particle density of the material is specified.

APPLICABILITY This command is available only for the PORFLOW™ Software Tool.

COMMENTS This mode of the command has been superseded by the DENSITY SOLID command. Please refer to that command.
MODE 2: Specification of Material Porosity

SYNTAX MATE {PORO}

PORO The material porosity is specified.

APPLICABILITY This command is currently available only for the PORFLOW™ Software Tool.

COMMENTS This mode of the command has been superseded by the POROSITY command. Please refer to that command.
MODE 3: Specification of Material Density and Porosity

SYNTAX MATE [PROP] \{\rho_S, \Theta_E, \Theta_T, \Theta_D\} [subrgn]

PROP

The material properties are specified. In this mode both density and porosity are specified on one command. If this specification is omitted and the modifier TYPE is not present, and the number of numerical values on the command is less than 5, then the specification is assumed to be for material properties. This mode of the command is being retained only for backward compatibility. Its function has been superseded by the DENSITY SOLID and POROSITY commands which are recommended for use instead of this mode of the command.

\rho_S

The density of a dry, solid component, \(\rho_S (> 0)\). The default value is 1.

\Theta_E

The effective (or flow) porosity, \(\Theta_E\). The default value is 1.

\Theta_T

The total porosity, \(\Theta_T\). If no value is specified, total porosity is set equal to the effective porosity.

\Theta_D

The diffusional porosity, \(\Theta_D\). If no value is specified, diffusional porosity is set equal to the effective porosity.

APPLICABILITY

This command is currently available only for the PORFLOW™ Software Tool.

COMMENTS

This mode of the command has been superseded by the DENSITY SOLID and POROSITY commands. Please refer to those commands.

EXAMPLES

MATERIAL density = 1; porosities: effective = 0.1, total 0.2, diffusive 0.15
MATERIAL density 2200, porosities: 3*0.15
MATERIAL density 2200, porosities: 0.2, 0.25, 0.21
MODE 4: Material Type for a Subregion

SYNTAX  

MATE [TYPE] {NMat} [subrgn] [FIEL] [dir]

TYPE  Identifies a material type with unique properties. This mode of the command is being retained only for backward compatibility. It is no longer required. Its function has been superseded by the LOCATE command which is recommended for use instead of this mode of the command.

NMat  A number that designates the material type or zone. A distinct number should designate each different material that has its own unique properties. The default value is 1.

For PORFLOW™, by default, the maximum assigned material type is limited to 100. If more than 100 material types are required, then the ALLOCATE MATERIAL command must be used to specify the maximum number. Though the material numbers may be assigned arbitrarily, most efficient use of memory results if these are defined sequentially.

For TIDAL™ this number indicates the type of the element. A value of 0 indicates open water and value greater than 7 indicates land. A value of 4 implies that the water height is specified by the user and the fluid velocity at the open boundary of the element is computed from the condition of zero normal gradient.

subrgn  The subregion for which the input is specified. If no subregion is specified, then the entire computational domain is selected.

FIEL  Unless the subrgn was specified by a LOCATE command with the FIELD modifier, the values are set at all nodes in the subregion and any nodes at the exterior boundary that are right next to the subrgn (see the LOCATE command). If this modifier is present, then only the interior field nodes are set by the command.

dir  By default, the input is applied to all the elements or nodes in the subregion defined by the subrgn modifier. If a modifier denoting a boundary orientation index is present, then the input is applied only to the nodes at the subregion boundary where the outward normal matches the specified modifier. See Table 3.5.1 for available choices.

APPLICABILITY  

This command is currently used only by the PORFLOW™ and TIDAL™ Software Tools; it is not used by the ANSWER™ Software Tool.

COMMENTS  

For PORFLOW™ the material type is used to provide a unique numerical identity to each material type. It is used primarily only for output purposes. For TIDAL™ the material designation is used to impose land or water boundary conditions for water height and velocity components.

EXAMPLES  

MATErial type 1! Total domain  
MATErial type 5 as the currently SELECTed subregion  
MATErial type 3 as subregion ID=COARSE_SAND  
MATErial type 5 for only the Y+ boundary of ID=GRAVEL  
MATErial type 6 for only the FIELD nodes of ID=GRAVEL
MODE 5: Material Type Data Input from a File

SYNTAX MATE {fname}

fname The name of the file from which the material type information is obtained. See Section 3.3 for additional information. In this mode, the zone designation for the entire domain of computation must be read from the file sequentially in the manner of the increasing x, y and z grid nodes, in that order. This mode can also be used to provide input only for the porous matrix zone. Any fracture or borehole features must be defined explicitly by Mode 1 input.

APPLICABILITY

This command is currently available only for the PORFLOW™ and TIDAL™ Software Tools.

EXAMPLES

MATErial type information from 'TYPE.DAT'
COMMAND  MATRIX

PURPOSE  To select the method of solution for the matrix of algebraic equations.

MODE 1:  ADI Matrix Solver

SYNTAX  MATR {ADI} [NORM] [Φ =N₁, Φ =N₂, ..., Φ =Nₙ] [ADI_dir] [ADI_options]

ADI  Matrix is solved by an alternating direction implicit method. This is the default option.

NORM  By default, the matrix is solved as computed where the coefficients of the matrix equations are in units of the computed fluxes. For example, if a species is in mass fraction units, the coefficients will be in units of [M t⁻¹]. If this modifier is present, then the matrix is normalized so that the diagonal coefficient is unity and other coefficients are non-dimensional.

Φ  One or more symbols that denote the variable(s) for which ADI matrix solver will be invoked. Valid symbols are listed in Table 2.7.1.

N₁,..., Nₙ  Number of times the matrix is “swept” for the variable denoted by the symbol immediately preceding the value. The default value may vary with each installation though it is generally set to 1 for most of the variables.

ADI_dir  One or more of the characters: X, Y, Z to denote the direction in which the matrix sweeps are made. For example, a specification of X results in the matrix equations being solved for the x-direction nodes in increasing order of the I grid index, for fixed values of the J and K indices. By default, the matrix is swept in all active coordinate directions.

ADI_options  OLD  By default the ADI rows are formed by starting from a boundary and searching for a string of element that connect that boundary with a boundary at an “opposite” face. If this modifier is present then an older element-based algorithm to be used to search for these strings. The use of this modifier is not recommended. It is retained only for compatibility with older versions.

SING  The ADI row consists of a single string of meandering elements throughout the computational domain.

COOR  The ADI rows are formed by a search based on physical coordinates rather than on the element connectivity. This is the default method for the Hybrid grids and the Gridless method.

FACE  This modifier overrides the default COOR based search for the Hybrid grids and the Gridless method. The rows are formed from a face-based algorithm.

COMMENTS

Each “sweep” through the matrix consists of one pass through the matrix of equations. A sweep is thus equivalent to a single inner iteration through the matrix described in Mode 2 of this command. During these sweeps the matrix coefficients stay fixed. The primary difference between a “sweep” and “Inner Iteration” is that during a sweep no checks are made to determine if the norm of the matrix residue meets any specified convergence criterion (CONVERGENCE command). The specified number of sweeps is always carried out. A sweep is more efficient than a full inner iteration because no matrix residue norms are computed. On the other hand a large number of sweeps may prove wasteful because, the sweeps are forced irrespective of the state of the solution.

EXAMPLES

MATRix sweeps in X and Y directions: T=3! Sweep T equation 3 times
MATRix sweeps: P=3, T=1, C=2 also perform REDBlack split
MATRix for T to be solved 3 times by the ADI method with OLD row forming algorithm
MATRix for T ADI; REDBlack file for elements based on OLD method
MODE 2: SOR Matrix Solver

SYNTAX MATR {SOR} [NORM] [EXPL] [Φ =N₁, Φ =N₂, ..., Φ =Nₙ]

SOR Matrix is solved by implicit successive over relaxation where values from the current iteration are used where available.

NORM See Mode 1 specification.

EXPL Matrix is solved by explicit successive over relaxation where only the values from the old iteration are used.

Φ One or more symbols that denote the variable(s) for which SOR matrix solver will be invoked. Valid symbols are listed in Table 2.7.1.

N₁,..., Nₙ Number of times the matrix is “swept” for the variable denoted by the symbol immediately preceding the value. This input is ignored if the EXPLICIT modifier is present. The default value may vary with each installation though it is generally set to 1 for most of the variables.

COMMENTS

In general the SOR solver is not recommended for any except the simplest of problems. However, with the EXPLICIT modifier, it provides an effective method for time-explicit solution of a transient problem. It can also prove very useful to monitor the behavior and progress of the solution front in case of lack of convergence of a matrix.

See also comments under Mode 1 for importance of the numerical input given by N₁,..., Nₙ etc.

EXAMPLES

MATRix SOR for P=7 sweeps and T=3 sweeps
MATRix for P=3, T=2 SOR and generate REDBlack file
MATRix for T to be solved by EXPLICIT SOR
MODE 3:  Built-In ACRi Matrix Solvers

SYNTAX  \texttt{MATR \{\Phi\} \{solver\} [precon] [N_{\text{Degree}} | N_{\text{Block}}]}

\(\Phi\) \quad \text{One or more symbols that denote the variable(s) for which specified matrix solver will be invoked. Valid symbols are listed in Table 2.7.1.}

\text{solver} \quad \text{BICG} \quad \text{Matrix is solved by the bi-conjugate gradient stabilized method.}
\text{BICO} \quad \text{Matrix is solved by the bi-conjugate gradient stabilized method.}
\text{CONJ} \quad \text{Matrix is solved by the conjugate gradient method. To be used for symmetric matrices only.}
\text{CG} \quad \text{Matrix is solved by the conjugate gradient method. To be used for symmetric matrices only.}
\text{CGNR} \quad \text{Matrix is solved by the conjugate gradient for normalized equations method. This method may be inferior to the BICG method.}
\text{LUDE} \quad \text{Matrix is solved by sparse direct LU decomposition method. This method can be slow and memory intensive if the problem size exceeds 20000 elements.} \text{MATR} \text{IX ITER mode of the command is ineffective with this option.}
\text{BLOC} \quad \text{Matrix is solved by a block by block version of sparse direct LU decomposition method. The main purpose is to overcome the performance limitations of the LUDE method. The block size can be specified on the same command.}
\text{USER} \quad \text{Matrix is solved by an algorithm supplied by the user. See Section 4.7.}

\text{precon} \quad \text{NEUM} \quad \text{The default pre-conditioner for the BICG, CG, and CGNR methods. Uses a Neumann matrix polynomial (approximate inverse) pre-conditioner. The degree of the polynomial can be specified on the same command.}
\text{SSOR} \quad \text{The symmetric SOR pre-conditioner for the BICG, CG, and CGNR methods.}

\text{NORM} \quad \text{See Mode 1 specification.}

\text{N_{\text{Block}}} \quad \text{The size of the block if BLOC modifier is present; the specified value must be greater than 99. The default value is 2000.}

\text{N_{\text{Degree}}} \quad \text{The degree of the polynomial if NEUM pre-conditioner is specified. The default value is 4.}

COMMENTS
Currently, the \texttt{CONJ}ugate gradient and \texttt{BICO}njugate gradient methods are optimized to work in co-operation with the CPU command. These methods will use multiple processors if the CPU command is used to specify the number of processors.

EXAMPLES
\texttt{MATR}ix for T USER option 5! Matrix Solver supplied by User
\texttt{MATR}ix for T accelerator: \texttt{BICO}njuate gradient preconditioner: \texttt{NEUMann degree 7}
\texttt{MATR}ix for T accelerator: \texttt{BICO}njuate gradient preconditioner: \texttt{SSOR}
\texttt{MATR}ix for P by sparse \texttt{LUDE}composition (only for less than 20000 elements)
\texttt{MATR}ix for P by \texttt{BLOCk} size=1000 elements
\texttt{MATR}ix for P accelerator: \texttt{CONJ}ugate gradient preconditioner: \texttt{SSOR} (symmetric matrices only)
MODE 4: Number of Inner Matrix Iterations

SYNTAX
MATR {ITER} [MAX | MIN] {N1 | Φ = N1, Φ = N2, ..., Φ = Nn} [NORM]

ITER The input pertains to the maximum or minimum number of inner iterations for the matrix. This mode of the command is ineffective if MATRIX LUDE command for the same variable is specified.

MAX The input applies to maximum number of inner iterations for the matrix. By default the input pertains to the maximum number of inner iterations. If no maximum iterations for a variable are specified, then the maximum iterations are set equal to the maximum iterations specified on the CONVERGENCE command for the variable.

MIN The input applies to minimum number of inner iterations for the matrix. If no minimum iterations for a variable are specified, then the minimum iterations are set equal to the minimum iterations specified on the CONVERGENCE command for the variable.

Φ Symbols that denote the variable(s) for which the N1, N2, ..., etc. are effective. Valid symbols are listed in Table 2.7.1. If no symbol is specified, and only one numerical value is present, then the input is applied to all variables for which a transport equation is solved.

N1, ..., Nn Number of times (≥1) per time step that the matrix is solved for the variable denoted by the symbol immediately preceding the value. The default value is 1.

NORM See Mode 1 specification.

COMMENTS
Once the matrix coefficients are assembled, the matrix is solved iteratively till the specified convergence criterion (CONVERGENCE command) is satisfied. During this process the matrix coefficients stay constant even though the value of the computed variable is changing. This process of solution is here named the “Inner Iteration”. Each inner iteration consists of one pass through the matrix of equations followed by a check on the matrix residue. If the norm of the residue is larger than the specified tolerance, and the number of iterations is less than the maximum specified, then another pass follows.

EXAMPLES
MATRix ITERations for all variables = 10
MATRix ITERations: P=8, T=2, C=2
MATRix MINIMUM ITERations for all variables = 3
MODE 5: Matrix Solvers from the University of Texas NSPCG Package

SYNTAX

MATR {NSPC} [Φ [precon] [accel] [ELIM [OFF]]] [option] [NORM] [Ndegree]

NSPC

One of the matrix solvers, consisting of a preconditioner and an accelerator, from the NSPCG package (NSPCG User's Guide Version 1.0, by T.C. Oppe, W.D. Joubert and D.R. Kincaid, Report No. CNA-216, April 1988, Center for Numerical Analysis, Univ. of Texas, Austin, TX 78713-8510) is used. The source code and manuals are available at http://www.netlib.org/itpack. A special agreement is required for use of this package.

ELIM

Integer parameter IPARM (1) is set to 1. This implies that equations below a threshold level are dropped from the matrix system.

ELIM OFF

Integer parameter IPARM (1) is set to 0. This turns off any previously specified ELIM modifier. This is also the default setting.

Φ

One or more symbols that denote the variable(s) for which the specified options are effective. Valid symbols are listed in Table 2.7.1.

precon

Preconditioner component of the Matrix Solver.

<table>
<thead>
<tr>
<th>precon</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEUM</td>
<td>Neumann matrix polynomial. This is the default option.</td>
</tr>
<tr>
<td>LEAS</td>
<td>Least squares matrix polynomial.</td>
</tr>
<tr>
<td>DEGR</td>
<td>Degree of NEUMann or LEASt squares polynomial (integer) default: 3</td>
</tr>
<tr>
<td>REDU</td>
<td>Reduced System preconditioner.</td>
</tr>
<tr>
<td>CHOL</td>
<td>Incomplete Cholesky Factorization.</td>
</tr>
<tr>
<td>JACO</td>
<td>The point Jacobi preconditioner.</td>
</tr>
<tr>
<td>SOR</td>
<td>The Successive Over-Relaxation preconditioner and accelerator</td>
</tr>
</tbody>
</table>

accel

Accelerator Component of the Matrix Solver

<table>
<thead>
<tr>
<th>accel</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONJ</td>
<td>Conjugate Gradient accelerator.</td>
</tr>
<tr>
<td>BCGS</td>
<td>The Biconjugate Gradient Squared accelerator.</td>
</tr>
<tr>
<td>GMRE</td>
<td>GMRES accelerator. This is the default option.</td>
</tr>
<tr>
<td>ORTH</td>
<td>ORTHOMIN accelerator.</td>
</tr>
<tr>
<td>CGNR</td>
<td>Conjugate Gradient applied to Normal Equations.</td>
</tr>
<tr>
<td>LANC</td>
<td>Lanczos with ORTHOMIN accelerator.</td>
</tr>
</tbody>
</table>

option

Modifier for the specification or matrix or solver method

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODI</td>
<td>If CHOLESKY preconditioner is selected, then modified incomplete Cholesky decomposition is used; otherwise this input is ignored.</td>
</tr>
<tr>
<td>PERM</td>
<td>If CHOLESKY preconditioner is selected, then matrix is red-black permuted; otherwise this input is ignored.</td>
</tr>
</tbody>
</table>

NORM

See Mode 1 specification.

TRUN

If GMRE modifier is specified, then the number of solution vectors saved is the smaller of the number of matrix iterations (MATRIX ITER command) and 200. If TRUN modifier is present, then the maximum of solution vectors is set to 5.

Ndegree

The degree of the polynomial if NEUMANN modifier is present.

EXAMPLES

MATR for P by NSPCG (PERMUTED CHOLESKY).
MATR for P from NSPCG with JACOBI preconditioner and BCGS accelerator
MATR U V W P use NSPCG preconditioner: NEUMANN poly of DEGREE 3 GMRES accelerator
MATR P NSPCG NEUMANN DEGREE 3 GMRES
MATR NSPCG P NEUMANN DEGREE 2 TRUNCated GMRES ELIMINATE equations below threshold.
MATR NSPCG turn previously specified ELIMINATE OFF
MODE 6: Matrix Solvers from the HYPRE Library, Lawrence Livermore National Laboratory

SYNTAX

MATR {HYPR} [Φ] [precon] [accel] [option] [VECT=N\text{\textit{Vector}}] [NORM]

HYPR


Φ

One or more symbols that denote the variable(s) for which the specified options are effective. Valid symbols are listed in Table 2.7.1.

precon

Preconditioner component of the Matrix Solver.

<table>
<thead>
<tr>
<th>precon</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMG</td>
<td>Algebraic Multi-Grid Preconditioner. This is the default option.</td>
</tr>
<tr>
<td>CHOL</td>
<td>Incomplete Cholesky Factorization.</td>
</tr>
<tr>
<td>DIAG</td>
<td>Diagonal Scaling Preconditioner</td>
</tr>
<tr>
<td>SPAR</td>
<td>The Sparse Approximate Inverse Preconditioner.</td>
</tr>
</tbody>
</table>

accel

Accelerator Component of the Matrix Solver

<table>
<thead>
<tr>
<th>accel</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMGA</td>
<td>The AMG accelerator.</td>
</tr>
<tr>
<td>BICG</td>
<td>The Bi-Conjugate Gradient accelerator</td>
</tr>
<tr>
<td>CONJ</td>
<td>Conjugate Gradient accelerator.</td>
</tr>
<tr>
<td>GMRE</td>
<td>GMRES accelerator. This is the default option.</td>
</tr>
</tbody>
</table>

option

Modifier for the specification of matrix or solver method

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>SYMM</td>
<td>By default the matrix is assumed to be non-symmetric. If this modifier is present, then the matrix is assumed to be symmetric.</td>
</tr>
<tr>
<td>INDE</td>
<td>By default the matrix is assumed to be positive definite. If this modifier is present, then the matrix is assumed to be indefinite. This may be the case if Central Difference Integration method is used (see INTEGRATION Command).</td>
</tr>
<tr>
<td>STAT</td>
<td>By default the working memory required for the AMG method is set up for each solution level on the fly. However, if the matrix is not changing for a variable (such as for pressure equation under certain conditions) then the use of the STATic modifier will lead to a more efficient set up strategy. This modifier is ignored if any preconditioner other than AMG is specified.</td>
</tr>
</tbody>
</table>

VECT

This modifier defines the number of vectors in the Krylov space that are saved.

N\text{\textit{Vector}}

The number of previous vectors that are stored to derive the new iterate of the solution. The typical values are between 5 and 20. The default is set at 5.

NORM

See Mode 1 specification.
EXAMPLES

MATRix by HYPRE solver
MATRix for P from HYPRE solver print detailed DIAGnostics
MATRix for P from HYPRE with AMG preconditioner and CONJ accelerator and AMORtized set up
MATRix for P is SYMMetric; use HYPRE with CHOLesky with CONJugate Gradient
MATRix U V W use HYPRE: SPARse preconditioner with GMRES accelerator
MATRix U V W use HYPRE CHOLesky with GMRES and 10 VECTors
MODE 7: Global Matrix Control Parameters

SYNTAX MATR [COEF=V\text{Coef}] [ZERO=V\text{Zero}] [NORM]

COEF The minimum value for the matrix diagonal coefficient is specified. The magnitude of the diagonal coefficient for any row of the matrix must be greater than zero otherwise the matrix is indeterminate. However due to limitations of digital arithmetic and round off, the value may become very small. This input allows the user to tune the minimum threshold to the machine accuracy. Currently this is applicable only to the ADI and SOR solvers.

\( V_{\text{Coef}} \) The minimum threshold for any of the diagonal coefficients of the matrix of equations. The default value is 1.E-20.

ZERO The machine zero parameter is specified. This parameter is used by the NSPCG and HYPRE matrix solver packages to perform various numerical tests. In general, it treats any real number smaller in magnitude than the specified value as equivalent to machine zero. It is useful to modify this parameter in the instances where the right hand side of the equation system is less than the default value. If the tests indicate that normalized values of the right side of the matrix are smaller than this number then the matrix system may return without solving the system.

\( V_{\text{Zero}} \) The numerical value for the machine zero. The default values are given in the table below.

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.192 x 10^{-7}</td>
<td>IEEE real with 32-bit precision.</td>
</tr>
<tr>
<td>2.22 x 10^{-16}</td>
<td>IEEE real with 64-bit precision. This is the default.</td>
</tr>
<tr>
<td>7.1 x 10^{-15}</td>
<td>Cray XMP.</td>
</tr>
<tr>
<td>1.49 x 10^{-8}</td>
<td>Dec 10 (single precision)</td>
</tr>
<tr>
<td>4.768 x 10^{-7}</td>
<td>IBM 370 / 158 (single precision)</td>
</tr>
</tbody>
</table>

NORM See Mode 1 specification.

EXAMPLES

MATRix COEFicient minimum value = 1.E-30
MATRix machine ZERO = 1.0E-300

! Above is useful if NSPCG thinks that the \|RHS\| < machine zero and returns prematurely.
MATRix machine ZERO set to 1.0E-300, COEFicient=1.E-30.
MODE 8:  Tolerance Threshold for Minimum Value of Matrix Elements

SYNTAX  MATR {TOLE} {V_{Tole} | \Phi = V_{Tole1}, \Phi = V_{Tole2}, \ldots, \Phi = V_{Tolen}} [NORM]

TOLE  The tolerance or threshold for the minimum value of matrix elements. Matrix elements with numerical values below the specified tolerance are dropped. For the AMG preconditioner in the HYPRE solver, this modifier controls the connections between matrix elements in constructing a coarse level.

V_{Tole}  The numerical value for the threshold. For the SPAR preconditioner, the typical values are between 0.01 and 0.1 and the default is set at 0.05. For the CHOLESKY preconditioner, the typical values are between 0.001 and 0.01 and the default is set at 0.01. For the AMG preconditioner, the default value is 0.25 for 2D problems and 0.5 for 3D problems.

\Phi  Symbols that denote the variable(s) for which the N1, N2, ..., etc. are effective. Valid symbols are listed in Table 2.7.1. If no symbol is specified, and only one numerical value is present, then the input is applied to all variables for which the CHOLESKY, SPAR or AMG methods have been selected (that is, the same numerical value is used for these methods if several of them are selected for different variables in a given simulation).

NORM  See Mode 1 specification.

EXAMPLES

MATRix for P from HYPRE with AMG preconditioner and CG accelerator
MATRix for U from HYPRE with SPAI preconditioner and GMREs accelerator
MATRix for V and W from HYPRE with CHOLesky preconditioner and GMREs accelerator
MATRix TOLErance for P=0.25, for U=0.1, for V=0.001 and for W=0.01
MODE 9: Number of levels for AMG and SPAR Preconditioners for HYPRE

SYNTAX MATR \{LEVE\}\{N_{Level}\}|\Phi=N_{Level1}, \Phi=N_{Level2}, \ldots, \Phi=N_{Leveln}\} [NORM]

LEVE For the SPAR preconditioner, this modifier controls the level of the pattern matrix. The pattern matrix is computed from the matrix $A$ by dropping small amplitude elements. For the AMG preconditioner, this modifier controls the maximum number of coarse levels. This modifier is ignored for other preconditioners.

$N_{Level}$ The numerical value for the number of levels. For the SPAR preconditioner, values in the range of 1 to 3 are recommended and the default is set at 1. For the AMG preconditioner, values in the range of 10 to 15 are recommended and the default is set at 12. In this case, generally, the number of levels needs to be increased with the problem size.

$\Phi$ Symbols that denote the variable(s) for which the $N_{Level}$ numerical values are effective. Valid symbols are listed in Table 2.7.1. If no symbol is specified, and only one numerical value is present, then the input is applied to all variables for which the SPAI or AMG methods have been selected (that is, the same numerical value is used for both methods if several of them are selected for different variables in a given simulation).

NORM See Mode 1 specification.

EXAMPLES

MATRix LEVELS = 10 for all relevant solvers
MATRix LEVELS U = 5, V=5, P=10 for
MODE 10: Maximum Number of Non-zero Elements for Any Row of Modified Matrix

SYNTAX

```
MATR {ELEM} {N0|Φ=N01, Φ=N02, ..., Φ=N0n} [NORM]
```

ELEM

This modifier controls the maximum number of non-zero elements that are to be retained in any row of the modified matrix during factorization. Currently it is applicable only to the CHOLESKY Preconditioner of the HYPRE package.

N0

The maximum number of non-zero elements in any row of the modified matrix. Typical values are between 15 and 25 and the default is set at 15. This input is effective if no symbol is specified, and it is then applied to all variables for which the CHOLESKY, method has been selected.

N01, N02, N0n

As for N0 above except that the input is effective if one or more variable (Φ) is specified.

Φ

Symbols that denote the variable(s) for which the N01, N02, N0n are effective. Valid symbols are listed in Table 2.7.1.

NORM

See Mode 1 specification.

EXAMPLES

```
MATRix maximum non-zero elements = 10 for all solvers
MATRix non-zero ELEMents for P=15 and for W=5
```
MODE 11: Maximum Number of Non-zero Elements for Any Row of Modified Matrix

SYNTAX MATR {RESI} {ABSO} [NORM]

RESI For the NSPCG solvers, by default the specified convergence tolerance (CONVERGENCE command) is normalized with the larger of the machine zero or a norm of the current matrix residue. If this command along with the ABSO modifier is present, then the specified convergence tolerance is used as an absolute measure.

ABSO The modifier to select the absolute measure of convergence tolerance.

NORM See Mode 1 specification.

EXAMPLES

MATRix RESIdue in ABSOlute mode
MODE 12: Matrix Diagnostic Output for NSPCG and HYPRE Solvers

SYNTAX

MATR [DIAG] [SUMM] [OFF] [NORM]

DIAG
Produces detailed diagnostic output consisting of parameter values and informative comments from the matrix solver.

DIAG SUMM
Produces diagnostic output in a compact and summarized form.

DIAG OFF
Turns any previously specified diagnostic output off.

NORM
See Mode 1 specification.

COMMENTS

This mode of the MATRIX command may be combined with any of the other modes also. That is the modifiers above can also appear with any of the other previous modes.

EXAMPLES

MATRix DIAGnostic output to be generated
MATRix DIAGnostic SUMMary form output to be generated
MATRix DIAGnostic output OFF from now on
Keyword Commands

**COMMAND**  META

**PURPOSE**  To Generate Multiple Simulations from a Master File and a Meta Command File.

**SYNTAX**  META {fname}

**fname**  The name of a meta-command file that contains the commands that will replace the meta-commands in the master file to generate a sequence of simulations. This command must occur before the “GRID” command is encountered.

**COMMENTS**

This option works by replacing commands in a Master File with corresponding commands from a Meta-command File “fname”. Each meta-command contains a distinctive name that is enclosed between a starting and ending “%” character. The structure of the meta-command is:

```
%metacomand_name <valid ACRi FreeForm™ Command>
```

Where the metacomand_name is an alphanumeric string with up to 32 characters and it is followed by a valid ACRi FreeForm™ command. At run time the prefix %metacomand_name% is stripped from the front of the command and the actual command becomes the effective input. Each meta-command in the Master File is replaced by a corresponding command starting with the same metacomand_name in the Meta-command File fname. If no corresponding command is found in the Meta-command File, then the ACRi FreeForm™ command in the Master File is retained. Each set of meta-commands in the fname terminates with the END command and the whole sequence is terminated if a STOP command is encountered. Thus the typical contents of a Meta-command File, fname, are as follows:

```
%metacomand1% <valid ACRi FreeForm™ Command>
%metacomand2% <valid ACRi FreeForm™ Command>
END
%metacomand1% <valid ACRi FreeForm™ Command>
%metacomand2% <valid ACRi FreeForm™ Command>
END
%metacomand1% <valid ACRi FreeForm™ Command>
%metacomand2% <valid ACRi FreeForm™ Command>
STOP
```

Consider, for example, a set of statements in the Master file:

**TITLE:** Test Problem for Parametric Analysis by Creating Multiple sets of Input Data
**META Command file “meta_commands.fil”**
**GRID:** 22 in x and 12 in y direction
%1% BOUNDARY T at X- value = 100  !for Master File Problem
(Other input commands follow here)
%DENSITY% DENSITY = 990  !for Master File Problem
(Other input commands follow here)
**SOLVE** in STEADY mode for maximum of 1000 steps
%SAVE% SAVE in file ‘problem_1.sav’  !for Master File Problem
END

Assume now that the commands in the file “meta_commands.fil” are:

```
%1% BOUNDARY T at X- value = 100  !for 2nd problem
%DENSITY% DENSITY = 1000  !for 2nd problem
%SAVE% SAVE in file ‘problem_2.sav’  !for 2nd problem
END
%1% BOUNDARY T at X- value = 120  !for 3rd problem
%SAVE% SAVE in file ‘problem_3.sav’  !for 3rd problem
END
%1% BOUNDARY T at X- value = 150  !for 4th problem
%DENSITY% DENSITY = 990  !for 4th problem
%SAVE% SAVE in file ‘problem_4.sav’ !for 4th Problem
STOP
```

The above Meta-command File will then generate 4 simulations; the 1st simulation is that defined in the Master File and the other 3 are those in the Meta-command File. The resulting “unfolded” data set is saved in
a file that has the same name as the Master File but with "_META_UNFOLD.DAT" appended to the file name. For the above example, this file shall contain 4 problems with input as follows:

```
** Unfolded ** META Command file "meta_commands.fil"
!
********************************************************************************

! Problem # 1 created from Meta Command File
********************************************************************************

TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data

METACommand file "meta_commands.fil"
GRID: 22 in x and 12 in y direction
BOUNDARY T at X- value = 100  !for Master File Problem
(Other input follows here)
DENSITY = 990  !for Master File Problem
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE in file 'problem_1.sav'  !for Master File Problem
END
!
********************************************************************************

! Problem # 2 created from Meta Command File
********************************************************************************

TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data

METACommand file "meta_commands.fil"
GRID: 22 in x and 12 in y direction
BOUNDARY T at X- value = 100  !for 2nd problem
(Other input follows here)
DENSITY = 1000  !for 2nd d problem
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE in file 'problem_2.sav'  !for 2nd problem
END
!
********************************************************************************

! Problem # 3 created from Meta Command File
********************************************************************************

TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data

METACommand file "meta_commands.fil"
GRID: 22 in x and 12 in y direction
BOUNDARY T at X- value = 120  !for 3rd problem
(Other input follows here)
DENSITY = 990  !for Master File Problem
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE in file 'problem_3.sav'  !for 3rd Problem
END
!
********************************************************************************

! Problem # 4 created from Meta Command File
********************************************************************************

TITLE: Test Problem for Parametric Analysis by creating Multiple sets of Input Data

METACommand file "meta_commands.fil"
GRID: 22 in x and 12 in y direction
BOUNDARY T at X- value = 150  !for 4th problem
(Other input follows here)
DENSITY = 990  !for 4th problem
(Other input follows here)
SOLVE in STEADY mode for maximum of 1000 steps
SAVE in file 'problem_4.sav'  !for 4th Problem
END
```

EXAMPLES
META command file “meta_command.fil”
COMMAND  MOVE

PURPOSE  To specify a moving coordinate system for the system geometry. This command is effective only for the ANSWER™ and PORFLOW™ Software Tools.

MODE 1:  Grid Coordinate Frame in Uniform Translation

SYNTAX  MOVE {dir} {V_{grid}} [ABSO|RELA] [MASS] [MOME]

dir  One of the X, Y, Z, R or THETA modifiers that, respectively, denotes the x, y, z, r or $\zeta$ coordinates for the axis along which the coordinate system is moving at a uniform speed. There is no default value; a value must be specified.

V_{grid}  The velocity of translation of the grid frame in the direction of the specified axis

ABSO  By default the numerical solution proceeds in terms absolute velocity – that is the velocity observed by a stationary observer. In this case all input must be specified in terms of absolute velocity. The component that is moving must be specified as a moving block (BLOCK command with MOVE modifier). The velocity of the moving component should be specified in the same sense as the direction of rotation so the moving component is stationary in the rotating coordinate system.

RELA  The solution is in terms of velocity relative to the rotating coordinate system. In this case all input must be specified in terms of relative velocity. The moving component must be specified as stationary and all initial and boundary conditions must be specified in terms of relative velocity. The velocity of the system boundaries should be specified in a sense opposite to that implied by the direction of rotation so the stationary fluid moves opposite to the rotating coordinate system.

MASS  By default the mass flux at the moving boundary is added to the mass continuity equation. This is required by the governing equations. If this modifier is present, then the mass flux at the moving boundary is not added. Its effect is to relieve local pressure changes next to moving body. The use of this modifier is intended as a debugging device and is not generally recommended.

MOME  By default the momentum flux at the moving boundary is automatically accounted for by the moving mass flux at the moving boundary. This is implied by the governing equations. If this modifier is present, then the momentum flux is explicitly added. This for example may be necessary if MASS modifier is present. The use of this modifier is intended as a debugging device and is not generally recommended.

COMMENTS

The ABSOLUTE velocity mode is recommended for most applications. In general it depicts better numerical behavior. The RELATIVE mode is prone to poor numerical behavior especially for problems with high rotation speed or large domains since the relative velocity grows without bounds away from the body.

EXAMPLES

MOVE coordinate frame along X-axis at 15 meters per second
MOVE coordinate frame along X-axis at 15 meters per second in Relative mode.
MOVE coordinate frame along X-axis at 15 meters per second do not add MASS; add MOMEtum.
Keyword Commands

MODE 2: Grid Coordinate Frame in Pure Rotation

SYNTAX

MOVE {dir} {ROTA} {ω} [RPM] [ABSO|RELA] [MASS] [MOME]

dir

One of the X, Y, Z, R or THETA modifiers that, respectively, denotes the x, y, z, r or θ coordinates for the axis around which it is rotating. There is no default value; a value must be specified.

ROTA

The coordinate frame is in simple rotation around the specified axis.

ω

The speed of rotation in radians per second or revolutions per minute. The value is positive if the axis is rotating in anti-clockwise sense for a right-handed coordinate system. For example for rotation around z-axis, the x and y components of velocity of rotation of the coordinate frame are defined by:

\[ u = -\omega y; \quad v = \omega x \]

RPM

By default the rotation speed is assumed to be in radians per second. If this modifier is present then the speed is taken to be in revolutions per minute.

ABSO

See Mode 1 of the command.

RELA

See Mode 1 of the command.

MASS

See Mode 1 of the command.

MOME

See Mode 1 of the command.

COMMENTS

The ABSOLUTE velocity mode is recommended for most applications. In general it depicts better numerical behavior. The RELATIVE mode is prone to numerical diffusion especially for problems with high rotation speed or large domains since the relative velocity grows without bounds away from the body.

EXAMPLES

MOVE grid by ROTAtion around Z-axis at 2.5 radians per second
MOVE coordinate frame by ROTAtion around Z-axis at 1000 RPM.
MOVE coordinate frame by ROTAtion around Z-axis at 2.5 radians per second in RELAtive velocity mode.
MODE 3: A Moving or Evolving Rectangular Subdomain

SYNTAX

MOVE {ID=subrgn} {LLC|URC} {X|Y|Z} {func [time]}

ID
The modifier to indicate that the input is for a previously defined subregion.

subrgn
The rectangular subregion for which the input is specified. The subregion must have been previously specified with a LOCATE MOVE COORDINATE command.

LLC
The input pertains to the coordinates of the “lower left” corner of the subregion.

URC
The input pertains to the coordinates of the “upper right” corner of the subregion.

X Y Z
The LLC or URC coordinate for which the functional input is specified.

func
One of the modifiers listed in Table 4.2.1, which denotes the functional form of the dependent variable. If no function is specified, the value is assumed to be constant.

time
The independent variable for the function.

COMMENTS
This mode of the command allows the input of an evolving or moving rectangular domain. The domain is always assumed to be the enveloping rectangle of the LLC and URC set of coordinates at any time. Multiple command may be specified for the same domain with any of the X, Y or Z modifiers.

EXAMPLES

MOVE ID=MOVING_REGION LLC coordinates: LINEAR function X = 0. + 0.001 * TIME
MOVE ID=MOVING_REGION LLC coordinates: LINEAR function Y = 0. + 0.0001 * TIME
MOVE ID=MOVING_REGION URC coordinates: Y = 1. EXP (0.1 * TIME +0.)
MODE 4: A Moving or Evolving Planar Fracture

SYNTAX

MOVE \{ID=subrgn\} \{N1\} \{X|Y|Z\} \{func \[TIME]\}

ID
The modifier to indicate that the input is for a previously defined subregion.

subrgn
The fracture subregion for which the input is specified. The subregion must have been previously specified with a LOCATE MOVE FRAC command.

N1
The input pertains to the N\textsuperscript{th} point defining the plane in order in which the points are specified by the LOCATE MOVE FRAC command. N1 can only be 1 or 2 for a 2D fracture. For 3D, N1 is between 1 and the number of points defining the fracture plane.

X|Y|Z
The input is specified for the corresponding x, y or z coordinates of the N\textsubscript{1} point. Multiple commands must be specified for movement of each of the x, y or z coordinate.

func
One of the modifiers listed in Table 4.2.1, which denotes the functional form of the dependent variable. Currently only functions of TIME can be specified. The combination of functions must ensure that the vertices of the fracture always define a plane.

The combination of functions must also ensure that the orientation of the fracture is not changed. The image above shows a valid moving fracture, with movement restricted to the plane of the fracture. The moving fracture shown below changes in orientation and so it is not a valid movement for the fracture.

TIME
The independent variable for the function. Currently only functions of time can be specified. This modifier must be specified.

COMMENTS
This mode of the command allows the input of an evolving or moving fracture. The points defining the fracture can only move in the fracture plane. Multiple commands may be specified for the same domain with any of the X, Y or Z modifiers, but the vertices must only move in the plane of the fracture and not out of the plane. The movement of the vertices is restricted by the condition that the orientation of the fracture plane must not change.

Currently this option is fully operational only for the fracture in a 2D geometry. Please contact ACRi for 3D implementation.

EXAMPLES

MOVE ID=MOVING_FRAC2D point no 1 coordinates: LINEAR function X = 0. + 0.001 * TIME
MOVE ID=MOVING_FRAC3D point no 4 coordinates: LINEAR function Z = 0. + 0.0001 * TIME
MOVE ID=MOVING_FRAC point no 2 coordinates: Y = 1. EXP (0.1 * TIME +0.)
Keyword Commands

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>MULTIPHASE</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To specify the nature of the characteristic curve and the values of the empirical characteristic constants for multiphase or variably saturated flow. This command automatically initiates the multi-phase mode of simulation. This command is effective only for the PORFLOW™ Software Tool.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>The Brooks &amp; Corey Soil Characteristic</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>MULT {BROO][SATU][COND][BURD][MUAL][COMP][phase] {λ, Ψa} {Sr, Sg, kmin} [subrgn]</td>
</tr>
<tr>
<td>BROO</td>
<td>The fluid phase saturation and the capillary pressure are related according to the Brooks and Corey expression given below.</td>
</tr>
<tr>
<td></td>
<td>[ S^n = (\Psi_a / \Psi^n)^\lambda ; \Psi &gt; \Psi_a ]</td>
</tr>
<tr>
<td></td>
<td>[ S^n = 1 ; \Psi \leq \Psi_a ]</td>
</tr>
<tr>
<td></td>
<td>[ \hat{S}^1 = \frac{S^1 - S_r}{1 - S_r - S_g} ; \hat{S}^2 = \frac{S^1 + S^2 - S_r}{1 - S_r - S_g} ; \hat{S}^3 = 1 ]</td>
</tr>
<tr>
<td></td>
<td>[ \Psi^n = P^n - P^{n+1} ]</td>
</tr>
<tr>
<td></td>
<td>[ \sum_{n=1}^{N} S^n = 1 ]</td>
</tr>
</tbody>
</table>

In these relations, the superscript “n” denotes the n<sup>th</sup> fluid phase, \( \hat{S} \) is the normalized saturation, \( \Psi \) is the capillary pressure, \( P \) is the computed fluid pressure, and \( \Psi_a, \lambda, S_r, S_g \) are empirical constants as defined below. The relations above assume a 3-phase system (such as water-oil-gas); the same relations apply to a 2 phase system except that the 2<sup>nd</sup> (rather than the 3<sup>rd</sup>) phase normalized saturation is then unity.

| SATU      | By default the moisture characteristic is used to compute both phase saturation and relative hydraulic conductivity. If the modifier SATU is present, the specification is used only to calculate the phase saturation. |
| COND      | By default the moisture characteristic is used to compute both phase saturation and relative hydraulic conductivity. If the modifier COND is present, the specification is used only to calculate the relative conductivity. |
| BURD      | The relative conductivity, \( k_r \), is computed from the Burdine (1953) predictive model which leads to the equations given below. This is the default option. |
|           | \[ k^n_r = \left( \hat{S}^n - \hat{S}^{n-1} \right)^2 \left[ \left( \hat{S}^{n-1} \right)^{1+2/\lambda} - \left( \hat{S}^n \right)^{1+2/\lambda} \right] ; \ n > 1 \] |
|           | \[ k^1_r = \left( \hat{S}^1 \right)^{3+2/\lambda} ; \ n = 1 \] |
| MUAL      | The relative conductivity, \( k_r \), is computed from the Mualem (1976) model which leads to: |
|           | \[ k^n_r = \left( \hat{S}^n - \hat{S}^{n-1} \right)^{1/2} \left[ \left( \hat{S}^{n-1} \right)^{2+2/\lambda} - \left( \hat{S}^n \right)^{2+2/\lambda} \right] ; \ n > 1 \] |
|           | \[ k^1_r = \left( \hat{S}^1 \right)^{5/2+2/\lambda} ; \ n = 1 \] |
| COMP      | If the modifier SECONd is also present then \( k_r \) for the second phase is computed from the complimentary function: |
|           | \[ k^2_r = 1 - k^1_r \] |
| phase     | The fluid phase for which the input is specified. See Section 3.6 for available options. If no phase modifier exists, the input is assumed to be for the first phase of the fluid. |
| λ         | The exponent (> 0) for Brooks and Corey relation. There is no default value. |
ψ_a The so-called air entry pressure (> 0) for Brooks and Corey relation. There is no default value.

Sr An empirical fitting constant (≥ 0) sometimes also called the residual saturation for the porous matrix. The default value is 0.

Sr An empirical fitting constant (≥ 0) sometimes also called residual gas-phase saturation. For a flow with 2 phases, this is always zero. The default value is 0.

k_rmin The minimum value of k_r. The default value is 10⁻⁶.

subrgn The subregion for which the input is specified. See Section 3.4 for more details. If no subregion is specified, then entire computational domain is selected.

EXAMPLES

MULTiphase flow: BROOks & Corey: lamda = 0.5; air entry p = 0.1
MULTiphase: BROOks with MUALem: lamda=4.5, h* = 5.4, 2*0
MULTiphase: BROOks for SECOnd phase with: N=3.5; Aow=0.100
MULTiphase: BROOks CONDuctivity SECOnd phase: lamda=3, psi=0.1
MULTiphase: BROOks CONDuctivity COMPlimentary SECOnd l=3, psi=0.2
MODE 2: The Van Genuchten Characteristic

SYNTAX
MULT {VAN} [SATU | COND] [MUAL | BURD] [COMP] [phase] {N, α} [S_r, S_g, M, k_{rmin}] [subrgn]

VAN
The saturation-capillary pressure characteristic is defined by the van Genuchten relations as shown below.

\[ \hat{S}^n = \frac{1}{\left[1 + (\alpha \psi^n)^N\right]^M} \quad ; \quad \psi^n > 0 \]
\[ \hat{S}^n = 1 \quad ; \quad \psi^n \leq 0 \]
\[ \hat{S}^1 = \frac{S^1 - S_r}{1 - S_r - S_g} \quad ; \quad \hat{S}^2 = \frac{S^1 + S^2 - S_r}{1 - S_r - S_g} \quad ; \quad \hat{S}^3 = 1 \]
\[ \psi^n = P^n - P^{n+1} \]
\[ \sum_{n=1}^{N} S^n = 1 \]

In these relations, the superscript “n” denotes the nth fluid phase, \( \hat{S} \) is the normalized saturation, \( \psi \) is the capillary pressure, \( P \) is the computed fluid pressure, and \( \alpha, N, M, S_r \) and \( S_g \) are empirical constants as defined below. The relations above assume a 3-phase system (such as water-oil-gas); the same relations apply to a 2-phase system except that the 2nd (rather than the 3rd) phase normalized saturation is then unity.

SATU
See Mode 1 specification.

COND
See Mode 1 specification.

MUAL
\( k_r \) is computed from the Mualem (1976) model. This is the default option.

\[ k_r^n = (\hat{S}^n - \hat{S}^{n-1})^{1/2} \left[ \{1 - (\hat{S}^{n-1})^{1/M}\}^M - \{(1 - (\hat{S}^n)^{1/M})^M \}^2 \right] ; \quad n > 1 \]
\[ k_r^1 = (\hat{S}^1)^{1/2} \left[ \{1 - (1 - (\hat{S}^1)^{1/M})^M \}^2 \right] ; \quad n = 1 \]

By default: \( M=1-1/N \) for this choice; it is overwritten if \( M \) is specified below.

BURD
\( k_r \) is computed from the Burdine (1953) predictive model.

\[ k_r^n = (\hat{S}^n - \hat{S}^{n-1})^2 \left[ \{1 - (\hat{S}^{n-1})^{1/M}\}^M - \{(1 - (\hat{S}^n)^{1/M})^M \}^{1/2} \right] ; \quad n > 1 \]
\[ k_r^1 = (\hat{S}^1)^2 \left[ \{1 - (1 - (\hat{S}^1)^{1/M})^M \} \right] ; \quad n = 1 \]

By default: \( M=1-2/N \) for this choice; it is overwritten if \( M \) is specified below.

COMP
See Mode 1 specification.

phase
See Mode 1 specification.

N
The \( N \ (> 0) \) of the equation above. There is no default value for this input.

α
The \( \alpha \ (> 0) \) of the above equation. There is no default value for this input.

S_r
An empirical fitting constant \( (\geq 0) \) sometimes also called the residual saturation for the porous matrix. The default value is 0.

S_g
An empirical fitting constant \( (\geq 0) \) sometimes also called residual gas-phase saturation. For a flow with 2 phases, this is always zero. The default value is 0.

M
The exponent, \( M \), in the above equation. The default value is 1-1/N if the Mualem model is selected and 1-2/N if the Burdine model is selected.

k_{rmin}
The minimum value of \( k_r \). The default value is \( 10^{-6} \).
**subrgn**  The subregion for which the input is specified. See Section 3.4 for more details. If no subregion is specified, then entire computational domain is selected.

**EXAMPLES**

MULTiphase flow VAN Genuchten: n = 2.0, alpha = 0.5  
MULTiphase: VAN Genuchten BURDine: N=3.5; Alfa=0.167, sr=0.067, sg=0.090  
MULTiphase: VAN Genuchten: N=3.5 a=0.167 sr=0.067 Sg=0.09, M=0.5 kr=0.02  
MULTiphase: VAN Genuchten for CONDuctivity only with: N=3.5; Aow=0.1  
MULTiphase: VAN Genuchten COND SECOnd COMPlimentary: N=3.5; a=0.1
MODE 3: Tabulated Data Input

SYNTAX MULT {TABL} [COND] [HEAD] [COMP] [phase] \{N_{sets}\} \{N_i, ..., N_n\} [fname] [subrgn]

TABL The moisture characteristic is specified in tabular form.

COND By default, the tabulated data are for the S-Ψ characteristic. If the modifier CONDUCTIVITY is present, the specification is assumed to be for the S-k_r characteristic.

HEAD By default, the relative moisture characteristic is assumed to be specified as S vs. k_r. If the modifier HEAD is present, the characteristic is assumed to be tabulated values of Ψ vs. k_r.

COMP See Mode 1 specification.

phase See Mode 1 specification.

N_{sets} The number of sets of tabulated values which follow.

N_1 The first value of S for the S-Ψ or S-k_r characteristic or the first value of the Ψ for the Ψ-k_r characteristic. The numerical value must be ≥ 0.

N_2 The first value of ψ for the S-Ψ or the first value of k_r for the S-k_r or Ψ-k_r characteristic. The input value may be scaled internally by the SCALE command. The numerical value must be ≥ 0.

N_3, ..., N_n The sets of values of S, ψ or k_r in a manner similar to N_1 and N_2. A total of N_{sets} sets (including N_1 and N_2) must be specified.

fname The name of the file from which numerical values N_1 through N_n for the moisture characteristic curve are read. See Section 3.3 for additional information.

subrgn The subregion for which the input is specified. See Section 3.4 for more details. If no subregion is specified, then entire computational domain is selected.

EXAMPLES

MULTi phase flow: TABLe of 4 sets: (0,1.E6), (0.1,1.E3), (0.9,1.E2), (1.,1.)
MULTi phase: COND: TABLe 4 sets: (0,0), (0.2,0.4), (0.8,0.7), (1,1) ! S vs. k_r
MULTi phase CONDuctivity COMPlimentary SECOnd phase: TABLe of 4 sets: (0,0), (0.2,0.4), (0.8,0.7) (1., 1.)
MULTi COND vs HEAD: TABLe 4: (100,0) (60,0.4) (40,0.7) (0, 1) ! Ψ vs. k_r
MULTi COND vs HEAD: TABLe of 40 sets from file 'SVSKRH'
MODE 4: Saturation as an Exponential or Logarithmic Function of Capillary Pressure

SYNTAX
MULT {EXPO | LOGA} [phase] {N, α} [C] [S_r, S_g, k_{rmin}] [subrgn]

EXPO Saturation is an exponential function of Ψ as shown in below equation

\[ \hat{S} = \frac{C}{C + \left[ \exp(\alpha \Psi) \right]^N - 1}; \quad \Psi > 0 \]
\[ \hat{S} = 1; \quad \Psi \leq 0 \]

LOGA Saturation is a logarithmic function of Ψ given in below equation (*) as

\[ \hat{S} = \frac{C}{C + \left[ \ln(\alpha \Psi) \right]^N}; \quad \Psi > 1/\alpha \]
\[ \hat{S} = 1; \quad \Psi \leq 1/\alpha \]

phase See Mode 1 specification.

N The exponent N of the equations above. There is no default value.

α The constant α of the equations above. There is no default value.

C The constant C the equations above. The default value is 0.

S_r An empirical fitting constant S_r in the definition of the normalized saturation (see Mode 1 specification)

S_g An empirical fitting constant S_g in the definition of the normalized saturation (see Mode 1 specification)

k_{rmin} The minimum value of k_r. The default value is 10^{-6}.

subrgn See Mode 1 specification.

EXAMPLES
MULTiphase EXPOnential characteristic: N=2., alpha=0.2
MULTiphase LOGArithmic relation: n = 1.0, alpha = 1, C=200, sr=0.05, sg=0.
Keyword Commands

MODE 5: Capillary Pressure as a Polynomial Function of Saturation

SYNTAX

MULT {POLY} [phase] {A, B, C, D, E} [Sr, Sg, kmin] [subrgn]

POLY

Ψ is a 4th order polynomial function of saturation as given below.

\[ \Psi = A + B \hat{S} + C \hat{S}^2 + D \hat{S}^3 + E \hat{S}^4 \]

Where A, B, C, D and E are empirical constants.

phase

See Mode 1 specification.

A

The constant A of above equation. There is no default value for this input.

B

The constant α of the above equations or the constant B of above equation. There is no default value for this input.

C

The constant C of the above equations. The default value is 0 for the above equation and is 1 otherwise.

D

The fitting constant, Sr in the definition of the normalized of saturation (see Mode 1)

E

The residual saturation, Sg of the above equation (≥ 0), for the exponential or logarithmic relations, or the constant, E, for the polynomial relation. The default value is 0.

Sr

An empirical fitting constant Sr in the definition of the normalized saturation (see Mode 1 specification)

Sg

An empirical fitting constant Sg in the definition of the normalized saturation (see Mode 1 specification)

kmin

The minimum value of kr. The default value is 10^-6.

subrgn

See Mode 1 specification.

EXAMPLES

MULTiphas POLYnomial: a = 1., b = -1.
MULTiphas POLYnomial: a=10, b=-5., c=-2.5, d=-1.5, e=-1, sr=0.1, sg=0.05
MODE 6: Tabulated Saturation Characteristic with Hysteresis

SYNTAX

MULT {TABL} [HYST] \{N_{sets}\} \{f_{name} \mid N_1, ..., N_n \mid f_{name}\} [subrgn]

TABL The moisture characteristic is specified in tabular form.

HYST The moisture characteristic is specified with hysteresis; that is, with separate wetting and drying cycles. A typical soil characteristic with hysteresis is shown below. The moisture characteristics consist of discrete values of saturation, $S$, and capillary pressure, $\Psi$. See comments below.

![Graph showing moisture characteristic with hysteresis](graph.png)

$N_{sets}$ The number of sets of tabulated values which follow. Three values must be specified for each set in the order of $(S$, wetting $\Psi$ and drying $\Psi)$.

$N_1$ The first value of $S$ ($\geq 0$) for the $S$- $\Psi$ characteristic.

$N_2$ The first value of $\Psi$ for wetting cycle. The input value may be scaled internally if a SCALE command is specified immediately preceding the command.

$N_3$ The first value of $\Psi$ for drying cycle.

$N_4, ..., N_n$ The sets of values of $S$, $\Psi_{\text{wet}}$, $\Psi_{\text{dry}}$, in a manner similar to $N_2$, $N_3$ and $N_4$. The total number of values specified must of 3 times $N_{sets}$.

$f_{name}$ The name of the file from which numerical values $N_1$ through $N_n$ for the moisture characteristic curve are read. See Section 3.3 for additional information.

$subrgn$ The subregion for which the input is specified. See Section 3.4 for more details. If no subregion is specified, then entire computational domain is selected.

COMMENTS

Capillary pressure as defined in ACRI Software Tools is the negative of the commonly sued soil moisture potential that is defined as a negative quantity. The input value for capillary pressure may be scaled internally if a SCALE command is specified immediately preceding the command.

The relation between soil saturation and relative conductivity must be separately specified. Care must be taken that if an analytical form (such as van Genuchten) relation is specified, then it must specify the modifier COND on the command and that the characteristic curve specified here is not overwritten.

EXAMPLES

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
100 200 300 400 500 600 700 800

Saturation

Wetting
Drying

Capillary Pressure

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MULTiphase flow: TABLE of 4 sets: (0,1.E6), (0.1,1.E3), (0.9,1.E2), (1.,1.)
MULTiphase: COND: TABLE 4 sets: (0,0), (0.2,0.4), (0,8,0.7), (1,1) ! S vs. k,
MULTiphase CONDuctivity COMPlimentary SECOnd phase: TABLE of 4 sets:
(0,0), (0,2,0.4), (0,8,0.7) (1., 1.)
MULTi COND vs HEAD: TABLE 4: (100,0) (60,0.4) (40,0.7) (0, 1) ! $\Psi$ vs. k,
MULTi COND vs HEAD: TABLE of 40 sets from file 'SVSKRH'
MODE 7: Saturation as a Function of Temperature

SYNTAX MULT {WHEE} {λ, Td} [Sr, Sg] [subrgn]

WHEE Saturation relation is that of Wheeler (1973) equation as shown below

\[
\hat{S} = \begin{cases} 
\frac{1}{1 + (T_F - T)/T_D^\lambda} & ; \quad T \leq T_F \\
0 & ; \quad T > T_F 
\end{cases}
\]

In the equation above, \(T\) is the fluid temperature; \(T_F\) is the freezing temperature; \(T_D\) is a characteristic delay temperature for freezing and \(\lambda\) is an empirical power-law exponent. The normalized saturation is defined in Mode 1 of this command.

\(\lambda\) The exponent, \(\lambda\), of the above equation (> 0). The default value is 10.

\(T_D\) The delay temperature, \(T_D\) (> 0), for the freezing/thawing algorithm. The default value is 1.E-30.

\(S_r\) An empirical fitting constant \(S_r\) in the definition of the normalized saturation (see Mode 1 specification)

\(S_g\) An empirical fitting constant \(S_g\) in the definition of the normalized saturation (see Mode 1 specification)

subrgn See Mode 1 of command

EXAMPLES

MULTiphase flow: with WHEEler option: \(n=4, Td=0.1\)
MULTiphase flow: WHEEler option: \(n=4, Td=0.1, Sr=0.2, Sg=0.02\)
Keyword Commands

MODE 8: Relative Hydraulic Conductivity as a Function of Saturation.

SYNTAX

```
MULT {COND} {POWE} {N, A [B, C]} [S_r, S_g, k_rmin] [COMP] [phase] [subrgn]
```

COND

The input is for the relative hydraulic conductivity, k_r.

POWE

k_r is a power law of saturation as shown in below equation

\[ k_r = A (B + \hat{S})^N + C \]

N

The exponent N of the power law relation. There is no default value.

A

The constant A for the power law (default value=1) or the constant, B, for the polynomial relation (default value=0).

B

The constant B for the power law. The default value is 0.

C

The constant C for the power law. The default value is 0.

S_r

An empirical fitting constant S_r in the definition of the normalized saturation (see Mode 1 specification)

S_g

An empirical fitting constant S_g in the definition of the normalized saturation (see Mode 1 specification)

k_rmin

The minimum value of k_r. The default value is 10^-6.

COMP

See Mode 1 specification.

phase

See Mode 1 specification.

subrgn

See Mode 1 specification.

EXAMPLES

```
MULTiphase CONDuctivity: POWEr law: N=4.
MULTiphase CONDuctivity POWEr: N=4, A=1 (B, C, sr, sg) =4*0. min =1.E-7
MULTiphase COND COMPlimentary SECOnd POWEr law: N=4. A=1. sr =0.2
```
MODE 9: Relative Hydraulic Conductivity as a Function of Saturation.

SYNTAX

```
MULT {COND} {POLY} {A} [B, C, D, E] [S_r, S_g, k_{r min}] [COMP] [phase] [subrgn]
```

COND
The input is for the relative hydraulic conductivity, \( k_r \).

POLY
\( k_r \) is a 4th-order polynomial of saturation as shown in below equation

\[
 k_r = A + B \hat{S} + C \hat{S}^2 + D \hat{S}^3 + E \hat{S}^4
\]

A
The constant \( A \) of the polynomial relation. **There is no default value.**

B
The constant \( B \) for the polynomial relation. **The default value is 0.**

C
The constant \( C \) for the polynomial relation. **The default value is 0.**

D
The constant \( D \) for the polynomial relation. **The default value is 0.**

E
The constant \( E \) for the polynomial relation. **The default value is 0.**

S_r
An empirical fitting constant \( S_r \) in the definition of the normalized saturation (see Mode 1 specification).

S_g
An empirical fitting constant \( S_g \) in the definition of the normalized saturation (see Mode 1 specification).

k_{r min}
The minimum value of \( k_r \). **The default value is 10^{-6}.**

COMP
See Mode 1 specification.

phase
See Mode 1 specification.

subrgn
See Mode 1 specification.

EXAMPLES

MULTiphase POLYnomial: \( a = 1., b = -1., c=0.5, d=-0.5 \)
Keyword Commands

**MODE 10:** Relative Hydraulic Conductivity as a Function of Capillary Pressure.

**SYNTAX**

MULT {COND} {EXPO|LOGA|INVE} [COMP] [phase] {N, α} [C] [Sr, Sg, k_{min}] [subrgn]

**COND**
The input is for the relative hydraulic conductivity, k_r.

**EXPO**
Relative conductivity is an exponential function of Ψ as defined by equation given below:

\[
k_r = \frac{C}{C + (\exp(\alpha \psi))^N} \quad ; \quad \psi > 0
\]

\[
k_r = 1 \quad ; \quad \psi \leq 0
\]

**LOGA**
Relative conductivity is a logarithmic function of Ψ as defined by the below equation:

\[
k_r = \frac{C}{C + [\ln(\alpha \psi)]^N} \quad ; \quad \psi > 1/\alpha
\]

\[
k_r = 1 \quad ; \quad \psi \leq 1/\alpha
\]

**INVE**
Relative conductivity is an inverse power law function of Ψ as shown by below equation:

\[
k_r = \frac{C}{C + [\alpha \psi]^N} \quad ; \quad \psi > 0
\]

\[
k_r = 1 \quad ; \quad \psi \leq 0
\]

**COMP**
See Mode 1 specification.

**phase**
See Mode 1 specification.

**N**
N is Exponent of the above equations. There is no default value.

**α**
α is constant of the above equations. There is no default value.

**C**
C is constant, of the above equations. The default value is 1.

**k_{min}**
Minimum permissible value of k_r. Any computed value smaller than this value is set equal to this value. The default value is $10^{-6}$.

**subrgn**
See Mode 1 of command

**EXAMPLES**

MULT phase EXPOnential CONDuctivity characteristic: N=2., alpha=0.2

MULT phase LOGArithmic CONDuctivity: n = 1.0, alpha = 1, C=200.

MULT phase CONDuctivity INVERsre power law: N=2., alpha = 0.05, C=1.

MULT phase COND INVERSE COMPlimentary SECOnd phase: N=2, alpha=0.05
COMMAND: NOZZLE

PURPOSE: To specify properties and parameters relating to injection of liquid droplets through nozzle. This command is effective only for the ANSWER™ Software Tool.

MODE 1: Location and Properties for Individual Droplets

SYNTAX: NOZZ {DROP} [FUEL|WATE] {Qm} [option] [[ABSO] RATE=Q_{Evap}] [STAR=t_{Start}] [STOP=t_{Stop}] [STOR=N_{Stor}] [TEMP=T_{NZL}] [FREQ=N_{Frq}] [SETS=N_{Sets}] {datatype [ELEM]} [UNIF] {fname|N_1,...,N_n}

DROP: The starting location and properties of each droplet injected by the nozzle are specified. The transport and evaporation of droplets is computed by the built-in algorithm.

FUEL: Nozzle injects fuel droplets. This is the default option.

WATE: Nozzle injects water droplets.

Q_m: The total mass flow rate [MT^{-1}] of fuel injected by the nozzle. This must be the first numerical value on the command. There is no default value.

option: Droplet options to be activated or deactivated.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description of Corresponding Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>DISA</td>
<td>The specified option(s) listed below is (are) deactivated</td>
</tr>
<tr>
<td>EVAP</td>
<td>The droplets evaporate during move. The option is active by default.</td>
</tr>
<tr>
<td>DRAG</td>
<td>The droplets undergo drag during move. The option is active by default.</td>
</tr>
<tr>
<td>OUTP</td>
<td>A diagnostic message is printed if the injected and evaporated amount from the nozzle differ by more than 0.1%. The option is active by default.</td>
</tr>
</tbody>
</table>

ABSO: This modifier is effective only if the RATE modifier is present, otherwise it is ignored. In the presence of this modifier, the specified rate of evaporation is computed from the original rather than the current remaining mass of the droplet.

RATE: If this modifier is present, then the number immediately following the modifier is interpreted as the rate of evaporation to be forced on the droplets from this nozzle. By default the evaporation rate is computed automatically from the droplet algorithm. This modifier and the corresponding numerical value, if present, may be placed anywhere after Q_m but before the actual droplet information (N_1,...,N_n). If SETS modifier is missing, then it must occur before the N_Sets value.

Q_{Evap}: The rate of evaporation as a fraction of the droplet mass. In the presence of the ABSOLUTE modifier, the specified fraction of the original droplet is forced to evaporate at each droplet time step (see NOZZLE command with TIME modifier for droplet time step). For example, a specification of 0.1 will result in complete evaporation in 10 droplet steps. If the ABSOLUTE modifier is not present, then the fraction is applied to the remaining mass of the droplet; that is with a specification of 0.1, the evaporated fractions will be 0.1, 0.09, 0.081, and so on.

STAR: If this modifier is present, then number immediately following the modifier is interpreted to be the starting time for the discharge of droplets from the nozzle. This modifier and the corresponding numerical value, if present, may be placed anywhere after Q_m but before the actual droplet information (N_1,...,N_n). If SETS modifier is missing, then it must occur before the N_Sets value.

T_{Start}: The starting time for the discharge of droplets from the nozzle if START modifier is present. By default for transient flow, the default discharge time is set to zero.

STOP: If this modifier is present, then number immediately following the modifier is interpreted to be the stopping time for the discharge of droplets from the nozzle. This modifier and the corresponding numerical value, if present, may be placed anywhere after Q_m but before the actual droplet information (N_1,...,N_n). If SETS modifier is missing, then it must occur before the N_Sets value.

T_{Stop}: The stopping time for the discharge of droplets from the nozzle if STOP modifier is present. By default, there is no stopping time for discharge.
STOR  For transient mode of computations, by default, it is assumed that the droplets that are discharged from the nozzle evaporate relatively fast compared to the computational time step. This implies that for each time step a set of droplets with the same characteristic are discharged; any previous droplets are assumed to have been evaporated or moved out of computational domain. This assumption preserves computational resources in that only one set (generation) of droplets is tracked (determined by $N_{\text{Set}}$ and $N_{\text{Frq}}$) and stored at each time step. However, if the droplet evaporation time-constant is larger than the computational time step, then some of the droplets released may not fully evaporate during the current time step and need to be kept track of during subsequent time steps.

The STOR modifier allows for storage and tracking of multiple generations of droplets. If this modifier is present then the number immediately following the modifier is interpreted to be the number of generations of droplets that are kept track of. This modifier and the corresponding numerical value, if present, may be placed anywhere after $Q_{m}$ but before the actual droplet information $(N_1, ..., N_n)$. If SETS modifier is missing, then it must occur before the $N_{\text{Sets}}$ value.

$N_{\text{Stor}}$  The maximum number of generations of droplets that are tracked during the computational process. An estimate of the required number can be arrived at by dividing the characteristic evaporation time for largest droplet by the computational time step. A value of 10 is estimated to be adequate for most typical applications. A diagnostic message is printed in the Standard Output File if droplets are removed from storage due to lack of storage space.

TEMP  If this modifier is present, then number immediately following the modifier is interpreted to be the temperature of the droplets. This modifier and the corresponding numerical value, if present, may be placed anywhere after $Q_{m}$ but before the actual droplet information $(N_1, ..., N_n)$. If SETS modifier is missing, then it must occur before the $N_{\text{Sets}}$ value.

$T_{\text{NZL}}$  The temperature of the droplets discharged from the nozzle if TEMP modifier is present. The temperature may also be specified individually for each droplet by using the T modifier (see datatype below). The temperature must be specified in absolute SI units for the evaporation algorithm to work correctly. The default value is set to 300 degrees.

FREQ  If this modifier is present, then the number immediately following the modifier is interpreted as the skip frequency ($N_{\text{Frq}}$) for processing the droplets data. This modifier and the corresponding numerical value, if present, may be placed anywhere after $Q_{m}$ but before the actual droplet information $(N_1, ..., N_n)$. If SETS modifier is missing, then it must occur before the $N_{\text{Sets}}$ value.

$N_{\text{Frq}}$  The skip frequency for processing the droplets. A value of 2 for example, results in the record number, 1, 3, 5, ..., etc. to be read from the file. If no skip frequency is specified, then all droplets are processed.

SETS  If this modifier is present, then the number immediately following the modifier is interpreted as the number of sets of droplets injected by the nozzle ($N_{\text{Sets}}$) for processing the droplets to be read from the data. This modifier and the corresponding numerical value, if present, may be placed anywhere after $Q_{m}$ but before the actual droplet information $(N_1, ..., N_n)$.

$N_{\text{Sets}}$  The number of sets of droplets injected by the nozzle. Each set is assumed to be composed of multiple droplets (see UNIF below). There is no default value. If the droplet data is read from a file then this number may not be specified; in this case the file is read to the end of data.
datatype

Symbols denoting the information contained in each record. The order in which data occurs corresponds to the order of the symbols. The valid symbols are listed below.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description of corresponding datatype</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>The X-coordinate location of the droplet is specified</td>
</tr>
<tr>
<td>Y</td>
<td>The Y-coordinate location of the droplet is specified</td>
</tr>
<tr>
<td>Z</td>
<td>The Z-coordinate location of the droplet is specified</td>
</tr>
<tr>
<td>M</td>
<td>Element number for the location of the droplet is specified</td>
</tr>
<tr>
<td>I</td>
<td>Grid index I for the location of the droplet is specified</td>
</tr>
<tr>
<td>J</td>
<td>Grid index J for the location of the droplet is specified</td>
</tr>
<tr>
<td>K</td>
<td>Grid index K for the location of the droplet is specified</td>
</tr>
<tr>
<td>N</td>
<td>The corresponding field is not processed</td>
</tr>
<tr>
<td>Skip</td>
<td>The corresponding field is not processed</td>
</tr>
<tr>
<td>Dia</td>
<td>The diameter of the droplet, in microns, is specified</td>
</tr>
<tr>
<td>Φ</td>
<td>The property denoted by the symbol Φ is specified. Any of the properties listed in Table 2.8.1-3 may be specified.</td>
</tr>
</tbody>
</table>

The location of droplet may be specified by its \((x, y, z)\) coordinates, its grid element number \((M)\), or its \((I, J, K)\) grid indices. If multiple modes of location are present, then the coordinate location takes precedence over other forms, and element location takes precedence over the grid indices. For 2D flows, the coordinate \(Z\) and the grid index \(K\), if present, are ignored. The symbol \(Φ\) may specify any combination of droplet properties. Currently only the droplet diameter, \(\text{Dia}\), the velocity components, \(U, V, W\) and the temperature, \(T\), are processed. Other input is ignored. For reactive flow, it is assumed that the droplets consist entirely of fuel species in liquid form.

**ELEM**

For a structured grid, if the droplet location is specified by its \((I, J, K)\) indices, then by default it is assumed that the \(I, J, K\) refer to the grid nodes. If this modifier is present along with the \(I, J, K\) modifiers, then it is assumed that the \(I, J, K\) refer to the element numbers rather than the grid nodes (see GRID Command). For unstructured grids this input is ignored.

**UNIF**

If this modifier is present, then the number of droplets in each of the \(N_{\text{Set}}\) sets is assumed to be the same. The number of droplets in the \(n^{th}\) set, \(N_n\), is computed as:

\[
N_n = \frac{Q_m}{\rho L \sum_{n=1}^{N_{\text{Set}}} \frac{\pi}{6} d_n^3}
\]

Here \(Q_m\) is the injected mass, \(N_{\text{Set}}\) is the number of sets, \(\rho L\) is the liquid density and \(d_n\) is the diameter of the \(n^{th}\) set. If this modifier is not present, then the fuel is equally distributed in the \(N_{\text{Set}}\) sets and the number of droplets in the \(n^{th}\) set is computed as:

\[
N_n = \frac{Q_m}{N_{\text{Set}} \rho L \frac{\pi}{6} d_n^3}
\]

**fname**

The name of the file containing the droplet location and properties. The file must contain \(N_{\text{Set}}\) records. Each record must have the same number of values in the same order as the datatype symbols on the command.

**\(N_1, \ldots, N_n\)**

The data for the droplets if a file name is not specified. \(N_{\text{Set}}\) records of data must be present. Each record must have the same number of values in the same order as the datatype symbols on the command.
The evaporation algorithm works correctly only if SI units are used for all quantities except for the droplet diameter, which must be specified in microns \((10^{-6} \text{ m})\).

**EXAMPLES**

```plaintext
NOZZle DROPllets q_fuel= 0.02, 500 records; data order: N I J K DIA U V W T file 'Droplets.NZL'
NOZZle DROPllets q_fuel= 0.02, 500 sets. ELEMents N I J K DIA U V W T file 'Droplets.NZL'
NOZZle with WATER DROPllets q=0.02, 500 sets. ELEMents N I J K DIA U V W T file 'Droplets.NZL'
NOZZle DROPllets data on 'Nozz2D.FIL' q_fuel= 0.02, 500 records Data order is: DIA J I V U T
NOZZle DROPllets data on 'NOZZLE.FIL' q_fuel= 0.02, SETS=500, FREQuency = 2
  Data order is: N DIA I J K SKIP U V W T RHO 1st & 6th columns skipped; RHO ignored.
NOZZle DROPllets data on 'Nozz2D.FIL' q_fuel= 0.02, FREQuency =2, SETS=500 records
  Data order is: N DIA I J SKIP SKIP U V N T N! 1st, 5th, 6th, 9th & 11th columns skipped.
NOZZle DROPllets on 'NOZZ3D.FIL' q = 0.02, 500 sets ELEMent based
  Data order is: N DIA K I J SKIP W U V T RHO! 1st & 6th columns skipped; RHO ignored.
NOZZle DROPllets data from 'NOZZ3D.FIL' q = 0.02, evaporation RATE = 0.1 FREQ=2, SETS=500
  Data order is: N DIA K I J SKIP W U V T RHO! 1st & 6th columns skipped; RHO ignored.
```
**ACRi™ Software Tools**  

### Keyword Commands

**MODE 2:** Nozzle Location and Injection Parameters (3D Geometry)

| SYNTAX | NOZZ {LOCA|DEGR} [FUEL|WATE] {X_o, Y_o, Z_o} {Q_m} {Rad, θ} {n_x, n_y, n_z} {Θ_o, Θ_f} {d_SMD} {N_Ray} [option] [[ABSO] RATE=Q_{Evap} ^] [STAR=\text{t}_{\text{Start}} ] [STOP=\text{t}_{\text{Stop}} ] [STOR=N_{\text{Stor}}] [TEMP=T_{\text{NZL}} ] {N_{vel}} \{v_1, .., v_{nvel}\} |
|---|---|
| LOCA | The location of the nozzle discharge flow is specified. Individual droplets are internally generated. |
| DEGR | By default all angles specified with this mode of command are in radians. If this modifier is present then all angles are in degrees. See Figure below for a schematic of the nozzle. |
| FUEL | Nozzle injects fuel droplets. This is the default option. |
| WATE | Nozzle injects water droplets. |
| X_o, Y_o, Z_o | The x, y, and z coordinates of the location of the nozzle. If the geometry is radial, then Z_o must be in radians or degrees. There is no default value. |
| Q_m | The mass flow rate injected through the nozzle. There is no default value. |
| Rad | The nozzle radius. There is no default value. |
| θ | The nozzle cone angle. There is no default value. |
| n_x, n_y, n_z | Direction cosines of nozzle orientation in the X, Y, and Z-directions, respectively). There is no default value. |
| Θ_o, Θ_f | Initial and final spray cone angles. There is no default value. |
| d_SMD | Sauter mean diameter (SMD) in microns. The actual distribution of droplet diameter for each ray (see N_{Ray} below) is controlled by the NOZZLE command with DISTRIBUTION modifier. There is no default value. |
| N_Ray | Number of spray cone rays issuing from the nozzle. Each is then subdivided into individual droplets (sub rays) with different diameters. The diameter distribution is controlled by the NOZZLE command with DISTRIBUTION modifier. There is no default value. |
| option | Same as Mode 1. |
| ABSO | This modifier is effective only if the RATE modifier is present, otherwise it is ignored. In the presence of this modifier, the specified rate of evaporation is computed from the original rather than the current remaining mass of the droplet. |
| RATE | If this modifier is present, then the number immediately following the modifier is interpreted as the rate of evaporation to be forced on the droplets from this nozzle. By default the evaporation rate is computed automatically from the droplet algorithm. This modifier and the corresponding numerical value, if present, may be placed anywhere after N_{Ray} but before the location of N_{vel}. |
| Q_{Evap} | The rate of evaporation as a fraction of the droplet mass. In the presence of the ABSOLUTE modifier, the specified fraction of the original droplet is forced to evaporate at each droplet time step (see Mode 8 of command for droplet time step). For example, a specification of 0.1 will result in complete evaporation in 10 droplet steps. If the ABSOLUTE modifier is not present, then the fraction is applied to the remaining mass of the droplet; that is with a specification of 0.1, the evaporated fractions will be 0.1, 0.09, 0.081, and so on. |
| STAR | If this modifier is present, then number immediately following the modifier is interpreted to be the starting time for the discharge of droplets from the nozzle. This modifier and the corresponding numerical value, if present, may be placed anywhere after N_{Ray} but before the location of N_{vel}. |
| T_{Start} | The starting time for the discharge of droplets from the nozzle if START modifier is present. By default for transient flow, the default discharge time is set to zero. |
STOP
If this modifier is present, then number immediately following the modifier is interpreted to be
the stopping time for the discharge of droplets from the nozzle. This modifier and the
the corresponding numerical value, if present, may be placed anywhere after NRay but before the
location of NVel.

TStop
The stopping time for the discharge of droplets from the nozzle if STOP modifier is present. By
default, there is no stopping time for discharge.

STOR
For transient mode of computations, by default, it is assumed that the droplets that are
discharged from the nozzle evaporate relatively fast compared to the computational time step.
This implies that for each time step a set of droplets with the same characteristic are
discharged; any previous droplets are assumed to be have been evaporated or moved out of
computational domain. This assumption preserves computational resources in that only one
set (generation) of droplets is tracked (determined by NVel and NFreq) and stored at each time
step. However, if the droplet evaporation time-constant is larger than the computational time
step, then some of the droplets released may not fully evaporate during the current time step
and need to be kept track of during subsequent time steps.

The STOR modifier allows for storage and tracking of multiple generations of droplets. If this
modifier is present then the number immediately following the modifier is interpreted to be the
number of generations of droplets that are kept track of. This modifier and the corresponding
numerical value, if present, may be placed anywhere after NRay but before the location of NVel.

NStor
The maximum number of generations of droplets that are tracked during the computational
process. An estimate of the required number can be arrived at by dividing the characteristic
evaporation time for largest droplet by the computational time step. A value of 10 is estimated to
be adequate for most applications; a warning is printed if droplets remain unevaporated
even at the end of NStor computational time steps.

TEMP
If this modifier is present, then number immediately following the modifier is interpreted to be
the temperature of the droplets. This modifier and the corresponding numerical value, if present,
may be placed anywhere after NRay but before the location of NVel.

TNZL
The temperature of the droplets discharged from the nozzle if TEMP modifier is present. The
temperature must be specified in absolute SI units for the evaporation algorithm to work
correctly. The default value is set to 300 degrees.

NVel
The number of values (2t) in the spray velocity distribution. There is no default value.

V1...Vnvel
Spray velocity distribution; the specified number of values must equal NVel. These values are
sampled in succession for each sub-ray within each ray. See COMMENTS for further
explanation of how the starting velocity of each droplet is computed.

COMMENTS
The individual droplets issued by this command and their characteristics are controlled by the
input given on this command and the droplet distribution specified by the NOZZLE
DISTRIBUTION mode of the command. For example if 7 values for droplet distribution, say,
0.5, 0.8, 1.0, 1.2, 1.5, 1.8 and 2.1, are specified on the NOZZLE DISTRIBUTION command
and 10 rays (NRay) are specified on this command, then each ray will contain 7 sub-rays and a
total of 70 droplets will be injected from the nozzle at each step. Further if the droplet SMD
(dSMD) is 40 then each of 10 rays will inject 7 droplets with respective diameters of 20, 32, 40,
48, 60, 72 and 80 microns. The total amount of fuel injected is divided equally between these
droplets; in this case each of the droplets represents 1/70th of the total injected fuel (Qm).

The location of droplets in each ray is computed so as to cover the total range of spray cone
angles in a uniform manner. For example if the number of rays is 10 and the initial and final
spray cone angles (Θ0, ΘF) are 45 and 315, then the 1st through the 10th rays will emit from
locations corresponding to the angles of 45, 75, 105, 135, 165, 195, 225, 255, 285 and 315
degrees, respectively. The actual coordinates, of course, will depend on the location, radius
and direction cosines of the nozzle.

The velocity of each droplet that issues determined by the NVel values of velocity distribution
(V1...Vnvel), the NRay values of the number of rays and the Nsubray values on the NOZZLE
DISTRIBUTION command. The starting velocity of each droplet is computed from the logic
given below.
IV = 0
do n = 1, N_Ray
  do ns = 1, N_subray
    IV = MOD(IV, N_Vel) + 1
    Vdroplet(n,ns) = Vspecified(IV) ! Vspecified() = V_1 to V_nvel
  enddo
enddo

EXAMPLES

NOZZle LOCAted at (0.1,1.0,0.02), 0.1 kg/s, 0.005 radius, 0.05 radian cone angle, dir cosines=(0,1,0),
(0 6.28), 20 microns, 8 rays, 1 velocity value, 100 m/s

NOZZle with angles in DEGRees, at (0.1,1.0,0.02), 0.1 kg/s, 0.005 radius, 10 deg cone angle, dir
   cosines=(0,1,0), (0 360) deg, 20 microns, 8 rays, 1 velocity value, 100 m/s
MODE 3: Nozzle Location and Injection Parameters (2D Geometry)

SYNTAX

```
NOZZ {LOCA|DEGR} [FUEL|WATE] {X₀, Y₀} {Qₘ} {H₀, φ} {nₓ, nᵧ} {dSMD} {NRay} [option]
     [[ABSO] RATE=Qₑvap] [STAR=tₘₖₜ] [STOP=tₘₖₜ] [STOR=Nₘₖₜ] [TEMP=Tₐₜₜ] {Nₙₑₙₜ} {N₁,...Nₙ}
```

LOCA
The location of the nozzle and flow parameters are specified. Individual droplets are internally generated.

DEGR
Same as Mode 2.

FUEL
Nozzle injects fuel droplets. This is the default option.

WATE
Nozzle injects water droplets.

X₀, Y₀
The x, and y coordinates of the location of the nozzle. There is no default value.

Qₘ
The mass flow rate injected through the nozzle. There is no default value.

H₀
The nozzle opening height in cross-section. There is no default value.

φ
The included angle of the spray cone. There is no default value.

nₓ, nᵧ
Direction cosines of nozzle orientation in the X and Y directions, respectively). There is no default value.

dSMD
Same as Mode 2.

NRay
Same as Mode 2.

option
Same as Mode 2.

ABSO
Same as Mode 2.

RATE
Same as Mode 2.

Qₑvap
Same as Mode 2.

STAR
Same as Mode 2.

Tₘₖₜ
Same as Mode 2.

STOP
Same as Mode 2.

Tₘₖₜ
Same as Mode 2.

STOR
Same as Mode 2.

Nₘₖₜ
Same as Mode 2.

TEMP
Same as Mode 2.

Tₐₜₜ
Same as Mode 2.

Nₑₙₜ
Same as Mode 2.

N₁,...Nₙ
Same as Mode 2.

EXAMPLES

```
NOZZle DEGRees: (0.1, 1.0) Q=0.1, R=0.005, cone=45 deg, dir cosines (0.707, 0.707), 40, 5,1,100
NOZZle LOCAted at (0.1, 1.0) Q=0.1, R=0.005, cone=0.75, dc's (0.707, 0.707), 40, 5, TEMP =350, 1,100
```
MODE 4: User Specified Droplet Algorithm with Atomization

SYNTAX

NOZZ {ATOM} {Q_m} {N_Sets}

ATOM

The droplet computation algorithm is specified by the user and the droplet location and properties will be computed by an atomization algorithm specified by the user. The built-in droplet transport and evaporate algorithm is by-passed. This option requires source code access or license from ACRi.

Q_m

The total mass flow rate [M T^{-1}] of fuel injected by the nozzle. There is no default value.

N_Sets

The number of individual droplets injected by the nozzle. There is no default value.

EXAMPLES

NOZZle ATOMization algorithm with q_fuel= 0.02 and 500 droplets
MODE 5: Nozzle Sauter Mean Diameter Distribution.

SYNTAX

NOZZ {DIST} { N1, Nm}

DIST Distribution of droplets emanating from the nozzle as a fraction of the given sauter mean diameter (SMD) is specified. This is applicable only to the NOZZLE command with LOCATION or DEGREE modifier.

N1, Nm The numerical values to compute the droplet diameters for each subset (ray) of droplets issuing from the nozzle. Each ray of droplets is sub-divided into this many sub-rays for tracking the spray droplets to compute the rate and location of phase change. Each sub-ray has a droplet diameter equal to the product of the SMD (dSMD specified by NOZZLE command with LOCATION or DEGREE modifier) and the distribution specified here. The number of values (each >0) must lie between 1 and 20. The default values are 0.6, 0.9, 1.2, 1.5 and 2.1.

COMMENTS

This command applies ONLY to the Mode 2 or 3 NOZZLE commands that follow this command. Any Mode 2 or 3 NOZZLE command that precedes this command will use the previously supplied (or default) droplet distribution. Thus each Mode 2 or 3 NOZZLE command may have its own droplet distribution. The number of values specified on this command determines the number of “sub-rays” that each spray “ray” is divided into. The number of rays is specified on the corresponding Mode 2 or 3 command.

This command is ignored if droplet information is directly specified by Mode 1.

EXAMPLES

NOZZle SMD DISTRIBUTION with values: 0.4, 0.8, 1.2, 1.6, and 2.0
NOZZle DISTRIBUTION with values: 0.1, 0.4, 0.6, 0.8, 1.0, 1.2, 1.6, 1.8, 2.0, and 2.5
MODE 6: Nozzle Spray Computations Parameters

SYNTAX

NOZZ \{FREQ\} \{V_{frq}\} [TIME] [N_{Begin}, N_{End}] 

FREQ  The spray computation frequency parameters are specified.

V_{frq}  The frequency (step or time interval) at which the droplet computations are performed. The default value is 10.

TIME  By default, V_{frq} is the frequency of computations in terms of number of steps. If this modifier is present, then V_{frq} is interpreted to be time interval between successive computations.

N_{Begin}  The first computational step at which the droplet computations are performed. The default value is 1.

N_{End}  The last computational step at which droplet computations is performed. The default frequency is set to 9999999.

COMMENTS

Spray droplet computations are automatically triggered if a NOZZLE command in Mode 1 through 3 is encountered. This input is required only if the user wants to modify the default values.

EXAMPLES

NOZZle FREQuency of calculations: 1 start at step number 10
NOZZle FREQuency of calculations: 10 start at step number 10 and stop at step 500
Mode 7: Nozzle Output Options

Syntax

```
NOZZ {TRAJ} [fname] [N_{start}, N_{end}, N_{frq}]
```

**TRAJ**

A detailed file of trajectory and evolving particulars for each droplet is generated. The frequency of output is controlled by $N_{start}$, $N_{end}$, and $N_{frq}$. A NOZZLE command with this modifier must be present to generate the trajectory output.

**fname**

The name of the file to which the output is directed. See Section 3.3 for additional information. If no name is specified then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by “_NOZZLE.TMP”. For example, if the Standard Output file is “PROBLEM.OUT”, then the file is named “PROBLEM NOZZLE.TMP”. At any time only one nozzle file can be open. If a new file name is given, then the previous file is closed and output is directed to the new file.

**N_{start}**

The first computational step at which the trajectory output is generated. If no value is specified, or the value is less than the nozzle computation frequency (see NOZZLE FREQUENCY mode of command), then output is obtained only once at the start of the droplet computations.

**N_{end}**

The last computational step at which the trajectory output is generated. If no value is specified, then the default value is set to 9999999 steps.

**N_{frq}**

The frequency of output in terms of computational steps. If both $N_{end}$ and $N_{frq}$ are missing, then the default value is set to 9999999 so that the output is obtained only once as determined by $N_{start}$. If on the other hand, $N_{end}$ is specified but $N_{frq}$ is missing, then the default value is set to unity so that the output is obtained at every step between $N_{start}$ and $N_{end}$.

Examples

- **NOZZle TRAjectory output the first time droplet computations are performed**
- **NOZZle TRAjectory output on file ‘TRAJ.NZL’**
- **NOZZle TRAjectory output on file ‘TRAJ.NZL’ at step number 50**
- **NOZZle TRAjectory output on file ‘TRAJ.NZL’ start at step# 50 up to step 100 with frequency 20,**
MODE 8: Droplet Time Step Factors and Tracking Options

SYNTAX

```
NOZZ [TIME=V_{dt}] [STEP] [INCR=\alpha_{dt}] [ITER=N_{iter}]
```

TIME

A suitable time step for moving each droplet is computed by examination of the kinetic and dynamic time scales. This modifier indicates that additional input for time step control is specified by the user.

\( V_{dt} \)

If the STEP modifier is absent then the time step computed internally is multiplied by \( V_{dt} \). If the STEP modifier is also present, then the droplet computation time step is forced to be equal to \( V_{dt} \); any internal computations are ignored.

STEP

The modifier to assist in the interpretation of \( V_{dt} \) input.

INCR

The time step increase factor, \( \alpha_{dt} \), is specified. If the droplet stays at its current element location after a time step, then the next step is increased by the specified factor. The default value is 1.4142.

\( \alpha_{dt} \)

The time step increase factor as defined above.

ITER

If this modifier is present, then the maximum number of iterations for each droplet is set by \( N_{iter} \). Each droplet is moved continuously in its trajectory unless it:

- Completely evaporates,
- Hits a solid boundary or object,
- Moves out of the computation domain or
- Completes a specified number of iterations (by default set to 500.).

\( N_{iter} \)

The maximum number of iterations for droplet. The numerical value must be >0; otherwise the input is ignored and the default or any previously specified value is used.

EXAMPLES

```
NOZZle TIME 2.0! Multiply internally computed value by 2
NOZZle TIME STEP is = 1.E-6 seconds! Force this time step for droplet Movement
NOZZle TIME multiplier is 2 and INCREASE factor is = 1.
NOZZle ITERations=200
NOZZle TIME STEP = 1.E-6, ITERations=200
NOZZle ITERations=200, TIME STEP = 1.E-6, INCrease factor 1.0
```
MODE 9: Droplet Temperature and Evaporation Factors

SYNTAX: NOZZ {MINI=$T_{min}$} [MAXI=$\delta_{T_{max}}$] [EVAP=$\delta_{q_{max}}$] [RANZ] [FUEL] [WATE] [GRAV] [STOC] [AUTO]

MINI
If the liquid droplet evaporation rate exceeds the heat input rate, then the liquid temperature can drop. This modifier is used to set the minimum permitted liquid temperature.

$T_{min}$
The minimum droplet temperature in absolute units. The default value is 273.15.

MAXI
This modifier sets the maximum change in the temperature of the droplet in a single time step as a fraction of the current liquid temperature.

$\delta_{T_{max}}$
The maximum change in temperature of the droplet as a fraction of current liquid temperature. The default value is 0.1.

EVAP
This modifier sets the maximum fraction of the mass of the droplet that can evaporate in any single time step.

$\delta_{q_{max}}$
The maximum permitted value of evaporated mass of the droplet in any single step as a function of its current mass. The default value is 0.1.

RANZ
By default the heat and mass transfer rates for droplets are computed from the Abramzon-Sirignano (1989) correlation. If this modifier is present then the more commonly used Ranz-Marshall (1952) correlation is used. If neither FUEL nor WATeR modifier is present, then the correlation is used for all nozzles.

FUEL
The Ranz-Marshall correlation is applied to the nozzles with fuel injection.

WATE
The Ranz-Marshall correlation is applied to the nozzles with water injection.

GRAV
By default the effect of gravitational force on the droplets is ignored. If this modifier is present then the droplet velocity is modified by the gravitational force.

STOC
By default the droplets move only due to the deterministic convective movement due to fluid and droplet velocity. If this modifier is present then the droplet movement due to turbulent motion is also accounted for. A random walk algorithm, coupled with the local state of turbulence, is used to generate the stochastic component of particle motion.

AUTO
A fixed evaporation rate for droplets may be explicitly set by the Mode 1 of the command with RATE modifier. This AUTO modifier disables the specified evaporation rate and switches back to the built-in thermal and mass transfer based computation of droplet evaporation rate. One of the uses of this option is to allow the droplets to be forced to evaporate in the early stages of a computation when the flame is not yet established. Once the flame is established, the forced evaporation rate can be disabled.

EXAMPLES

NOZZle MINimum temperature=300 degrees
NOZZle MINimum temperature=300 degrees; MAXimum temperature change=0.01
NOZZle MINimum temperature=300 degrees; Evaporated fraction in one step=0.01
NOZZle MINimum temp=300; AUTOmatic mode
NOZZles with GRAVitational and STOChastic forces and RANZ marshall correlation
NOZZles of WATER type with RANZ Marshall correlation
NOZZle switch back to AUTOmatic mode
COMMAND  OPEN

PURPOSE  To specify an open boundary through which fluid may enter or leave based upon prevailing flow conditions. This command is effective only for the ANSWER™ Software Tool.

MODE 1:  Open Boundary with Default Boundary Conditions

SYNTAX  OPEN  {dir} [subrgn] [FREE] [DIAG]

dir  The orientation index for the open boundary. There is no default value; a value must be specified.

subrgn  The subregion to be identified as an open boundary. If no subregion is specified, the outermost "dir" oriented boundary of the entire computational domain is selected.

FREE  By default, diffusion at an OPEN boundary is set to zero. If this modifier is present then no assumption is made about diffusion and the boundary diffusion is computed from the specified boundary conditions and the diffusivity coefficient.

DIAG  By default only summary statistics of total boundary area, average density and velocity, and flow rate are printed to the standard output device. If this modifier is present then a complete detail of area, velocity components, density and flow rate for each segment of the boundary is printed.

COMMENTS  An open boundary, by definition, is assumed to be a boundary where the values of all dependent variables are fixed if fluid enters through the boundary but the normal gradients of all dependent variables are zero if fluid leaves through the boundary. If the fluid enters through the boundary then the value of the variable for the entering fluid is taken to be that existing at the boundary. This value may be specified (or subsequently changed) by the INITIAL, READ or SET commands and is maintained even if the fluid leaves through the boundary.

EXAMPLES  

OPEN  at Y+ boundary at maximum y
OPEN  at X+ boundary for most recently SELECTed subregion
OPEN  at Y- boundary for subregion ID = OPEN
OPEN  OFF at Y- boundary for subregion ID = OPEN
MODE 2: Open Boundary with flow based on Pressure and drag Coefficient.

SYNTAX

OPEN \{DISC|GATE \} \{dir\} \{subrgn\} \{C_D\} \{P|PRES=P_B\} \{AREA=A_B\} \{IN|OUT\}

DISC | GATE

The flow at the boundary is computed from:

\[ Q_t = C_D \rho \sqrt{\frac{2}{\rho}} (P_B - P) A_B \]

Where \( Q_t \) is the mass flow, \( C_D \) is a discharge or drag coefficient, \( A_B \) is the boundary area, \( P_B \) is the boundary pressure, \( P \) is the computed pressure in the flow field interior to the boundary and \( \rho \) is the fluid density at the boundary. If the boundary comprises more than one element face, then the total mass flow is the sum of the individual components.

With \( A \) as the total area of the face, and \( A_i \) as its vector components, the velocity components, \( v_i \), at the element face are computed from:

\[ v_i = \frac{Q_t}{\rho} \frac{A_i}{A} \]

dir

The orientation index for the open boundary. There is no default value; a value must be specified or must be implicit in the subrgn definition.

subrgn

The subregion to be identified as an open boundary. If no subregion is specified, the outermost “dir” oriented boundary of the entire computational domain is selected.

\( C_D \)

The discharge coefficient for the boundary

\( P|PRES \)

The modifier to indicate that the pressure at the boundary is being specified explicitly.

\( P_B \)

By default it is assume that the boundary pressure is equal to zero. If the \( P \) or PRES modifier is present, then this is taken to be the value of the boundary pressure.

\( AREA \)

The modifier to indicate that the effective flow at the boundary is being specified explicitly.

\( A_B \)

By default it is assumed that the area through which the flow occurs is the actual area of the face of the element; that is \( A_B = A \). If the modifier AREA is present, then this is taken to be area through which the flow occurs.

IN

If this modifier is present, then only inflow is allowed at the boundary. Any pressure gradient that indicates an outflow is set to zero.

OUT

If this modifier is present, then only outflow is allowed at the boundary. Any pressure gradient that indicates an inflow is set to zero.

EXAMPLES

OPEN at ID=OPEN surface: DISCHARGE coef = 0.5
OPEN at ID=OPEN surface: DISCHARGE coef = 0.5 , P=100
OPEN at ID=OPEN surface: DISCHARGE coef = 0.5 , P=100, AREA=0.02
MODE 3: Turn Off a Previously Specified OPEN Port

SYNTAX

OPEN {dir} {subrgn} {OFF}

dir The orientation index for the open boundary. There is no default value; a value must be specified.

subrgn The subregion to be identified as an open boundary. If no subregion is specified, the outermost “dir” oriented boundary of the entire computational domain is selected.

OFF Previously specified open boundary for the identified subregion is deactivated. A new specification for this subregion may follow.

EXAMPLES

OPEN at Y+ boundary OFF
<table>
<thead>
<tr>
<th>COMMAND</th>
<th>OPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To select or modify built-in default options.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>Geometry, Interpolation and Solver Options</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>OPTI [NEW</td>
</tr>
<tr>
<td>NEW</td>
<td>The volume fractions and interpolation factors for computing interface values are computed as the vector dot product of the interface areas and the direction vector connecting the two adjoining element. <strong>This is the default option.</strong></td>
</tr>
<tr>
<td>OLD</td>
<td><strong>Use of this modifier is not recommended.</strong> The volume fractions and interpolation factors for computing interface values are obtained from the fraction of volume contained between the interface and the element node.</td>
</tr>
<tr>
<td>QUAD</td>
<td>By default the values of a field variable such as pressure at the element interface are computed as a linear function of the distance of the interface from the two nearest element values. If this modifier is present, then the values are computed as inverse square function of the distance of the interface from the two nearest element values. <strong>This modifier is effective only if the OLD modifier is not present.</strong></td>
</tr>
<tr>
<td>VOLU</td>
<td>The values of a field variable at the element interface are computed as a volume-weighted function of the two nearest element values. <strong>This modifier is effective only if the OLD modifier is not present.</strong></td>
</tr>
<tr>
<td>INTE</td>
<td>By default the distance of the element nodal point to the element interface is computed as the Euclidian distance from the node to the center of the face. If this option is selected, then the node to interface distance is computed as the projected normal distance of the node to the plane of the interface. For orthogonal grids the two are equal.</td>
</tr>
<tr>
<td>ROBU</td>
<td>By default the solvers related settings are optimized for computational speed rather than numerical stability and robustness. If this option is specified, then the initial settings are optimized for robustness of the solution procedure.</td>
</tr>
</tbody>
</table>

**EXAMPLES**

**OPTI**on NEW geometry computations with QUADratic interpolation
MODE 2: Mach Number Computation Options

SYNTAX

```
OPTI {MACH} {SONI|GAMM|T|GAS} [V₁]
```

MACH
This modifier selects the method used to compute the Mach number for the flow. If must be present for one of these options to be invoked.

SONI
The Mach number is computed from the relation

\[ Ma = \frac{V}{c} \]

Here \( V \) and \( c \) are the fluid and the sound speeds. The latter can be specified with the GAS SONIC command. This is the default option unless COMPRESSIBLE or REACTION command is specified.

GAMM
The Mach number is computed from the relation:

\[ Ma = \frac{V}{\sqrt{\frac{\gamma C_p}{\rho}}} \]

Here \( V \) is the fluid speed, \( \gamma \) is the ratio of specific heat at constant pressure to that at constant volume, \( C_p \) is the specific heat at constant pressure, \( P \) is the gas pressure and \( \rho \) is the gas density. The \( \gamma \) can be specified by N1 or the GAS GAMMA command.

T
If this modifier is present without the GAMM modifier then with, \( R \) as the gas constant and \( T \) as the temperature in absolute units, the Mach number is computed from:

\[ Ma = \frac{V}{\sqrt{\frac{R}{C_p} - \frac{R}{C_p} T}} \]

T
If this modifier is present together with the GAMM modifier, then the Mach number is computed from the relation:

\[ Ma = \frac{V}{\sqrt{(\gamma - 1) C_p T}} \]

GAS
The Mach number is computed from:

\[ Ma = \frac{V}{\sqrt{C_p - \frac{P}{\rho}}} \]

Here \( V \) is the fluid speed, \( R \) is the gas constant, \( C_p \) is the specific heat, \( P \) is the pressure and \( \rho \) is the gas density. \( R \) is computed from the mass fractions and molecular weights of the gas components. This is the default option if COMPRESSIBLE or REACTION command is specified.

V₁
The sonic speed if the SONI modifier is present; the default value is 300. The specific heat ratio \( \gamma \) if the GAMM modifier is present; the default value is 1.4.

EXAMPLES

```
OPTI on MACH number from GAMMA
```

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Keyword Commands
MODE 3: Pressure Related Options for ANSWER™

SYNTAX

OPTI [LINE|GRAD|FIXE|FIX] [P|PRES]

LINE
For ANSWER™, pressure at inlet, outlet and open boundaries is computed from linear extrapolation. This is the default option for hexahedral grids. This is equivalent to assuming that the 2nd gradient normal to the boundary is zero. This selection may be numerically unstable if the grid quality is poor or if the pressure gradients near the boundary are very high.

GRAD
For ANSWER™, pressure at inlet, outlet and open boundaries is computed by assuming that the normal gradient at the boundary is zero. This option is numerically more stable than the LINEar extrapolation. This is the default option for unstructured non-hexahedral grids.

FIXE
For ANSWER™, pressure at inlet, outlet and open boundaries is assumed to be fixed. This option is more suited for compressible flow computations. In this case the boundary pressure must be explicitly specified by the user.

FIX
Same as the FIXED modifier.

P
If the FIXE option is selected, then by default it is assumed that the pressure at the specified boundary is fixed and the change in pressure ($p'$, computed from the continuity equation) is zero. If this modifier is present, then it is assumed that while the boundary $P$ is fixed, the $p'$ can vary based on the other default settings – such as linear extrapolation at the boundaries. This modifier is effective only in the presence of the FIXE modifier.

PRES
Same as the P modifier.

EXAMPLES

OPTlon GRAD for pressure ! For extrapolation of pressure for this highly skewed grid
MODE 4: Enthalpy Related Options for ANSWER™

SYNTAX

OPTI [ENTH|NORM|GRAD] [DIFF] [ARIT|SOLI|FLUI|OFF]

ENTH
If this modifier is present with the NORM modifier, then its interpretation is as described under NORM. If it is present with the GRAD modifier, then its interpretation is as described under GRAD. If this modifier is present by itself, then it activates the computation of thermal energy equation with enthalpy as the dependent variable.

NORM
If this modifier is present together with the ENTH modifier, then thermal energy equation is solved in terms of normalized enthalpy which is enthalpy divided by reference specific heat (see REFERENCE command). This has the advantage that the computed value is on the order of the temperature. Since specific heat in metric units can be large (~1000), enthalpy variable can have values on the order of $10^5$ or higher which can increase truncation errors with real number arithmetic. This is the default mode of solving thermal energy equation.

GRAD
The thermal diffusion term is computed as the product of effective thermal conductivity and the temperature gradient. This formulation is the correct expression of the Fourier’s Law of Conduction. However, if it is desired to compute thermal diffusion from gradients of enthalpy, then this modifier must be specified together with the ENTHalpy modifier.

DIFF
In ANSWER™ Software Tool, the thermal conductivity is multiplying by dividing the diffusivity with the specific heat. This modifier along with the modifiers described below selects the manner of computation of the interface thermal conductivity.

ARIT
The specific heat at the element interface is computed as the arithmetic average of the values at the two nodes that straddle the interface. This is the default option. This modifier is effective only in the presence of the DIFF modifier for the ANSWER™ Software Tool.

SOLI
The specific heat at the interface between a fluid and solid is taken to be value for solid. If the interface is between two solid (blocked) elements or two fluid elements, then the interface specific heat is computed as the arithmetic average between the two nodes that straddle the element. This modifier is effective only in the presence of the DIFF modifier for the ANSWER™ Software Tool.

FLUI
The specific heat at the interface between a fluid and solid is taken to be value for fluid. If the interface is between two solid (blocked) elements or two fluid elements, then the interface specific heat is computed as the arithmetic average between the two nodes that straddle the element. This modifier is effective only in the presence of the DIFF modifier for the ANSWER™ Software Tool.

OFF
The interface diffusion is set to zero. This modifier is effective only in the presence of the DIFF modifier for the ANSWER™ Software Tool.

EXAMPLES

OPTIon use ENTHalpy ! Formulation for conjugate heat transfer
OPTIon use TEMPerature formulation for heat transfer even though there are no solid blocks.
OPTIon thermal DIFFusion with specific heat of SOLId at the interface
MODE 5: Flow Related Options for ANSWER™

SYNTAX

OUTL

For all incompressible flow simulations and for steady state compressible flow simulations, the flow at OUTLET boundaries is corrected so that the total outflow equals the net global inflow into the domain. For incompressible flow, the convergence of the solution process may be adversely affected if this correction is not performed. For compressible flow, this may or may not be necessary based on the specified boundary conditions for pressure and/or density. This option is available only for ANSWER™ Software Tool.

OFF

The outflow correction indicated by the OUTLET modifier is suppressed. For incompressible flow, convergence of the solution process may be adversely affected and is strongly influenced by the boundary conditions for pressure and/or density. On the other hand, for compressible flow, this modifier may improve the convergence of the solution process. This modifier is effective only in the presence of the OUTLET modifier for the ANSWER™ Software Tool.

VELO

By default the corrections relating to the OUTLET boundaries are made by directly modifying outgoing convective flux; the outlet velocity is not corrected to correspond to the local values of density and boundary orientation. The outlet velocity is controlled by the specified or default boundary conditions. If this modifier is specified, then the outlet velocity is corrected so that it corresponds to the outflow flux. This modifier is effective only in the presence of the OUTLET modifier for the ANSWER™ Software Tool. The use of this modifier is not generally recommended.

EXAMPLES

OPTI on OUTLET VELOCITY from convective flux
MODE 6:  Salt Dissolution Options

SYNTAX  

\[ \text{OPTI} \{\text{SALT}\} \{\text{FORC}\mid \text{CONS}\mid \text{VELO}\mid \text{OFF}\} \{Z_{\text{min}}\} \{Z_{\text{max}}\} \{\alpha\} \{\beta\} \]

SALT  This option is applicable only for ANSWER™ software. This option affects the dissolution rate of the salt. By default, the dissolution is determined from the correlation given under the BLOCK SALT command. That correlation was developed for flows that are dominated by natural convection. In some situations, forced convection may strongly influence the dissolution rate. One such circumstance is when the location of injection is higher than the that of outflow. In this case descending heavy brine near the wall may be assisted by the injected flow traveling towards the lower outflow point.

FORC  Implements the forced convection enhancement that occurs in salt caverns when the injection point of fresh water is located above the brine outflow point. In this case the velocity of injected fluid is co-directional with the downward movement of heavy brine. This is the default option.

With \( \text{Nu}_e \), \( \text{Nu}_{fc} \) and \( \text{Nu}_{nc} \), respectively, the effective, the forced convection and the natural convection Nusselt numbers, the forced convection enhancement is based on the correlation:

\[
(\text{Nu}_e)^3 = (\text{Nu}_{fc})^3 + (\text{Nu}_{nc})^3
\]

The discussion below will be carried out in terms of Nusselt numbers but the same arguments apply to Mass transfer if Nusselt number is replaced by Sherwood number. For fully developed turbulent flow in tubes, with \( V \) as the characteristic velocity and \( R \) as the radius, the \( \text{Nu}_{fc} \) is given by:

\[
\text{Nu}_{fc} \propto [V R]^{0.8}
\]

We may further assume that the characteristic velocity, \( V \), is related to the injection velocity, \( \beta \), and the radius, \( R \) as:

\[
V \propto \frac{\beta}{R^2}
\]

From these equations, we obtain:

\[
\frac{\text{Nu}_e}{\text{Nu}_{nc}} = \left[ 1 + \left( \frac{C V^{0.8}}{R^{0.8} \text{Nu}_{nc}} \right)^3 \right]^{-1/3}
\]

We write the \( \text{Nu}_{nc} \) as:

\[
\text{Nu}_{nc} = \frac{h_{nc} L}{\Gamma} = \frac{q L}{\Gamma \Delta C_s}; \quad h_{nc} = \frac{q}{\Delta C_s}
\]

Where, \( h_{nc} \) is a transfer coefficient, \( L \) is a characteristic length, \( \Gamma \) is a diffusivity, \( q \) is the mass transfer rate and \( \Delta C_s \) is a driving force based on the salt concentration in the fluid. The ratio of mass transfer rate to driving force can be determined from the Sandia correlation for mass transfer rate (see BLOCK SALT command). It is graphically represented in the figure below where the transfer coefficient is in metric units. This can be expressed as:

\[
\text{Nu}_{nc} = \frac{L}{\Gamma} (67.856 - 52.807C_s)
\]
Therefore the forced convection enhancement factor, $f_{fc}$, can be written:

$$f_{fc} = \frac{\text{Nu}_e}{\text{Nu}_nc} = \left[1 + \left(\frac{\alpha \beta^{0.8}}{R^{0.8} L (67.856 - 52.807 C_s)}\right)^3\right]^{1/3}$$

The constant of proportionality, $\alpha$, must be determined from empirical data. In metric units, its value is expected to be on the order of 100.

**CONS**

Forced convection enhancement is based on a user specified constant rather than on a computed function based on Nusselt numbers. The enhancement factor is given as:

$$f_{fc} = \alpha$$

**VELO**

Forced convection enhancement is based on a representative cavern velocity. The enhancement factor is computed from:

$$f_{fc} = 0.98077 - 5.15405 V + 74.73588 V^2 - 108.98371 V^3; \quad V > 0.008467; \quad f_{fc} \leq 4$$

$$= 1; \quad V \leq 0.008467$$

The $V$ is in m/s and it is taken as the velocity just upstream of the outflow location.

**OFF**

Forced convection enhancement is deactivated.

**Z_{min}**

The minimum value of the ending value of the axial coordinate of the salt cavern where the forced convection effects are significant.

**Z_{max}**

The ending value of the axial coordinate of the salt cavern where the forced convection effects are significant. It should be noted that the $L$ required for the forced convection enhancement option is computed as: $L = Z_{max} - Z_{min} > 0$.

**$\alpha$**

The forced convection enhancement constant if the modifier FORC or CONS is present.

**$\beta$**

The injection velocity if the modifier FORC is present. If the injection velocity is not specified, its default value is assumed to be 5.

**EXAMPLES**

**OPTI**n SALT FORCed convection with $Z_{min}=0$. $Z_{max} = 200$, $\alpha=100$, $\beta=5$

**OPTI**n SALT CONStant enhancement factor for $Z_{min}=0$. $Z_{max} = 200$, $\alpha=3$
**COMMAND**  OUTLET

**PURPOSE**  To specify an outflow boundary for the domain of computation. This command is effective only for the ANSWER™ Software Tool.

**MODE 1:**  Outflow at an External Boundary or Boundary Next to an Obstacle

**SYNTAX**  OUTL  [(subrgn), [dir]] [FREE] [FLUX | AREA | MASS | Qf] [DIAG]

**subrgn**  The subregion to be identified as an outlet. The subregion, together with any orientation specified with the dir modifier, must point to a surface or boundary of a region. See Section 3.5 for further details.

For unstructured grids, a subregion defined as a surface (such as with a LOCATE PAIR command) must be specified. For structured grids the subregion may consist of a surface or a volume (such as with a LOCATE COORDinate or LOCATE LIST command). Volume type of subregions specified with a LOCATE command with FIELD, STATion or CORrelation modifiers cannot be used with this command. For structured grids, if no subregion is specified, then entire computational domain is selected.

**dir**  This input is only relevant for structured grids. It specifies the orientation index for the outlet boundary if the subregion specified is not a surface but is of the volume type as described above.

**FREE**  By default it is assumed that at an OUTLET boundary, no inflow can occur in any part of the boundary. If inflow is detected then it is set to zero. If this modifier is present, then parts of the outlet boundary that have inflow are left uncorrected and the outflow correction is applied only to that part of the boundary that has outflow.

**FLUX**  For steady state or incompressible flow, the flow rate at each outlet port is adjusted so that the total outflow equals the total inflow to the computational domain (See Comments below). If this modifier is present, then the outflow is distributed in proportion to the computed outflow flux rate. This is the default option. The default practice is equivalent to treating all the outlets as a single outlet. The outflow through the mth port, \( Q_m \) is computed from:

\[
Q_m = Q_{\text{out}} \frac{\sum_{n=1}^{N} \sum_{i=1}^{3} (\rho u_i A_i)_m}{\sum_{m=1}^{M} \sum_{n=1}^{N} \sum_{i=1}^{3} (\rho u_i A_i)_m}
\]

Here subscript \( i \) denotes the \( i \)th coordinate direction, \( n \) the element number, \( N \) is the total number of elements in the \( m \)th outflow port with a total of \( M \) outflow ports. The velocity and area vectors, \( u \) and \( A \), and the density, \( \rho \), are taken at the element outlet boundary of the element which is defined by the dir modifier.

**AREA**  The outflow rate at each port is distributed in proportion to the ratio of its area to the total outflow area. This modifier is effective only if multiple OUTLET commands are specified. The outflow through the \( m \)th port, \( Q_m \) is computed from:

\[
Q_m = Q_{\text{out}} \frac{\sum_{n=1}^{N} A_{n,m}}{\sum_{m=1}^{M} \sum_{n=1}^{N} A_{n,m}}
\]

Where \( A_{n,m} \) is the area of the \( n \)th element of the \( m \)th port.

**MASS**  The total mass flow rate at the outlet boundary for the \( m \)th port is set equal to the specified \( Q_f \); that is: \( Q_m = Q_f \).

**Qf**  If the MASS modifier is specified, then this input is treated as mass flow rate at the outlet port. In the absence of the MASS modifier, this is the flow fraction that exits through the \( m \)th port as a fraction of the total outflow through all outlet ports. The outflow rate through the port is computed as:
\[ Q_m = Q_{out} \frac{Q_f}{\sum_{m=1}^{N} Q_f} \]

**DIAG**  
By default only summary of total boundary area, average density and velocity, and flow rate are printed to the standard output device. If this modifier is present then a complete detail of area, velocity, density and flow rate for each boundary segment is printed.

**COMMENTS**
An outlet boundary, by definition, is assumed to be a boundary where the normal gradients of all dependent variables are zero. This command provides a compact way to specify the zero normal gradient boundary conditions for all variables at a given boundary.

For incompressible flow, the only other action that is specific to the outflow boundary is the correction of outflow so that the total outflow from all ports equals the total inflow to the computational domain. Some further details of the correction procedure are given in Section 3.14.2 checkup.

Though it is possible to specify, a mix of these options, it is recommended that a consistent practice be followed for specification of outflow if more than one outflow port is specified.

**EXAMPLES**

- OUTLet at X+ boundary at right (maximum x)
- OUTLet at Y+ boundary for most recently SELECTed subregion
- OUTLet port at Y+ for SELECTed subregion; outflow fraction = 0.5
- OUTLet port at Y+ for SELECTed subregion; outflow fraction in proportion to AREA
- OUTLet at X-: FIXED pressure boundary for subregion ID = OUTFlow
- OUTLet at X-: MASS flow = 0.1 at ID = OUTFlow
MODE 2: Outflow at an External Boundary or Boundary Next to an Obstacle to Match Inflow at Another Boundary

SYNTAX

OUTL {[subrgn],[dir]} {[subrgn_in],[dir_in]} [DIAG]

subrgn See Mode 1 of the command.
dir See Mode 1 of the command.

subrgn_in The subregion at which the mass inflow will be computed to set the mass flow at the specified outlet boundary. The subregion, together with any orientation specified with the dir modifier, must point to a surface or boundary of a region. See Section 3.5 for further details.
dir_in This input is only relevant for structured grids. It specifies the orientation index for the outlet boundary if the subregion specified is not a surface but is of the volume type.

DIAG See Mode 1 of the command.

EXAMPLES

OUTL et at X+ boundary of ID=DOMAIN equal to X- boundary of ID=DOMAIN
OUTL et flow at X+ boundary of ID=OUTLET to be equal to X- boundary of ID=INLET
OUTL et flow ID=OUTLET_SURFACE = ID=INLET_SURFACE !Both sub regions defined as surfaces
**MODE 3:** Outflow from an Internal Element

**SYNTAX**

```
OUTL {SOUR} {subrgn} [dir] [FLUX|AREA|VOLU]
```

**SOUR**
The outflow occurs from one or more elements in the interior of the domain. Internally the outflow is treated as a (negative) source.

**subrgn**
The subregion to be identified as an outlet. The subregion may represent either a volume subregion or a surface. The latter is necessary if a flux or AREA modified is specified. See Mode 1 command.

**dir**
This input is only relevant for structured grids. It specifies the orientation index for the outlet boundary if the subregion specified is not a surface but is of the volume type as described above. There is no default value; a value must be specified.

**FLUX**
The outgoing flow is divided according to the relation:

\[
Q_m = Q_{out} \frac{\sum_{n=1}^{N} \sum_{i=1}^{3} (\rho u_i A_i)_m}{\sum_{m=1}^{M} \sum_{n=1}^{N} \sum_{i=1}^{3} (\rho u_i A_i)_m}
\]

Here subscript \(i\) denotes the \(i^{th}\) coordinate direction, \(n\) the element number, \(N\) is the total number of elements in the \(m^{th}\) outflow port with a total of \(M\) outflow ports. The velocity and density, \(u\) and \(\rho\), are taken at the element node location and the area vector, \(A\), is taken at the outlet boundary of the element defined by the dir modifier which must be specified for this option. This is the default option.

**AREA**
The outgoing flux, \(q_m\), removed from the \(m^{th}\) element is computed according to the relation:

\[
Q_m = Q_{out} \frac{\sum_{n=1}^{N} A_{n,m}}{\sum_{m=1}^{M} \sum_{n=1}^{N} A_{n,m}}
\]

Where \(A_{n,m}\) is the area of the \(n^{th}\) element of the \(m^{th}\) port taken at the element boundary defined by the dir modifier which must be specified for this option.

**VOLU**
The outgoing flow is divided according to the relation:

\[
Q_m = Q_{out} \frac{\sum_{n=1}^{N} V_{n,m}}{\sum_{m=1}^{M} \sum_{n=1}^{N} V_{n,m}}
\]

Where \(V_{n,m}\) is the volume of the \(n^{th}\) element of the \(m^{th}\) port. The dir modifier must not be specified for this option.

**COMMENTS**

This command is useful for if outflow is to be extracted from interior of the domain so that the total outflow matches the inflow into the computational domain. The outflow specified by Mode and 2 of the command require that the outlet boundary be an exterior boundary or a boundary of an obstacle. This command can be used anywhere in the interior of the computational domain.

**EXAMPLES**

```
OUTL set SOURCE type at ID=OUTLET divide by VOLUME
OUTL set SOURCE type at X+ of ID=OUTLET divide by FLUX
OUTL set SOURCE type at ID=OUTLET_SURFACE divide by AREA
```
MODE 4: Turn Off a Previously Specified Outflow Port

SYNTAX OUTL {[subrgn], [dir]} [OFF]

subrgn See Mode 1 of the command.
dir See Mode 1 of the command.
OFF Previously specified outlet boundary for the identified sub region is deactivated. A new specification for this sub region may follow.

EXAMPLES

OUTL et OFF at X- boundary for subregion ID = OUTFlow
**Keyword Commands**

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>OUTPUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To select the field arrays to be written to the standard output device and to specify the extent, manner and frequency of output.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>Output of Phase Space Variables</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>OUTP [Φ] [plane] TABL [ADD] [STAN] [fname] [subrgn] [STAT] [NOST] [NOTA] [NARR] [WIDE] [TIME] [Vr] [IMME] [NOW] [ONLY] [OFF]</td>
</tr>
</tbody>
</table>

**Φ**

One or more of the symbols that represent the variables for which output is desired. The valid symbols are listed in Table 2.8.1-3. The output for listed variables is produced in the order of specification. If no symbols are specified, and the **ADD** modifier is not present, then a suitable default set is automatically selected after the 1st **SOLVE** command is encountered. The default set includes the variables for which equations are solved, and some important supporting variables based on the nature of the problem.

**plane**

One of the character strings: XY, XZ, YZ, XY, ZX, ZY, RX, RY, RZ and RZ. The strings XY, YX, XR and RX all denote the xy plane, YZ, ZY, and ZR denote the yz plane and, XZ and ZX denote the xz plane. By default, for structured grids, the output is generated for xy planes.

For structured grids the output is presented in a two-dimensional planar tabular form. For 2D geometry only one plane (xy) is possible; hence this modifier is redundant. For 3D geometry, the output can be presented plane-by-plane ordered as xy, yz or xz planes.

**TABL**

The output is generated in a linear columnar table of values ordered by element numbers, the default mode for unstructured grids.

**ADD**

One **OUTPUT** command is activated by default. If the **ADD** modifier is present, then the specified command is added to the list of active **OUTPUT** commands. On the other hand, if the **ADD** modifier is not specified, then the default command is modified or replaced by user specified command.

**STAN**

The output is directed to the Standard Output Unit. This is the default option. The default name for this file is the name of the Input Command file but with the extension changed to “OUT”. For example if the input command file name is “MYCASE.INP” or “MYCASE.DAT”, then the default output file name will be “MYCASE.OUT”.

**fname**

The name of the file to which the output is directed. If a file name is specified on an **OUTPUT** command with an **ADD** modifier, then this file name is uniquely attached to a unit for output from that command and any subsequent **OUTPUT** command that specifies the **fname**. The file name specification is case sensitive and the case must be consistent, otherwise some operating systems may report an error. See Section 3.3 for additional information.

Output from all **OUTPUT** command without an **ADD** modifier is directed to a single common file (by default, the Standard Output Unit). If any such command specifies a file name, then that file becomes the common output file for all commands without the **ADD** modifier. If a new file name or the **STANDARD** modifier is subsequently specified, then the previous file is closed and all subsequent output from all **OUTPUT** commands without an **ADD** modifier is directed to the new file or the Standard Output Unit.

**subrgn**

The subregion for which the output is required. For the **plane** type of output, the specified subregion must be in the mode of a grid index window (Mode 1 of LOCATE command). If any other type of subregion is specified, then the **TABLE** mode (MODE 2) of the command is automatically invoked. For **TABLE** type of output, any type of subregion can be specified. If no subregion is specified, the entire computational domain is selected. See Section 3.4.

**STAT**

Statistics of the selected variables are computed and printed at the end of the tabular outputs. The output includes minimum, maximum and mean values, standard deviation, mass weighted averages and other relevant information.

**NOST**

Output of statistics of the selected variables is suppressed. This is the default option.

**NOTA**

If this modifier exists together with the **STAT** modifier, then only the statistics for the variables are printed out; the tabular output is suppressed.

**NARR**

The output tables are produced in an 80-column (narrow) format.
The output tables are produced in a 132-column (wide) format. This is the default mode.

**TIME**

By default, \( V_{\text{req}} \) is the frequency of output in terms of number of steps. If this modifier is present, then \( V_{\text{req}} \) is interpreted to be time interval between successive outputs.

**\( V_{\text{req}} \)**

The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. The specified value is ignored if it is zero or negative. The default value is set so that output is obtained only at the end of simulations.

**IMME**

The output is produced immediately. This modifier is necessary only before the 1st **SOLVE** command is given. It then enables the output of the current value of specified variable(s) immediately. After the 1st **SOLVE** command, the output is always produced as soon as the command is encountered and this modifier is redundant. The symbol(s) for the output variable(s) must be specified with this modifier since the default output symbols are not available till after the 1st **SOLVE** command.

**NOW**

If this modifier is specified before the 1st **SOLVE** command, then the output is produced just before the 1st step of the solution but after all the initial and boundary conditions have been processed. Thus, this modifier provides the output of the initial conditions for the variable(s) at the start of the solution process. After the 1st **SOLVE** command, the output is always produced as soon as the command is encountered; this modifier is redundant.

**ONCE**

If this modifier is specified then the output is produced only once in response to a **NOW** or **IMMEDIATE** modifier or at the frequency determined by \( V_{\text{req}} \).

**OFF**

Output for any previous command(s) for the same subrgn and type (plane or **TABLE**) is subsequently suppressed.

**COMMENTS**

If no **OUTPUT** command is specified then a command is automatically invoked to produce output for active variables at the end of simulations. The active variables consist of all variables for which the equations are solved plus other variables that are of interest to the problem being solved. Successive commands may be used to accommodate changing output requirements.

**EXAMPLES**

```plaintext
OUTPut: U, V, W in NARRow tabular format
OUTPut: IMMEdiately the current values of U and V
OUTPut: T, V, U and P in WIDE tabular format NOW with variable STATistics
OUTPut: U, V, for subregion ID=OUTDomain in WIDE tabular format NOW with STATistics
OUTPut: U, V, T, P, K by XZ planes in WIDE format NOW for SELEcted subregion
OUTPut: OFF for all variables
OUTPut: NOW for subregion specified by the most recent LOCAte command
OUTPut: ONLY at step number 50
OUTPut: U, V, W as an element-by-element **TABLE**
OUTPut: **TABLE** of values for U, V and W NOW with STATistics
OUTPut: T, V, U and P in WIDE tabular format NOW as **TABLE**
OUTPut: **TABLE** for U and V for the SELECTed active subregion
OUTPut **TABLE**s for V, W, P and K and L by YZ planes every 15 steps
OUTPut **TABLE** OFF for all variables
```
MODE 2: Output of Properties and Coefficients for the Differential Equations

SYNTAX

```
OUTP {Φ} {{COND|DIFF|STOR|SOUR|MATR|RESI}} [plane|TABL] [ADD] [STAN |fname] [subrgn] [STAT|NOST|NOTA] [NARR|WIDE] [TIME] [Vfrq] [IMME|NOW|ONLY|OFF]
```

Φ One, and only one, of the symbols that denotes the dependent variable for which a differential equation is solved. The valid symbols are listed in Table 2.7.1. There is no default value; a valid symbol must be specified.

COND The conduction or diffusion coefficient for the variable is printed to the output file. If the conduction or diffusion coefficient is a tensor, then the output is produced for each component of the tensor.

DIFF Same as COND.

STOR The storage coefficient for the variable is printed to the output file.

SOUR The net source (algebraic sum of source and sink) for the variable is printed to the output file.

MATR The matrix coefficients for the variable are printed to the output file. The coefficients are printed in the order of the forcing function (rhs of the matrix), the diagonal coefficient and the influence coefficients for each of the neighboring elements.

RESI The residue of the matrix equation or the governing differential equation is printed to the output device. If the output is requested at an intermediate stage of computation, then the matrix residue \((B_j - A_{ij} X_i)\) is printed. If the output is requested at the final stage of computations, then the residue of the governing differential equation is printed.

plane See Mode 1 specification.

TABL See Mode 1 specification.

ADD This modifier is assumed by default. Each command in this mode, unless an OFF modifier is present, is treated as an additional command that adds to the active commands.

STAN See Mode 1 specification.

fname The name of the file to which the output is directed. See Section 3.3 for additional information. Since the ADD modifier is assumed by default, the filename, if specified, is considered unique for the command and any subsequent OUTPUT command that specifies the same file name.

plane See Mode 1 specification.

subrgn See Mode 1 specification.

STAT See Mode 1 specification.

NOST See Mode 1 specification.

NOTA See Mode 1 specification.

NARR See Mode 1 specification.

WIDE See Mode 1 specification.

TIME See Mode 1 specification.

Vfrq The frequency (step or time interval) at which the output is written to the output device. In this mode of the command, there is no default value. A value must be specified or the modifiers NOW or IMMEDIATE must be present for an output to be obtained. See COMMENTS below.

IMME The output is produced at the start of computations. In this mode of input, this modifier is equivalent to the NOW modifier because the coefficients and components of the transport equation are not available till the first SOLVE command is given and the computation process has started.

NOW See Mode 1 specification.

ONLY See Mode 1 specification.

OFF Output for any previous command(s) for the same subrgn, same type (plane or TABLE) and
same combination of COND, DIFF, STOR, SOUR, MATR, and RESI modifiers is subsequently suppressed.

**COMMENTS**

This mode of the OUTPUT command provides the ability to monitor the coefficients and contribution of the various components of the transport equation. Any combination of the modifiers COND, DIFF, STOR, SOUR, MATR, and RESI may be specified. At least one of these must be specified to trigger this mode of the command.

This command mode triggers output for quantities which are computed (and needed) only during the solution of the equations. Most of these quantities are not allocated permanent storage but are computed on as needed basis. Therefore this output is possible only during the solution of the equation for the corresponding variable. This command must therefore be given before the last SOLVE command. Also a frequency (Vfreq with or without the ONLY modifier) or NOW modifier must be specified for the output to be

Multiple commands may be used to obtain output for different variables. Output is generated after all the coefficients for the solution matrix have been computed. These commands essentially form a queue and are executed for each variable in order as the solution for that variable at the specified step is initiated.

This mode of the OUTPUT command may be combined with Mode 3 of the command. That is, the modifiers of Mode 2 may be simultaneously specified with those of Mode 3 on the same command.

**EXAMPLES**

\[\text{OUTPut: for U and P of DIFFusion coefficients at the final stage}\]
\[\text{OUTPut: for T DIFFusion, coefficients NOW and the end to file = ‘DIFFUSION.T’}\]
\[\text{OUTPut: for T STORage and MATRix coefficients NOW (at the next step)}\]
\[\text{OUTPut: for T CONDuction, STORage, SOURce, MATRIx and RESIDUe at step number 52 ONLY}\]
\[\text{OUTPut: for C: SOURce at step number every 52 steps}\]
\[\text{OUTPut: in TABLE format of MA TRIX for T and P at frequency of 75 steps}\]
\[\text{OUTPut: of RESIdue for T at the end}\]
**Keyword Commands**

**MODE 3:** Output of Convective, Diffusive and Total Flux for each Element

**SYNTAX**

```
OUTP {Φ} {FLUX} [CONV] [DIFF] [TOTA] [AREA] [plane] [TABL] [ADD] [STAN] [fname] [subrgn] [STAT] [NOST] [NOTA] [NARR] [WIDE] [TIME] [Vfrq] [IMME] [NOW] [ONLY] [OFF]
```

**Φ**

One, and only one, of the symbols that denotes the dependent variable for which a differential equation is solved. The valid symbols are listed in Table 2.7.1. There is no default value; a valid symbol must be specified.

**FLUX**

The total flux for each face of the elements of the computational domain is printed. The total flux is the sum of the convective and diffusive components.

**CONV**

The convective flux for each face of the elements of the computational domain is printed.

**DIFF**

The diffusive flux for each face of the elements of the computational domain is printed.

**TOTA**

The sum total of the convective and diffusive fluxes for each face of the elements of the computational domain is printed. This modifier is assumed by default if the CONV or DIFF modifiers are not present.

**AREA**

The computed flux is divided by the projected area of the face for output.

**plane**

See Mode 1 specification.

**TABL**

See Mode 1 specification.

**ADD**

This modifier is assumed by default. Each command in this mode, unless an OFF modifier is present, is treated as an additional command that adds to the active commands.

**STAN**

See Mode 1 specification.

**fname**

See Mode 2 specification.

**plane**

See Mode 1 specification.

**subrgn**

See Mode 1 specification.

**STAT**

See Mode 1 specification.

**NOST**

See Mode 1 specification.

**NOTA**

See Mode 1 specification.

**NARR**

See Mode 1 specification.

**WIDE**

See Mode 1 specification.

**TIME**

See Mode 1 specification.

**Vfrq**

The frequency (step or time interval) at which the output is written to the output device. In this mode of the command, there is no default value. A value must be specified or the modifiers NOW or IMMEDIATE must be present for an output to be obtained. See COMMENTS below.

**IMME**

The output is produced at the start of computations. In this mode of input, this modifier is equivalent to the NOW modifier because the coefficients and components of the transport equation are not available till the 1st SOLVE command is given and the computation process has started.

**NOW**

See Mode 1 specification.

**ONLY**

See Mode 1 specification.

**OFF**

Output for any previous command(s) for the same subrgn, same type (plane or TABL) and same combination of FLUX, CONV, DIFF and TOTA modifiers is subsequently suppressed.
COMMENTS

This mode of the OUTPUT command provides the output of the convective, diffusive and total fluxes at the faces of the elements. Any combination of the choice of fluxes may be specified. At least one of these must be specified to trigger this mode of the command.

This command mode triggers output for quantities which are computed (and needed) only during the solution of the equations. These quantities are not allocated permanent storage but are computed on as needed basis. Therefore this output is possible only during the solution of the equation for the corresponding variable. This command must therefore be given before the last SOLVE command. Also a frequency ($V_{frq}$ with or without the ONLY modifier) or NOW modifier must be specified for the output to be generated.

Multiple commands may be used to obtain output for different variables. Output is generated after all the fluxes required for solution of the transport equation have been computed. These commands essentially form a queue and are executed for each variable in order as the solution for that variable at the specified step is initiated.

This mode of the OUTPUT command may be combined with Mode 2 of the command. That is, the modifiers of Mode 2 may be simultaneously specified with those of Mode 3 on the same command.

Also, if the output of both the diffusion coefficients and the diffusive fluxes is desired through such a single command, then the modifier DIFF must be specified twice or both the COND and DIFF modifiers must appear simultaneously on such a command.

EXAMPLES

OUTPut: FLUX for T for each element at the final stage
OUTPut: CONVective FLUX for T NOW (at the next step) to file ‘CFLUX.TMP’
OUTPut: CONVective and DIFFusive FLUX for T at step number 50 ONLY
OUTPut: CONVective, DIFFusive and TOTAL FLUX divided by AREA for T every 50 steps
OUTPut: FLUX divided by AREA for T at step# 52 ONLY in NARROW mode for ID=SUBREGION
OUTPut: in TABLE mode FLUX for T in NARROW mode for ID=SUBREGION at end of simulations
Keyword Commands

**MODE 4:** Output of Special Derived Flow Based Variables

**SYNTAX**

```
OUTP \{ [GRAD] [VORT] [STRUCTURE] [STRAIN] [STRESS] [LIGHTHILL] \} \{plane\} \{TABL\} \{ADD\} \{STAN\} \{fname\} \{subrgn\} \{STAT\} \{NOST\} \{NOTA\} \{NARR\} \{WIDE\} \{TIME\} \{V_{frq}\} \{IMME\} \{NOW\} \{ONLY\} \{OFF\}
```

**GRAD**

The tensor components of the gradients of velocity, $\varphi_{ij}$ are output, where:

$$\varphi_{ij} = \frac{\partial u_i}{\partial x_j}$$

Here $u_i$ is the $i^{th}$ component of velocity and $x_j$ is the $j^{th}$ coordinate. The gradient consists of 4 components for 2D and 9 for 3D.

**VORT**

Output of the components of vorticity vector, $\omega$, is obtained, where:

$$\omega_1 = \frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_3}; \quad \omega_2 = \frac{\partial u_1}{\partial x_3} - \frac{\partial u_3}{\partial x_1}; \quad \omega_3 = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}$$

There are 3 components of vorticity for 3D flow but only one for 2D flow.

**STRUCTURE**

Output of a “vorticity” structure variable, $\Omega$, is obtained. It is defined as:

$$\Omega = -\frac{\partial u_1}{\partial x_2} \frac{\partial u_2}{\partial x_1}$$

for 2D

$$\Omega = \frac{\partial u_1}{\partial x_2} \frac{\partial u_2}{\partial x_1} - \frac{\partial u_2}{\partial x_2} \frac{\partial u_3}{\partial x_1} - \frac{\partial u_3}{\partial x_2} \frac{\partial u_1}{\partial x_3}$$

for 3D

**STRAIN**

Output of the components of strain tensor, $S_{ij}$, is obtained, where:

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

There are 3 components for 2D and 6 for 3D flow.

**STRESS**

Output of the components of stress tensor, $\tau_{ij}$, is obtained, where:

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \sum_k \frac{\partial u_k}{\partial x_k} \right) - \delta_{ij} \rho$$

Here $\mu$ is viscosity and $\rho$ is the pressure. There are 3 components for 2D and 6 for 3D flow.

**LIGHTHILL**

Output of the components of “lighthill” stress tensor, $L_{ij}$, is obtained, where:

$$L_{ij} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \sum_k \frac{\partial u_k}{\partial x_k} \right) + \rho u_i u_j$$

Here $\mu$ is the viscosity and $\rho$ is the density. There are 3 components for 2D and 6 for 3D flow.

**Additional Notes**

- **ADD** This modifier is assumed by default. Each command in this mode, unless an **OFF** modifier is present, is treated as an additional command that adds to the active commands.
- **plane** See Mode 1 specification.
- **TABL** See Mode 1 specification.
- **STAN** See Mode 1 specification.
- **fname** See Mode 2 specification.
- **subrgn** See Mode 1 specification.
- **STAT** See Mode 1 specification.
- **NOST** See Mode 1 specification.
- **NOTA** See Mode 1 specification.

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NARR See Mode 1 specification.
WIDE See Mode 1 specification.
TIME See Mode 1 specification.
V_{frq} See Mode 1 specification.
IMME See Mode 1 specification.
NOW See Mode 1 specification.
ONLY See Mode 1 specification.
OFF Output for any previous command(s) for the same subrgn, same type (plane or TABLE) and same combination of GRAD, VORT, STRUCTURE, STRAIN, STRESS and LIGHTHILL modifiers is subsequently suppressed.

EXAMPLES

Output: VORTICITY and GRADients of velocity at the final stage to file ‘VORTGRAD.FIL’
Output: VORTICITY STRUCTure, STRESS and LIGHTHILL stress at frequency of 100 steps
Output: in TABLE mode VORTICITY STRUCTure, STRESS and LIGHTHILL every 100 steps
MODE 5: Output of Partitioning for Species Variables

SYNTAX

```
OUTP {SECO} {PHAS} {Φ} {plane [TABL]} [ADD] [STAT | name] [subrgn] [STAT | NOST | NOTA] [NARR | WIDE] [TIME] [Vfrq] [IMME | NOW] [ONLY] [OFF]
```

SECO

The output for the inventory (amount in storage at a element) of a species in phases other than the primary phase is generated. The output is computed as:

\[
Q_{φs} = Q_{φ} - Q_{f} \Phi
\]

Here \(Q_{φs}\) is the inventory of property in an element in phases other than the primary phase, \(Q_{φ}\) is the total inventory and \(Φ\) is the species concentration in the primary phase for the element.

PHAS

A companion modifier that must be present to invoke this mode of the command.

\(Φ\)

One or more of the symbols that represent the variables for which output is desired. The valid symbols are the species symbols listed in Table 2.7.1. This output can only be obtained for species variables for which a transport equation is solved. There is no default value; a valid symbol must be specified.

plane
See Mode 1 specification.

TABL
See Mode 1 specification.

ADD
This modifier is assumed by default. Each command in this mode, unless an OFF modifier is present, is treated as an additional command that adds to the active commands.

STAN
See Mode 1 specification.

fname
See Mode 2 specification.

plane
See Mode 1 specification.

subrgn
See Mode 1 specification.

STAT
See Mode 1 specification.

NOST
See Mode 1 specification.

NOTA
See Mode 1 specification.

NARR
See Mode 1 specification.

WIDE
See Mode 1 specification.

TIME
See Mode 1 specification.

Vfrq
See Mode 1 specification.

IMME
See Mode 1 specification.

NOW
See Mode 1 specification.

ONLY
See Mode 1 specification.

OFF
Output for any previous command(s) for the same subrgn, same type (plane or TABL) and same combination variable is subsequently suppressed.

COMMENTS

This mode of the command is active only for the PORFLOW™ Software Tool where some of the property may be present in secondary phases (solid and gas components of the porous matrix). The partitioning between different phases is specified by the TRANSPORT, DISTRIBUTION or RETARDATION commands.

The output from this mode of the command can be generated only after the start of the solution process. At the initial stage, before the solution process starts, the meaningful values of the inventory of variables may not be available. This mode of the command operates independently of any other modes of the command and essentially adds to any other commands that are specified.

EXAMPLES

```
OUTPut: SECOndary PHASe partitioning for variables C and C2.to file ‘SOLIDC.FIL’
OUTPut: SECO PHAS for C and C2.to file ‘SOLIDC.FIL’ every 100 steps
```
COMMAND  OXIDIZER

PURPOSE  To specify the proportion of inert substance to active substance in the oxidizer for reactive flows. This command is effective only for the ANSWER™ Software Tool.

SYNTAX   OXID {N1}

N1      The molar ratio of inert to active substance in the oxidizer. The default value is 3.76.

COMMENTS

The default oxidizer is "air" which consists of oxygen and nitrogen in a molar ratio of 3.76 moles of N₂ per mole of O₂. Any other proportion of diluent nitrogen, including zero, may be set by this command.

EXAMPLES

OXIDizer is pure oxygen
OXIDizer with N₂:O₂ = 2.5 by molar ratio
COMMAND  PAUSE

PURPOSE  To cause a temporary halt in the calculations.

SYNTAX  PAUS

COMMENTS

Operator intervention is required to restart the calculation process. This command allows for operator action during interactive execution.

EXAMPLES

PAUSe and await operator action
**COMMAND** PERIODIC

**PURPOSE** To select the periodic boundary option for boundary conditions of the domain.

**MODE 1:** Periodic Boundary Without Velocity Transformation

**SYNTAX** PERI {X|Y|Z|fname} [option]

**X|Y|Z** The boundary conditions for the corresponding x, y or z direction boundaries are determined automatically from the requirement of periodicity. A BOUNDARY command with a corresponding boundary index (X-, X+, Y-, Y+, or Z-, Z+) must not be specified if this option is selected.

**fname** The name of the file which contains the information about the periodic boundary locations. This file must contain a list with one record for each pair of matching periodic surfaces (called “lower” and “upper”). Each record must consist of only 4 integers in the order:

1. Element number for the periodic surface at “lower” periodic boundary.
2. Surface number for the periodic surface (or face) of the element above.
3. Element number containing the periodic surface at “upper” periodic boundary.
4. Surface number for the periodic surface (or face) of the element above.

The definition of the “lower” or “upper” boundary is arbitrary. The element numbers that appear in the periodic list must consist only of the internal field elements. Boundary node numbers must not appear in this list. The surfaces are numbered from 1 to 4 for Quad and from 1 to 6 for Hex elements. For hybrid unstructured grids, the number of faces depends on the type of element. See LOCATE command with PAIR modifier and Section 3.4 for further details of the manner in which these surface numbers are assigned.

**option** Options selected for implementation of the PERIODIC command.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>LINE</td>
<td>For a structured grid, by default, an ADI cyclic solver is used in the periodic direction. If this modifier is present, then a linear form of the ADI solver is used. This modifier has no effect if the solver used does not have a cyclic option. Of the default solvers only the ADI has the cyclic option. Please check with ACRi for other solvers.</td>
</tr>
<tr>
<td>CYCL</td>
<td>For an unstructured grid, by default, a linear solver is used in the periodic direction. The periodicity is imposed explicitly by forcing the boundary values to be periodic. If this modifier is present, then the cyclic solver is used. The user must ensure that the unstructured grid is setup in a manner that the ADI “lines” in the periodic direction run unbroken from one boundary to the other. Otherwise the solution may be corrupted with unforeseen consequences.</td>
</tr>
<tr>
<td>Φ</td>
<td>One or more (≤ 54) symbols that denote the variables, which are periodic (or not periodic if OFF modifier is specified) at the θ₁ and θ₂ boundaries. By default all variables are assumed to be periodic.</td>
</tr>
<tr>
<td>OFF</td>
<td>The periodic boundary conditions are not applied to the variables specified by the Φ modifier. All variable not so identified are assumed to be periodic.</td>
</tr>
<tr>
<td>PRES</td>
<td>By default it is assumed that the pressure at a periodic surface is also cyclic; that is there is no net pressure loss in the direction of periodicity. If this modifier is present, then any initial pressure difference between the matched elements of the periodic surfaces is maintained.</td>
</tr>
</tbody>
</table>
EXAMPLES

PERIodic boundaries in X
PERIodic boundaries in X, Y and Z
PERIodic boundary in X for U, V, W, T, P only
PERIodic boundary at X option OFF for P and FU variable
PERIodic boundary surface data on file: ‘PERIODIC.DAT’
PERIodic boundary in Z direction with LINEar solver
PERIodic boundary unstructured grid but use CYCLic solver; data on file: ‘PERIODIC.DAT’
MODE 2: Periodic Boundary With Radial to Cartesian Velocity Transformation

SYNTAX

PERI {X|Y|Z|fname} {THET} [option] [\(\Psi, N_{VR}, N_{VC}\)]

X|Y|Z
The boundary conditions for the corresponding x, y or z direction boundaries are determined automatically from the requirement of periodicity. A BOUNDARY command with a corresponding boundary index (X-, X+, Y-, Y+, or Z-, Z+) must not be specified if this option is selected.

fname
See Mode 1 specification.

THET
This modifier denotes that the velocity components are Cartesian but the problem is periodic in the circumferential (\(\theta\)) direction of a cylindrical coordinate system. At times a problem which is periodic in cylindrical (x, r, \(\theta\)) coordinates is solved instead in a Cartesian (x, y, z) system. Then, the Cartesian (U, V, W) velocity components at the two periodic boundaries located at \(\theta = \theta_1\) and \(\theta = \theta_2\) obey the transformed periodicity relations:

\[
U_2 = U_1
\]

\[
V_2 = V_1 \cos \Psi - W_1 \sin \Psi
\]

\[
W_2 = W_1 \cos \Psi + V_1 \sin \Psi
\]

where

\[
\Psi = \theta_2 - \theta_1
\]

option
See Mode 1 specification.

\(\Psi\)
The angle of periodicity, \(\Psi\), in degrees. There is no default value, if the modifier THET is present, then a value must be specified.

\(N_{VR}\)
A number \((1 \geq N_{VR} \geq 3)\) that denotes the order of the radially directed component of velocity among the three velocity components (U, V, W). The default value is 2.

\(N_{VC}\)
A number \((1 \geq N_{VC} \geq 3)\) that denotes the order of the circumferentially directed component of velocity among the three velocity components (U, V, W). The default value is 3.

EXAMPLES

PERIodic boundaries in Z with \(THETa = 45\) degrees
PERIodic boundaries in Y with \(THETA = 45\) degrees v = 1, w = 2
PERIodic boundary in Z with \(THETa = 18\) degrees for U, V, W, T, P only
PERIodic boundary in Z with \(THETa = 18\) degrees but option OFF for P and FU variable
PERIodic boundary at \(THETA = 20\) degrees surface data on file: 'PERIODIC.DAT'
MODE 3: Periodic Boundary With General Velocity Transformation

SYNTAX  PERI {X|Y|Z|fname} {TRAN|STAC} [option] [V₁, ..., V₉]

X|Y|Z  The boundary conditions for the corresponding x, y or z direction boundaries are determined automatically from the requirement of periodicity. A BOUNDARY command with a corresponding boundary index (X-, X+, Y-, Y+, Z-, Z+) must not be specified if this option is selected.

fname  See Mode 1 specification.

TRAN  The velocity vector at the identified periodic boundaries is transformed according to:

\[
\begin{bmatrix}
U₂ \\
V₂ \\
W₂
\end{bmatrix} = \begin{bmatrix}
n₁ & n₂ & n₃ \\
n₄ & n₅ & n₆ \\
n₇ & n₈ & n₉
\end{bmatrix} \cdot \begin{bmatrix}
U₁ \\
V₁ \\
W₁
\end{bmatrix}
\]

STAC  The velocity vector at the identified periodic boundaries is transformed according to the transformation specified in the most recent STACK TRANSFORMATION command.

option  See Mode 1 specification.

V₁,..V₉  The transformation matrix to compute the velocity components at the “higher” (say, at Z+) periodic boundary from those at the “lower” (say, at Z-) periodic boundary if the TRAN modifier is present. This information is ignored otherwise. There is no default value, if the modifier TRAN is present, then a set of 9 values must be specified.

EXAMPLES

PERIODIC boundaries in Z Velocity TRANSformed by:
1.0 0.0 0.00.0 0.995004 -0.9983340.0 0.998334
0.995004

PERIODIC boundaries in Z Velocity TRANSformed by:
1.0 0.0 0.00.0 0.995004 -0.09983340.0 0.0998334
0.995004

PERIODIC boundaries in Z Velocity by STACK TRANSformation

PERIODIC boundary in X by STACK TRANSformation for U, V, W, T, P only

PERIODIC boundary TRANSformation as follows with surface data on file: ‘PERIODIC.DAT’
1.0 0.0 0.00.0 0.995004 -0.9983340.0 0.998334
0.995004

PERIODIC boundary by STACK TRANSformation surface data on file: ‘PERIODIC.DAT’
COMMAND  PERMEABILITY

PURPOSE  To specify permeability for a porous medium.

MODE 1:  Constant Permeability

SYNTAX  PERM  {K} [subrgn]

K  The numerical value (>0) for the permeability of the medium. The units are [L²]. The SI units are [m²]. There is no default value; a value must be specified.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

APPLICABILITY

This command is available only for the ANSWER™ and PORFLOW™ Software Tools.

EXAMPLES

PERMEABILITY for the medium is 1.E-6 square meter. For the entire domain
PERMEABILITY for the medium is 1.E-6 square meter for ID=POROUS subdomain.
MODE 2: Permeability as a General Function

SYNTAX

PERM \{func[\xi]\} \{N_1, N_2, \ldots, N_n\} [fname] [subrgn]

func
One of the modifiers listed in Table 4.2.1 that denotes the functional form of the value of the permeability for the porous medium.

\xi
One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N_1,\ldots,N_n
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname
The name of the file containing the numerical values N_2 through N_n. This option is available only for selected functions. See Section 3.3 for additional information.

subrgn
The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

APPLICABILITY

This command is available only for the ANSWER™ and PORFLOW™ Software Tools. For ANSWER™ Software Tool this command automatically triggers the inclusion of Brinkman-Forchheimer terms (BRINK command.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (PERM) must replace the keyword used in these examples.
MODE 3: Permeability from Carman-Kozeny Equation

SYNTAX

PERM \{CARM\} \{d_p\} \{C_{CK}\} \{subrgn\}

CARM

The permeability is computed from the Carman-Kozeny relationship:

\[
K = \frac{d_p^2 \theta^3}{C_{CK} (1 - \theta)^2}
\]

Where

- \(K\): is the permeability of the medium \([L^2]\),
- \(d_p\): is the representative particle diameter \([L]\),
- \(\theta\): is the porosity of medium \([0]\),
- \(C_{CK}\): is an empirical constant \([0]\)

- \(d_p\): The representative particle diameter for the porous medium. Typically it represents the ratio of the volume to the surface area of the particles. There is no default value; a value must be given.

- \(C_{CK}\): The empirical constant for the relationship. The default value is 180.

- \(subrgn\): The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

EXAMPLES

PERMEABILITY from CARMAN relationship diameter = 0.002 meters for the entire domain
PERMEABILITY from CARMAN relationship diameter = 0.002 m for ID=POROUS subdomain.
PERMEABILITY from CARMAN relationship diameter = 0.002 m with Cck=150.
**Keyword Commands**

**COMMAND**  PHASE

**PURPOSE**  To specify phase change option for multi-phase option. This command is effective for the ANSWER™ and PORFLOW™ Software Tools.

**MODE 1:**  Phase change at a Fixed Temperature.

**SYNTAX**  PHAS  (EVAP | FREE) [T_{phase}]

**EVAP**  Evaporation temperature is specified. This is the default mode.

**FREE**  Freezing temperature is specified.

**T_{phase}**  The temperature at which phase change occurs. If FREE modifier is specified; then it is the freezing temperature with a default value of 0 °C otherwise it is the evaporation temperature with a default value of 100 °C.

**EXAMPLES**

PHASE  change at 100 Degrees Celcius
PHASE  change is FREEZING at 0 Degrees Celcius
MODE 1: Phase Change (Evaporation) from Casius-Clapeyron Equation.

SYNTAX  

PHAS \{CLAP\} \[T_0, T_1, P_0, A\]

CLAY Phase change occurs according to Clayperon’s vapor-pressure relation:

$$T_s = T_0 + \frac{T_1}{A \ln(P/P_0)},$$

where, $T_s$ is the saturation temperature at pressure $P$, $T_0$ is a base temperature, $P_0$ is a base pressure and $A$ is an empirical constant. This relation can also be inverted to compute, saturation pressure, $P_s$, at any given temperature, $T$, according to:

$$P_s = P_0 \exp\left(A - \frac{T_1}{T - T_0}\right),$$

$T_0$ The base temperature $T_0$ of the vapor pressure equation above. The default value is 45 K.

$T_1$ The temperature $T_1$ of the vapor pressure equation. The default value is 3841.1954 K.

$P_0$ The pressure $P_0$ of the vapor pressure equation. The default value is 131.57894 pascal.

$A$ The constant $A$ of the vapor pressure equation. The default value is 18.3443.

COMMNETS

This relation is suitable for evaporation of a liquid. The default constants are tuned for water so that the computed vapor pressure is in good agreement with the experimental data in the 0°C to 350°C range as shown in the table below.

### TABLE: VAPOR PRESSURE FOR WATER

<table>
<thead>
<tr>
<th>°C</th>
<th>K</th>
<th>$P_s$ (pascals x 10^5)</th>
<th>Equation</th>
<th>Steam Tables</th>
</tr>
</thead>
<tbody>
<tr>
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</tbody>
</table>

EXAMPLES

PHASE Change according to default CLAPEYRON’s relation

PHASE Change CLAPEYRON’s equation: $T_0=45$, $T_1=3841.1954$, $p_0=131.57894$, $a_1=18.3443$
**COMMAND** POROSITY

**PURPOSE** To define the material porosity of the porous matrix.

**MODE 1:** Constant Porosity

**SYNTAX** PORO {Θ_E} [Θ_T, Θ_D] [ALWA] [sub rgn]

- Θ_E: The effective (or flow) porosity, Θ_E. The default value is 1.
- Θ_T: The total porosity, Θ_T. If no value is specified, total porosity is set equal to the effective porosity.
- Θ_D: The diffusional porosity, Θ_D. If no value is specified, diffusional porosity is set equal to the effective porosity.

**ALWA** By default the PORO command is implemented immediately and only once -- as soon as the command is encountered. If this modifier is present then the command is executed immediately as well as repeatedly at the beginning of each time step (or iterative step in steady state mode) of the solution procedure.

**sub rgn** The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

**APPLICABILITY**

This command is currently available only for the **ANSWER™** and **PORFLOW™** Software Tools.

**COMMENTS**

For **ANSWER™** Software Tool only the effective porosity is relevant and hence the Θ_T and Θ_D, if specified, are ignored. Also for **ANSWER™** this command automatically triggers the inclusion of Brinkman-Forchheimer terms (BRINK command).

**EXAMPLES**

POROSITY for the material is **0.35**

POROSITY porosities: effective = **0.1**, total **0.2**, diffusive **0.15**

POROSITY porosities: **3*0.15**

POROSITY porosities are **0.45, 1.50, 1.25** internal check
MODE 2: Porosity as a General Function

SYNTAX

PORO [ONLY] [EFFE] [TOTA] [DIFF] {func[ξ]} {N_1, N_2, .., N_n} [fname] [ALWA] [subrgn]

ONLY

By default, the effective, total and diffusional porosity are all set to the specified value. If this modifier is present, then only the components specified by one or more of the EFFE, TOTA, or DIFF modifiers are set to the specified value.

EFFE

If ONLY modifier is also present, then the effective porosity is set to the specified value.

TOTA

If ONLY modifier is also present, then the total porosity is set to the specified value.

DIFF

If ONLY modifier is also present, then the diffusional porosity is set to the specified value.

func

One of the modifiers listed in Table 4.2.1 that denotes the functional form of the value of the porosity of the porous medium.

ξ

One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N_1,...,N_n

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname

The name of the file containing the numerical values N_2 through N_n. This option is available only for selected functions. See Section 3.3 for additional information.

ALWA

By default, the PORO command is implemented immediately and only once – as soon as the command is encountered. If this modifier is present then the command is executed immediately as well as repeatedly at the beginning of each time step (or iterative step in steady state mode) of the solution procedure.

subrgn

The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

APPLICABILITY

This command is currently available only for the ANSWER™ and PORFLOW™ Software Tools.

COMMENTS

For ANSWER™ Software Tool only the effective porosity is relevant and hence the mode selecting modifiers are ignored. Also for ANSWER™ this command automatically triggers the inclusion of Brinkman-Forchheimer terms (BRINK command.

More than one mode of porosity may be set by a single command. In the presence of the ONLY modifier, any combination of the modifiers EFFE, TOTA or DIFF may be present on the command. If the specified function is a constant then Mode 1 of the command is activated.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (PORO) must replace the keyword used in these examples.
COMMAND PRANDTL

PURPOSE To specify Prandtl number for the fluid. This command is effective only for the ANSWER™ Software Tool.

SYNTAX PRAN [EFFE] {σ}

EFFE If the modifier EFFECTIVE is present on the command line then the input is assumed to be for the effective Prandtl number, \( σ_e \), otherwise it is assumed to be the molecular Prandtl number, \( σ \), for the fluid.

σ The effective or molecular Prandtl number \( (>0) \) for the fluid. The default value is 0.7.

EXAMPLES

PRANdtl number for fluid = 1.
PRANdtl number EFFEctive value = 0.5
COMMAND  PRECIPITATION

PURPOSE  To specify the precipitation or uptake reactions for dissolved species. This command is effective only for the PORFLOW™ Software Tool.

MODE 1: Precipitation Reaction with Constant or Variable Reaction Rate and Solubility.

SYNTAX  PREC {idreac} {Φ} {Ψ} {ω, ξ} [LIMI, {ζ}] [TOLE, {ε}] [POSI|NEGA] [subrgn]

idreac  A unique identifier for the precipitation (or uptake) reaction rate where the species Φ precipitates to generate species Ψ or the species Ψ is converted to species Φ by uptake. The reaction rate is computed as:

\[ R_Φ = ω (ξ - Φ) \]  \hspace{1cm} (1) 

The computed rate is algebraically added to the equation for Ψ and subtracted from the equation for Φ. The reaction rate units are the units of the species divided by time.

Φ  The symbol for the species that is precipitated or re-adsorbed by the reaction.

Ψ  The symbol for the species that is produced by precipitation or dissolved by uptake.

ω  The constant or the symbol for a variable that specifies the precipitation/uptake reaction time constant (units of frequency). There is no default value; either constant or a symbol must be specified.

ξ  The constant or the symbol that specifies the solubility limit for the species (units of Φ). There is no default value; either constant or a symbol must be specified.

C_S  The solubility limit for the species (units of Φ). There is no default value; a value must be specified.

LIMI  If this modifier is present, then the reaction rate is assumed to be influenced by the presence of a limitor species denoted by the symbol, ζ. If the limitor is present above a certain threshold, the reaction rate is assumed to be zero.

ζ  The symbol for the reaction limitor variable. If no tolerance (see TOLE) is specified then no reaction occurs if the value of the limitor variable exceeds \(10^{-30}\). There is no default value; a symbol must be specified.

TOLE  If this modifier is present, then it must be followed by the threshold value above which no precipitation reaction occurs.

ε  The threshold value of the limitor. There is no default value; a value must be specified.

POSI  The reaction rate is set to zero if Φ > C_S. This limits the reaction only to uptake.

NEGA  The reaction rate is set to zero if C_S > Φ. This limits the reaction only to precipitation.

subrgn  The subregion for which the idreac reaction is computed. If no subregion is specified, the reaction is computed for the entire computational domain. See Section 3.4.

EXAMPLES

PRECipitation reaction R1 from C1 to C2 with frequency = 1000; Solubility = 0.02
PRECipitation reaction R2 from C2 to C3 with time constant = 0.05; Solubility = 0.30
PRECipitation reaction R1 from C1 to C2 with solubility defined by C3 and a frequency = 1000
PRECipitation reaction R2 from C2 to C3 with C4 as solubility and time constant = 0.05
MODE 2: Precipitation Reaction with Variable Solubility

SYNTAX

\[
\text{PREC } \{\text{ELEM}\} \{\text{idreac}\} \{\phi\} \{\psi\} \{\omega\} \{\xi\} \{\text{C}_\text{Sat}\} \{\text{subrgn}\}
\]

ELEM

Element mode of the precipitation reaction is activated. In this mode, the solubility of the isotope is decreased by the presence of other elements according to a modified Raoult’s Law. With \(\text{C}_\text{Sat}\) as the solubility of the pure element, the solubility, \(\text{C}_s\), in the presence of other elements is given by:

\[
\text{C}_s = \text{C}_\text{Sat} \left( \frac{\sum_{j=1}^{n} (M_{\text{liquid}}^j + M_{\text{solid}}^j)}{M_{\text{liquid}}^i + M_{\text{solid}}^i} \right)
\]

where \(M_{\text{liquid}}^j\) and \(M_{\text{solid}}^j\) are, respectively, the molar concentration of elements in the liquid and solid phases.

idreac

A unique identifier for the precipitation (or uptake) reaction rate where the species \(\phi\) precipitates to generate species \(\psi\) or the species \(\psi\) is converted to species \(\phi\) by uptake. The reaction rate is computed as:

\[
\text{Rate} = \omega (\text{C}_s - \phi)
\]

The computed rate is algebraically added to the equation for \(\psi\) and subtracted from the equation for \(\phi\). The reaction rate units are the units of the species divided by time.

\(\phi\)

The symbol for the species that is precipitated or re-adsorbed by the reaction.

\(\psi\)

The symbol for the species that is produced by precipitation or dissolved by uptake.

\(\omega\)

The constant or the symbol for a variable that specifies the precipitation/uptake reaction time constant (units of frequency). There is no default value; either constant or a symbol must be specified.

\(\xi\)

The symbol for the variable that represents the sum of the molar concentrations of all the species that participate in reducing the solubility of the element; the denominator in the above equation for \(\text{C}_s\).

\(\text{C}_\text{Sat}\)

The solubility limit for the species (units of \(\phi\)) in its pure element form. There is no default value; a value must be specified.

subrgn

The subregion for which the idreac reaction is computed. If no subregion is specified, the reaction is computed for the entire computational domain. See Section 3.4.

COMMENTS

For this mode of input, it is preferable that all species concentrations be expressed in terms of moles. In this case the SET SUM command can be used to define the sum of molar concentrations, \(\xi\). If the species concentrations are in terms of mass units, then SET LINEAR command must be used to define \(\xi\) with appropriate coefficients.

EXAMPLES

PRECipitation ELEMENT form: R1 for C1 and C2 with molar variable C3 frequency = 1000, csat=0.05
PRECipitation ELEMENT form: R1 for C1, C2 molar variable C3 omega=1000, csat=0.05 ID=REAC1
PRECipitation ELEMENT form: R1 for C1, C2, sum=C3, omega=1000, csat=0.05 SELECted region
COMMAND       PRINT

PURPOSE        To generate output of details of mass flow rate and statistical measures of flow variables.

MODE 1:        Print Statistics for Flow and Selected Variable

SYNTAX         PRIN  [FLOW] [STAT] [Φ] [GEOM] [subrgn]

FLOW           The mass inflow into and, outflow from, all inlets, outlets, open boundaries and sources are computed and written to the standard output device as soon as the command is encountered.

STAT           The statistics related to the minimum, maximum and average value of specified variable(s) is computed and written to the standard output device as soon as the command is encountered. The variables for which the statistics are computed must be identified by the Φ modifier(s).

Φ              One or more symbols that denote the dependent variables for which the STAT modifier is effective. The valid symbols are listed in Table 2.8.1-3. There is no default value.

GEOM           The face areas and volume of the subregion identified on the command are printed on the output file.

subrgn         The subregion for which the output of face areas and volume is required. If no subregion is specified, the entire computational domain is selected. See Section 3.4.

EXAMPLES

PRINT FLOW immediately
PRINT STATistics for U, V, T now
PRINT FLOW and STATistics for U, V, T now
MODE 2: Integrated Averages for Selected Variables at Uniformly Spaced Locations

SYNTAX  
```
PRIN  {Φ} {AVER|PROF} {N1} {coordinate} [subrgn] [dir] [TOLE=Vtol] [NORM]

{BASE=Φ_base} [MASS|AREA|VOLU] [OUTP|fname] [Vfreq] [TIME]
```

Φ  One or more of the symbols that represent the variables for which output is desired. The valid symbols are listed in Tables 2.8.1-3 and 2.8.4. There is no default value.

AVER  The averages of the specified variable are computed at a number of specified locations.

PROF  Same as AVER modifier.

N1  The number of locations at which the averages are computed. It must be the first numerical value on the command. There is no default value; a numerical value (>0) must be specified.

coordinate  One of: X, Y, Z, R or THETA modifiers. It denotes the coordinate of locations at which the averages are computed. The Z, R or THETA can only be used for three-dimensional geometry. In this case is R = sqrt (y²+ z²) and THETA = arctan (z/y).

subrgn  The subregion for computations. If no subregion is specified, the entire domain is selected.

dir  The orientation index for the boundary of the sub-domain if averages are to be computed only at the boundary. See Section 3.5 for available choices. There is no default value.

TOLE  The coordinate tolerance for inclusion of the elements in averaging at a location. With $S_i$ as the coordinate of the $i^{th}$ location, all elements that satisfy: $S_i - V_{tol} \leq S \leq S_i + V_{tol}$ are included in averaging. By default, the tolerance is set equal to half the interval between successive uniformly spaced coordinates from 0 to 1. For example if N1 = 10, then interval will be 0.1 and $V_{tol}$ will be set of 0.05. However if the modifier TOLE is present, then the tolerance is set to the user specified value $V_{tol}$.

Vtol  The user specified value of tolerance. This input must be specified only if the TOLE modifier is present and then it must immediately follow the modifier.

STAT  By default, if the dir modifier is present, then the computed values are arithmetic, area-weighted and mass-flux-weighted mean values; otherwise the computed values are arithmetic, volume-weighted and mass-weighted mean values. If this modifier is present, then computed values include the arithmetic mean, minimum, maximum and standard deviation of the variable.

NORM  The output for the selected variable is normalized or non-dimensionalized as:

$$\Phi_{output} = \frac{\Phi_{computed}}{\Phi_{norm}}$$

where $\Phi_{base}$ and $\Phi_{norm}$ are normalizing values. By default these are set to the minimum and maximum values for the sub-domain selected by subrgn and dir modifiers. However other options are available as described below.

BASE  This modifier will automatically select the normalized (NORM) form of the output. If this modifier exists, then $\Phi_{base}$ must be specified and, in this case, only one variable (Φ) must be specified on the command.

$\Phi_{base}$  The user specified value for $\Phi_{base}$. This input must be specified only if the BASE modifier is present and then it must immediately follow the modifier.

MASS  This modifier is significant only if the BASE modifier is specified. By default $\Phi_{norm}$ is taken to be arithmetic mean of the values for the sub-domain. If this modifier is present, then $\Phi_{norm}$ is the mass or mass-flux-weighted mean of the variable.

AREA  This modifier is significant only if the BASE modifier is specified. By default $\Phi_{norm}$ is the arithmetic mean of the values for the sub-domain. If this modifier is present, then $\Phi_{norm}$ is the area-weighted mean in the presence of the dir modifier or volume-weighted mean otherwise.

VOLU  Same as the AREA modifier.

OUTP  The output is directed to the standard output file unit.

fname  The file name for output. If a file name is present then the output is directed to the named file, otherwise the output is directed to the standard output device. The total number of open files...
in any simulation cannot exceed 64.

\( V_{frq} \)

The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. If \( V_{frq} \) is specified, it must be the last numerical input on the command. The default value is set so that output is obtained only at the end of simulations.

\( \text{TIME} \)

By default, \( V_{frq} \) is the frequency of output in terms of number of steps. If this modifier is present, then \( V_{frq} \) is interpreted to be time interval between successive outputs.

**COMMENTS**

This command generates a series of profiles of integrated averages for a variable. For example, if the selected coordinate is \( X \), the subrgn denotes a 3D sub-domain and there is no dir modifier, then this command will generate integrated averages across the yz planes of the sub-domain at \( N1 \) uniformly spaced locations in the x-direction. If the subrgn and dir denote a xy plane, and the coordinate selected is \( X \), then it generates integrated averages across the y-direction at \( N1 \) locations along the x-coordinate of the plane.

This command with the BASE modifier can be used to generate the pattern and profile factors, which are commonly used in the aircraft and gas turbine industry to denote the variation of temperature at the outlet plane of the combustor. In this case, the variable \( \Phi \) should be the symbol \( T \) (for Temperature) and the base value, \( \Phi_{base} \), should be specified as the average inlet temperature (commonly called T3). The \( \Phi_{norm} \) is automatically selected to be the computed arithmetic mean (generally called T4). If T4 is to be mass-weighted mean then the modifier MASS must also be present.

**EXAMPLES**

```
PRINT Profile of T at 20 X locations! 20 values versus x for whole of the domain
PRINT PROFILE of U, V, T at 20 X locations! Multiple variables
PRINT AVERAGE of U at 20 X locations for ID=OUTLET in X+ direction! Output for outlet plane.
PRINT PROFILE of STATistics for T at 20 X locations for ID=OUTLET in X+ direction! Min, max & stats
PRINT PROFILE of NORMalized T at 20 X locations for ID=OUTLET in X+ direction
PRINT AVERAGE for T at 20 R for ID=OUTLET. In X+ direction BASE value = 375
PRINT AVERAGE for T at 20 R for ID=SECTION1 BASE value = 375 MASS weighted
PRINT AVERAGE for T at 20 Y locations with TOLERance=0.01 for SELECTed subregion in X+ direction
PRINT AVER for T at 20 Y locs with TOLERance=0.01 and BASE=375 for ID=OUTLET in X+ every 50 steps
PRINT AVER T 20 Y locs TOLERance=0.01, BASE=375, ID=OUTLET X+ at TIME interval of 0.05 units
```
MODE 3: Integrated Averages for Selected Variables at Specified Locations

SYNTAX

PRIN \{Φ\} \{AVER|PROF\} \{N_{Loc}\} \{x_{1},..., x_{n}\} \{coordinate\} \{subrgn\} \{dir\} \{TOLE=V_{tol}\} \{NORM\} \{BASE=Φ_{base}\} \{MASS\} \{AREA\} \{VOLU\} \{OUTP\} \{fname\} \{V_{frq}\} \{TIME\}

Φ
One or more of the symbols that represent the variables for which output is desired. The valid symbols are listed in Tables 2.8.1-3 and 2.8.4. There is no default value.

AVER
The averages of the specified variable are computed at a number of specified locations.

PROF
Same as AVER modifier.

N_{Loc}
The number of locations at which the averages are computed. It must be the first numerical value on the command. There is no default value; a numerical value (>0) must be specified.

x_{1},...,x_{n}
The coordinates of the locations at which averages are computed. There must be a total of N_{Loc} values and these must precede any other numerical input except N_{Loc}. The values must be specified in relative units. The relative units vary from 0 to 1, respectively, from the minimum to the maximum of the coordinate for the subrgn. There is no default value.

coordinate
Same as Mode 2 of the command.

subrgn
Same as Mode 2 of the command.

dir
Same as Mode 2 of the command.

TOLE
The coordinate tolerance, V_{tol}, for inclusion of the elements in averaging at a location. With S_{i} as the coordinate of the i^{th} location, all elements that satisfy: S_{i} – V_{tol} ≤ S < S_{i} + V_{tol} are included in averaging. By default, the tolerance is set equal to 0.01.

V_{tol}
Same as Mode 2 of the command.

STAT
Same as Mode 2 of the command.

NORM
Same as Mode 2 of the command.

BASE
Same as Mode 2 of the command.

Φ_{base}
Same as Mode 2 of the command.

MASS
Same as Mode 2 of the command.

AREA
Same as Mode 2 of the command.

VOLU
Same as the AREA modifier.

fname
Same as Mode 2 of the command.

V_{frq}
Same as Mode 2 of the command.

TIME
Same as Mode 2 of the command.

EXAMPLES

PRINT PROFile of U, V, T at 5 X locations 0.1, 0.3, 0.4, 0.5, 0.9
PRINT PROFile of STATistics for T at 4 Y values 0.1, 0.3, 0.5, 0.8 for ID=OUTLET in Y+ direction
PRINT PROFile of NORMalized T at 4 X stations 0.1, 0.3, 0.5, 0.8 for ID=OUTLET in X+ direction
PRINT AVERage for T at 4 R values 0.1, 0.3, 0.5, 0.8 for ID=OUTLET in X+ direction BASE value = 375
PRINT AVERAGE for T at 4 R values 0.1, 0.3, 0.5, 0.8 ID=SECTION1 BASE value = 375 MASS weighted
PRINT AVERage for T at 3 R values 0.2, 0.4, 0.8 TOLErance=0.01 SELECTed region in X+ direction
PRINT AVER for T at 4 R 0.1, 0.3, 0.5, 0.8 TOLErance=0.01 BASE=375 ID=OUTLET in X+ frq= 50 steps
PRINT AVER T 3 Y 0.2, 0.4, 0.8 TOLErance=0.01, BASE=375, ID=OUTLET X+ at TIME frq 0.05 units
MODE 4: Forges and Moments for a Selected Variable at a Specified Location

SYNTAX

PRIN [Φ] {FORC|MOME} [subrgn] [dir] [X_i] [Φ_0] [Vfreq] [TIME] [NOW] [OFF] [fname]

Φ
The symbol for the variable for which the “force” or “moment” is to be computed. The valid symbols are listed in Tables 2.8.1-3. If no symbol is specified then pressure, P, is selected.

FORC
“Force” and “Moment” of a variable for the surface of a selected subregion are defined as:

\[
F_i = \int (\Phi + \Phi_0) n_i \, dA \\
M_i = F_i \times (X_i - Y_i)
\]

Where

- \(F_i\) is the force vector for the \(\Phi\) variable,
- \(\Phi_0\) is a reference datum for the \(\Phi\) variable,
- \(n_i\) is the normal vector at the surface of the subregion,
- \(A\) is the area of the surface,
- \(M_i\) is the moment vector for the \(\Phi\) variable,
- \(\times\) denotes the cross product of vectors,
- \(X_i\) is the location of the pivot point around which the moment is computed,
- \(Y_i\) is the point of intersection of the vector from \(X_i\) and the force vector such that the vector from \(X_i\) is normal to force vector. This is automatically computed.

MOME
Same as FORC modifier.

subrgn
The subregion for computations. If no subregion is specified, the entire domain is selected.

dir
The orientation index for the boundary of the subregion for which the force is computed. See Section 3.5 for available choices. If no value is specified then the total (closed) boundary of the subregion is selected. In this case the computed force will be the net force on the selected body.

X_i
The coordinates of the pivot point around which the moment of the force is computed. Two values must be specified for 2D and three for 3D geometry. If specified these must be the first set of numerical values on the command. The default value is zero.

Φ_0
Datum for the selected variable \(\Phi\). If specified this must be the 3rd numerical value for 2D and 4th numerical value for 3D geometry. The default value is zero.

Vfreq
The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. If specified this must be the 4th numerical value for 2D and 5th numerical value for 3D geometry. By default the output is obtained only at the end of simulations.

TIME
By default, \(Vfreq\) is interpreted as the frequency of output in terms of number of steps. If this modifier is present, then it is interpreted as the time interval between successive outputs.

NOW
The force and moment are computed at the first step after the command.

OFF
Any previously specified command for the specified \(\Phi\) and subrgn is deactivated.

fname
The file name for output. A different output file may be specified for each command. If no file name is specified then the output is directed to the most recent previously specified file. If no previous file was specified, then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by “_FORCE.TMP”. For example, if the Standard Output file is “PROBLEM.OUT”, then the file is named “PROBLEM_FORCE.TMP”. A summary of output is also printed to the standard output device at the end of simulations.
EXAMPLES

PRINT FORCE for ID=BODY
PRINT FORCE of P for ID=BODY in X+ direction with moments around point (0., 2.354, 5.75)
PRINT FORCE of T for ID=BODY in X+ dir; around (0., 2.35, 5.7); add Pref = 1.E5 file="FORCE_FIL"
PRINT FORCE of U ID=BODY in Y+ dir with moments (0., 0.); add Pref = 1.E5 every 20 steps! 2D case
PRINT FORCE ID=BODY in Z+ dir; pivot (0., 2.35, 5.7); Pref = 1.E5, every 20 steps
PRINT FORCE Z+ of ID=BODY; pivot (0., 2.35, 5.7); Pref = 1.E5, every TIME = 100 'FORCE_OUT' NOW
PRINT FORCE of P OFF for Z+ direction of ID=BODY
MODE 5: Convective and Diffusive Fluxes for a Variable at Specified Boundaries

SYNTAX

PRIN {FLUX} [Φ] [DETA] [option] [subrgn] [dir] [fname] [Vfrq] [TIME] [NOW] [OFF]

FLUX
The convective and diffusive fluxes for the variable at specified boundaries are written to the output file. The output includes the mean, minimum and maximum values for the variable, and the flow rate at the boundary (or boundaries).

Φ
One or more symbols for the dependent variable for which output is required. Up to 10 symbols may be specified per command. The valid symbols are listed in Table 2.7.1. If no symbol is specified then output is obtained for each active variable for which a transport equation is solved.

DETA
By default only a summary of the total fluxes and variable values for each boundary is written to the output device. If this modifier is present, then output also contains the detail for each segment (element) of the boundary.

option
The boundary type for which output is required. More than one option may be selected. If an option is specified, then the subrgn and dir modifiers are ignored. If no option is specified, then the averages are computed for the specified subrgn and dir modifiers.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>INLE</td>
<td>Boundaries specified by the INLET command are selected.</td>
</tr>
<tr>
<td>OUTL</td>
<td>Boundaries specified by the OUTLET command are selected.</td>
</tr>
<tr>
<td>OPEN</td>
<td>Boundaries specified by the OPEN command are selected.</td>
</tr>
<tr>
<td>IO</td>
<td>All boundaries specified by INLET, OUTLET or OPEN command are selected.</td>
</tr>
<tr>
<td>WALL</td>
<td>Walls specified by WALL or BLOCK command are selected.</td>
</tr>
<tr>
<td>EXTE</td>
<td>All external (or outer) boundaries of the computational domain are selected.</td>
</tr>
<tr>
<td>ALL</td>
<td>All of the above boundaries are selected.</td>
</tr>
</tbody>
</table>

subrgn
The subregion for computations. This specification is ignored if any of the option modifiers is present. If no subregion is specified, the entire domain is selected.

dir
The orientation index for the boundary for which the output is required. See Section 3.5 for available choices. If no input is given, then the output is obtained for all boundaries of the subrgn. This specification is ignored if any of the option modifiers is present.

fname
The file name for output. If a file name is present then the output is directed to the named file, otherwise the output is directed to the standard output device. The total number of open files in any simulation cannot exceed 64.

Vfrq
The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the output is obtained only at the end of simulations.

TIME
By default, Vfrq is interpreted as the frequency of output in terms of number of steps. In the presence of TIME this is the time intervals between successive outputs.

NOW
A record of fluxes is written to the output device at the next time step when the equation for the dependent variable is solved. This is in addition to the output from the Vfrq specification.

OFF
Any previously specified PRINT FLUX commands for the specified variables and subregion are disabled. New commands may be subsequently specified.
EXAMPLES

PRINT FLUX for EXTERNAL boundaries for all variables
PRINT FLUX of U, V and T for INLET boundaries at every 100 steps
PRINT FLUX of U and T for X- direction of ID=OBJECT at every TIME=20 units
PRINT FLUX of T for X+ direction of currently SELECTed subregion at the end of simulations
PRINT FLUX of T for OUTLET boundaries at every 100 steps on file “FLUX_T_OUTLET.FIL”
PRINT FLUX of T for ALL boundaries NOW and at every TIME=20 units on file “FLUX_T_ALL.FIL”
PRINT FLUX of T OFF for X- direction of ID=OBJECT
MODE 6: Convective and Diffusive Fluxes for a Variable at Specified Boundaries

SYNTAX

PRIN {SHEA} [DETA] [option] [subrgn] [dir] [fname] [Vfrq] [TIME] [NOW] [OFF]

SHEA

The shear stresses and y' at specified boundaries are written to the output file. The y' is the normalized distance to the node, which is meaningful for turbulent boundary layer type of flows. For laminar flow, it is reported as zero. The output also includes the normal distance from the boundary to the nearest fluid node and the mean velocity at the near boundary nodes. Strictly speaking, the output consists of the momentum gain or loss at the boundary and not the shear stress. However, in most instances where a boundary-layer type of flow occurs, the two can be considered to be equivalent.

DETA

By default only a summary of the total fluxes and variable values for each boundary is written to the output device. If this modifier is present, then output also contains the detail for each segment (element) of the boundary.

option

The boundary type for which output is required. More than one option may be selected. If an option is specified, then the subrgn and dir modifiers are ignored. If no option is specified, then the averages are computed for the specified subrgn and dir modifiers.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>INLE</td>
<td>Boundaries specified by the INLET command are selected.</td>
</tr>
<tr>
<td>OUTL</td>
<td>Boundaries specified by the OUTLET command are selected.</td>
</tr>
<tr>
<td>OPEN</td>
<td>Boundaries specified by the OPEN command are selected.</td>
</tr>
<tr>
<td>IO</td>
<td>All boundaries specified by INLET, OUTLET or OPEN command are selected.</td>
</tr>
<tr>
<td>WALL</td>
<td>Walls specified by WALL or BLOCK commands are selected.</td>
</tr>
<tr>
<td>EXTE</td>
<td>All external (or outer) boundaries of the computational domain are selected.</td>
</tr>
<tr>
<td>ALL</td>
<td>All of the above boundaries are selected.</td>
</tr>
</tbody>
</table>

subrgn

The subregion for computations. This specification is ignored if any of the option modifiers is present. If no subregion is specified, the entire domain is selected.

dir

The orientation index for the boundary for which the output is required. See Section 3.5 for available choices. If no input is given, then the output is obtained for all boundaries of the subrgn. This specification is ignored if any of the option modifiers is present.

fname

The file name for output. If a file name is present the output is directed to the named file, otherwise the output is directed to the standard output device. The total number of open files cannot exceed 64.

Vfrq

The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. By default the output is obtained only at the end of simulations.

TIME

By default, Vfrq is interpreted as the frequency of output in terms of number of steps. In the presence of TIME this is the time interval between successive outputs.

NOW

A record of fluxes is written to the output device at the next time step when the equation for the dependent variable is solved. This is in addition to the output from the Vfrq specification.

OFF

Any previously specified PRINT SHEAR commands for the specified variables and subregion are disabled. New commands may be subsequently specified.
EXAMPLES

PRINT SHEAR stress for all WALLS
PRINT SHEAR for EXTERNAL boundaries every 100 steps
PRINT SHEAR T for X- direction of ID=OBJECT at every TIME=20 units
PRINT SHEAR for X+ direction of currently SELECTed subregion at the end of simulations
PRINT SHEAR for OUTLET boundaries at every 100 steps on file “SHEAR_T_OUTLET.FIL”
PRINT SHEAR for ALL boundaries NOW and at every TIME=20 units on file “SHEAR_T_ALL.FIL”
PRINT SHEAR OFF for X- direction of ID=OBJECT
COMMAND PROBLEM

PURPOSE To specify the general nature and type of problem to be solved.

MODE 1: Atmospheric Pressure Computation Mode

SYNTAX PROB {ATMO}

ATMO This command mode is applicable only to the ANSWER™ Software Tool. It invokes the “atmospheric” mode of ANSWER™. By default the body force in the momentum equations is computed as \( \rho^* g_j \) where \( g_j \) is the body force vector component in the \( x_j \) direction. If this modifier is present, then the body force is computed as \( (\rho - \rho^*) g_j \). This effectively adds hydrostatic pressure \( (\rho^* g_j x_j) \) to the computed pressure. In this case, the thermodynamic pressure, \( p \), is related to the computed pressure by:

\[
p = p_{computed} + \rho^* \sum (x^*_j - x_j) g_j
\]

where \( x^*_j \) is the coordinate datum in the \( j \)th direction which can be specified by the DATUM command. For this mode, all initial and boundary conditions for pressure must be specified in terms of the computed pressure, \( p_{computed} \), that is the pressure boundary values must be in terms of the thermodynamic pressure minus the hydrostatic pressure.

COMMENTS This command provides a convenient option for solving the problem with hydrostatic pressure. This is particularly convenient for atmospheric applications where often the boundary pressure is specified as a linear function of height from ground level.

EXAMPLES Problem to be solved with the ATMOSPHERIC mode of ANSWER™
MODE 2: Boussinesq Approximation for Natural Convection

SYNTAX

```
PROB {BOUS} {ξ} {β} {ξ₀}
```

**BOUS**

This command mode is applicable only to the ANSWER™ Software Tool. It invokes the “Boussinesq” approximation mode of ANSWER™. In this mode, a source term for body force is added to momentum equations. The source term, $S_i$, for the $i^{th}$ direction velocity component, $u_i$, is given by:

$$S_i = \beta \left( \xi - \xi_0 \right) g_i$$

where $g_i$ is the gravitational acceleration vector in the $i^{th}$ direction and the other symbols are defined below. See comments below for further discussion.

**ξ**

One, and only one, symbol to denote the variable which controls the body force. Most commonly, the body force is created by a variation of density due to temperature. In this case, $\xi$ is the symbol $T$ (for temperature). The valid symbols are listed in Table 2.8.1-3

**β**

The numerical value for the coefficient for the body force defined as:

$$\beta = \frac{\partial \rho}{\partial \xi}$$

where $\rho$ is the density of the fluid. If the working fluid is a gas and the perfect gas law applies, then $\beta$ can be estimated from:

$$\beta = -\frac{\rho_o}{T_o}$$

where $T_o$ is a reference temperature and $\rho_o$ is a reference density. For air at atmospheric pressure and 300K, $\beta \approx -0.004$ [kg/(m$^3$K)]. For water at 300K, $\beta \approx -0.2$ [kg/(m$^3$K)].

**ξ₀**

The numerical value for the reference state at which there is no net body force in the fluid. Typically this should be equal to the mean value of $\xi$ in the computational domain.

**COMMENTS**

This command provides a convenient way to incorporate body forces with Boussinesq assumption. In this case, the density for the fluid is assumed to be constant and the variation of density is accounted for only in the body force term which is specified as a linearized function of the controlling variable, say, temperature.

If the body force is a function of more than one variable (say, density is a function of both temperature and a species concentration) then the **ALLOCATE** command can be used to define a composite variable which is a function of these variables. For example if the source term is given by:

$$S_i = \left( \beta_1 \left( T - T_o \right) + \beta_2 \left( C - C_o \right) \right) g_i$$

Then the **ALLOCATE** command can be used to specify a composite variable $\xi$ with:

$$\xi = \beta_1 T + \beta_2 C; \quad \beta = 1; \quad \xi_0 = \beta_1 T_0 + \beta_2 C_0$$

The composite variable, $\xi$, in turn can be defined by an appropriate **SET** command with the **ALWAYS** modifier so that it is continuously updated as $T$ and $C$ change.

**EXAMPLES**

PROBLEM BOUSSINESQ approximation: function of $T$ with beta = -0.004, $T_0$=300
MODE 3: Other Geometry or Client Specific Options

SYNTAX PROB {RADI|option} [attributes] [N₁, ..., N₄]

RADI This command mode is applicable only to the ANSWER™ Software Tool. If the geometry is Cartesian then, by default, the velocity components are also Cartesian. If this modifier is present, then it is assumed that the velocity components are in cylindrical radial system. In this case, the velocity component in the x-direction is identical to that in the Cartesian system, but the components in the y and z direction are assumed to be the radial and circumferential components, respectively.

option One of the special options implemented by ACRi in response to specific user requirements. Please call ACRi for the exact option(s), if any, available for your installation.

N₁, ..., N₄ Numerical input relevant to the implemented option.

COMMENTS The purpose of this command is to provide users access to special options implemented by ACRi in response to user requests.

EXAMPLES

PROBlem with RADial velocity in a geometry specified by Cartesian coordinates
PROBlem special option for GEAE
PROBlem special option for DOE to read GRID
MODE 4:  Free Surface or Unconfined Flow

SYNTAX  PROB {UNCO | FREE SURF} [dir [kr]] [AREA]

UNCO  This command mode is applicable only to the PORFLOW™ Software Tool. It invokes the unconfined or free-surface mode PORFLOW™ where the Richard’s equation form of the pressure equation is solved. In this mode the hydraulic conductivity itself is a function of the pressure head or depth of saturation.

FREE  Same as UNCO but the modifier SURF must be simultaneously present.

SURF  Same as UNCO but the modifier FREE must be simultaneously present.

dir  The coordinate direction that is normal to the plane of the phreatic surface. This is the nominal “vertical” direction for the flow. This direction must be one of the X, Y, Z, R or THETA modifiers, which, respectively, denote the x, y, z, r or θ coordinates. By default, the y direction is assumed to be the direction of the normal to the phreatic surface for 2-D problems and the z direction for 3-D problems. In this case, the effective hydraulic conductivity for the soil is computed as:

\[ K_{\text{effective}} = S_i K_{\text{saturated}} \]

where \( K_{\text{effective}} \) is the hydraulic conductivity used in the governing equations, \( K_{\text{saturated}} \) is the value specified by the user and \( S_i \) is the local saturation of the soil. This relation leads to a hydraulic conductivity that is zero for soil above the water table. This is unsatisfactory if infiltration occurs at a boundary above the water table or if a source of flow is located above the water table. In this case, a better assumption is that the “vertical” component of hydraulic conductivity retains a minimum value. The above relation is then replaced by:

\[ K_{\text{dir}} = k_r K_{\text{dir,saturated}} ; \quad S_i < 1 \]

Where \( k_r \) is the relative hydraulic conductivity if the modifier dir is specified. The default value is 1.0. The default value is satisfactory for most cases. However it does lead to a thickening of the interface (fringe) between the saturated and the dry soil. It will also lead to transport of contaminants from the water table to the dry soil since there is a finite “vertical” hydraulic conductivity at the water table if \( k_r > 0 \). In such cases, provided there is no infiltration or source above the water table, the \( k_r \) should be set to a small number or even zero.

AREA  Unconfined areal mode is selected. In this mode, the equations are solved in a two-dimensional integrated form where the effect of the third direction appears as a dynamically variable depth of the water body.

COMMENTS

By default, the upper and lower limits for the pressure head are automatically computed from the coordinates and datum specifications. The default limits represent the phreatic surface when the surface reaches either the bottom of the aquifer or the top of the ground surface. However, the user may explicitly alter these limits. Alteration may be necessary, for example, when the bottom of the aquifer is not at the bottom of the grid system or when ponding occurs above the ground surface. In these cases, the lower value of the pressure head (representing the bottom of the aquifer) is specified as the P2 pressure field and the upper value (representing the top of the ponding surface) is specified as the P3 pressure field.

EXAMPLES

PROBLEM is UNCONFINED
PROBLEM with FREE SURFACE; bedding plane normal to direction Y
PROBLEM with FREE SURFACE in X direction; dry soil kr = 0.1 of the saturated value
PROBLEM with FREE SURFACE in AREAL mode
MODE 5: Active Two or Multiple Phase with Variable Saturation

SYNTAX

PROB \{TWO|MULT\}

TWO

This command mode is applicable only to the PORFLOW™ Software Tool. It invokes the active two-phase variable saturation mode. A pressure equation is solved for each of the two phases. The saturation of the 1st phase is determined from the capillary pressure (the difference between the 2nd and 1st phase pressure). The saturation of the 2nd phase is equal to one minus the saturation of the 1st phase.

MULT

This command mode is applicable only to the PORFLOW™ Software Tool. The general multi-phase variable saturation mode is selected. The number of pressure equations solved is determined from user input (see comments below). This mode is also automatically activated by a MULTIPHASE command. The saturation of the last phase is always obtained as one minus the sum of the saturation of the other phase.

COMMENTS

For a typical vadose zone problem, involving water as the primary phase and air as the secondary phase, there are two phases but only 1 pressure equation is solved. It is assumed that the pressure of air phase is constant for this type of flow only 1st (water) phase is active; the 2nd (air) phase is passive.

If the 2nd phase is also active and its pressure is not constant, then a second pressure equation must be solved. In this case the MULTiphase command with TWO modifier must be specified.

The next stage of complexity in multiphase flow is reached when there are two active phases of immiscible liquids (say, water and oil) and one passive phase (say, air). The pressure of the air phase is assumed constant and only 2 pressure equations, those for water and oil phase, are solved.

The most complex option involves three active phases. In this case 3 pressure equations, one for each phase, are solved.

With the exception of the two active phases, all other modes of solution can be automatically determined by PORFLOW™ from the user input.

EXAMPLES

PROBLEM is TWO phase with water and oil as the liquid
PROBLEM is MULTiphase with three phases
Keyword Commands

MODE 6: Phase Change with Freezing and Thawing

SYNTAX

PROB \{FREEZ\} [V₁]

FREEZ This command mode is applicable only to the PORFLOW™ Software Tool. It invokes the Freezing/thawing phase-change mode of PORFLOW™. All 5 characters must be specified.

V₁ An empirical constant to determine the maximum rate of freezing or thawing from step to step. A small value results in gradual changes in freezing/thawing behavior; a large value results in more abrupt changes from one time step to another. The default value is 1000.

EXAMPLES

PROBlem with phase change: FREEZing

PROBlem with phase change: FREEZing rate=500
MODE 7: Phase Change with Evaporation and Condensation

SYNTAX PROB {EVAP}

EVAP The Evaporation/condensation phase-change mode is selected.

APPLICABILITY

This command is available only for the ANSWER™ and PORFLOW™ Software Tools.

COMMENTS

The phase change is assumed to be in thermodynamic equilibrium and the phase saturation is computed from enthalpy equation.

EXAMPLES

PROBLEM with EVAPoration
**MODE 8:**  Phase Change with Thermodynamic Non-Equilibrium

**SYNTAX**

```
PROB \{EVAP\} [DYN\{A\}] [FIXE] [Cm, δT, α, Rf]
```

**EVAP**  The Evaporation/condensation phase change mode is selected.

**DYN\{A\}**  The non-equilibrium mode of phase change is employed (see **COMMENTS** below). The vapor formation rate is computed from:

\[
m_v = C_m \theta_E S^\alpha \frac{P_s - P_v}{P_g}
\]

Where:
- \(m_v\) is the rate of evaporation or condensation,
- \(C_m\) is an empirical constant (see below),
- \(\theta_E\) is the effective porosity
- \(S\) is the saturation fraction of the fluid,
- \(\alpha\) is an empirical exponent,
- \(P_s\) is the saturation pressure of the vapor at equilibrium,
- \(P_v\) is the actual thermodynamic pressure of the vapor, and
- \(P_g\) is the thermodynamic pressure of the gas phase.

**FIXE**  The time constant, \(C_m\), for phase change is adjusted for transient flow to account for the changes in time step. Presence of the **FIXE** modifier results in \(C_m\) being held at its specified value.

**\(C_m\)**  The time constant \(C_m\) in the equation above. The constant has units of \([t^{-1}]\) and represents the speed of phase change due to a balance between hydraulic conductivity (to replenish the fluid), thermal energy (to satisfy the enthalpy demand) and mass transfer (to restore equilibrium). The numerical value represents the limiting (slowest) process among these three. The default value is 0.0025.

**δT**  Thermal tolerance for phase change. If the local temperature differs from the equilibrium value by less than \(δT\), the effect of phase change on thermal energy balance is ignored. The default value is 0.01.

**α**  \(α\) is the exponent in the above equation. The default value is 0.0625.

**Rf**  The relaxation factor for the source term. The new source term at any stage is computed as a weighted average of the previous value and the newly computed value. The default value is 1.0.

**APPLICABILITY**

This command is available only for the **PORFLOW™** Software Tool.

**COMMENTS**

Most phase change applications stay within the bounds of thermodynamic equilibrium. The exception may be extremely fast and explosive rate of phase change. This mode is computationally very sensitive and must be employed only if there are strong indications of non-equilibrium phase change. If the equation that determines the rate of evaporation and condensation is known, then the source terms may be introduced in the appropriate phase equations to control the phase change.

**EXAMPLES**

**PROBLEM** DYNAMIC EVAPORATION: \(Cm=0.01\), \(dt=0.02\), \(power=0.20\), \(RF=0.5\)
**COMMAND**  PROPERTY

**PURPOSE**  To specify the mode of calculation of fluid or material properties at an interface that lies between two elements where the properties are known at the element nodes.

**MODE 1:**  The Interface Conductivity and Diffusivity Mode

**SYNTAX**  PROP [Φ] [ARIT|HARM|GEOM|UPWI|MINI|MAXI] [SATU] [Λ]

**Φ**  One or more symbols that represent corresponding variable(s) for which the input is effective. The valid symbols are listed in Table 2.7.1. If no symbol is specified, the input is assumed to be effective for all variables.

**ARIT:**  The interface value is the weighted arithmetic mean of the values at nodes B and P. This is the default option for the ANSWER™ Software Tool. With respect to the figure below, the interface value of a property, Γ, is obtained from the node values, Γ_B and Γ_P, by:

\[
Γ_F = αΓ_P + βΓ_B
\]

Where \( b \) is the distance from the node B to the interface and \( d \) is the distance from node B to P, respectively.

**HARM:**  The interface value is the weighted harmonic mean of the values at nodes B and P. This is the default option for the TIDAL™ Software Tool. It is also the default option for the PORFLOW™ Software Tool in the single-phase mode. The interface value of the property is computed as:

\[
Γ_F = \frac{Γ_PΓ_B}{αΓ_B + βΓ_P}
\]

**GEOM:**  The interface value is the weighted geometric mean of the values at nodes B and P which is computed as:

\[
Γ_F = Γ_P^αΓ_B^β
\]

**UPWI:**  The interface value is taken to be the upstream value. With \( V \) as the velocity vector directed
from B towards P; this value is given by:

\[ \Gamma_F = \Gamma_B \quad \text{if} \quad V > 0 \]
\[ = \Gamma_P \quad \text{if} \quad V < 0 \]
\[ = \alpha \Gamma_P + \beta \Gamma_B \quad \text{if} \quad V = 0 \]

**MINI:** The interface is the minimum of the values at nodes B and P; that is:

\[ \Gamma_F = \min(\Gamma_B, \Gamma_P) \]

**MAXI:** The interface is the maximum of the values at nodes B and P; that is:

\[ \Gamma_F = \max(\Gamma_B, \Gamma_P) \]

**SATU** The interface value is computed from a harmonic average weighted with the local phase saturation. This modifier is effective only if the **HARMONIC** modifier is also present. This is the default option in **PORFLOW™** if the multiphase problem mode is invoked. With S denoting the phase saturation, the interface value is computed as:

\[ \Gamma_F = \Gamma_P \gamma_B \frac{\alpha S_P^{1/\lambda} + \beta S_B^{1/\lambda}}{\alpha S_P^{1/\lambda} \gamma_B + \beta S_B^{1/\lambda} \gamma_P} \]

\( \lambda \) The inverse of the power exponent of saturation if the **SATURATED HARMONIC** option is invoked; otherwise this input is ignored. The specified value must be an integer between 1 and 9. The default value is 2.

**COMMENTS**

This command is effective in **PORFLOW™** for computing the interface hydraulic conductivity, thermal conductivity and diffusivity of the mass species. In **ANSWER™**, this command is effective only if the conductivity or diffusivity for a governing variable is declared to be a vector (See **CONDUCTIVITY** command). In **TIDAL™** software it is effective only for the thermal and species equations.

**EXAMPLES**

- **PROP**erty at interface for all variables by arithmetic average
- **PROP**erty for U use **GEO**metric mean
- **PROP**erty averages for T and C by **UPWInd** mean
- **PROP**erty for C by **MAXimum** method
- **PROP**erty at interface for all variables by arithmetic average
MODE 2: The Effective Fluid-Solid Matrix Property Mode

SYNTAX

PROP [Φ] [EFFE|TOTA]

Φ One or more symbols that represent corresponding variable(s) for which the input is effective. The valid symbols are those for the mass species listed in Table 2.7.1. If no symbol is specified, the input is assumed to be effective for all relevant variables. (See comments below for important information)

EFFE This modifier is effective only for the PORFLOW™ Software Tool. It modifies the interpretation of the 1st values given on the TRANSPORT commands. By default the 1st value is assumed to be the partition coefficient, \( k_d \), for the species. If this modifier is present then this input is assumed to be the retardation factor, \( R_d \).

TOTA This modifier is effective only for the PORFLOW™ Software Tool. The use of the TOTAL modifier on this command has been superceded by the DISTRIBUTION command which provides more flexibility in selecting the inputs to which it applies. It is being retained here only for backward compatibility and its use is not recommended. See the DISTRIBUTION command for interpretation of this modifier.

COMMENTS

This mode of the PROPERTY command must be specified before the TRANSPORT command to which it applies; it will then apply to all TRANSPORT commands that follow till the next PROPERTY command.

This command mode may be combined with the Mode 1 of the command.

EXAMPLES

PROPERTY in EFFECTive mode for C
PROPERTY in EFFECTive mode for P by HARMONIC SATURATED based with power 4.
PROPERTY C present in TOTAL: solid.
COMMAND  QUIT

PURPOSE  To signify the termination of a sequence of problems.

SYNTAX  QUIT

COMMENTS
This command terminates a sequence of problems. The FREEFORM™ command language does not process any input following this command. Thus, for a sequence of problems, an END command terminates each problem whereas the QUIT command terminates the entire segments of problems. An example of the use of this command is when, for example, there are, five problems in an input sequence but the user desires to solve only the first two. In this instance, a QUIT command may be inserted immediately after the END command for the second problem. The input for the other three problems will then be ignored.

EXAMPLES

QUIT  Termination of sequence. No more problems to solve.
COMMAND  RADIATION

PURPOSE  To activate thermal radiation calculations and specify radiation constants. This command is effective only for the ANSWER™ Software Tool.

MODE 1: Radiation Approach and Thermal Source Term

SYNTAX  RADI [VIEW] [PASS]

VIEW  By default the radiation flux is computed from the 6-flux radiation model. If this modifier is present, then the radiation flux is computed from the View Factor approach. While the 6-flux radiation approach is available as a standard option with the Professional Versions of ACRi Software, the View Factor approach is available only by special arrangement and under a consulting contract with ACRi.

The 6-flux approach is best suited for “participating” media where the absorption and/or scattering phenomena dominate radiative transport. This is the case, for example, for combustion systems with high concentrations of gases that absorb and re-emit (such as CO₂ and H₂O) and contain scattering particles (such as soot). For “non-participating” media (such as air), this approach is not well suited. In these cases the View Factor approach is more appropriate.

PASS  By default the net radiation flux contributes to the thermal source in the enthalpy equation. If this modifier is present, then the effect of radiative heat flux is ignored in the enthalpy equation. For all practically purposes this is equivalent to a non-participating fluid medium.

COMMENTS  The modifiers of this mode can be combined with any of the other modes.

EXAMPLES  RADIation by VIEW factor approach.
          RADIation computations in PASSive mode
          RADIation computations by VIEW factor method in PASSive mode
MODE 2: Radiation Computation Frequency

SYNTAX  RADI  {FREQ} [V_{frq}]

FREQ The frequency of computation of radiation fluxes.

V_{frq} The frequency in terms of number of steps of the solution process. The numerical value must be >0; otherwise the input is ignored and the default or any previously specified value is used. The default value is 10.

EXAMPLES

RADIation FREQency of computations is 20 steps.
MODE 3: Specification of Gas Absorptivity

SYNTAX

`RADI {ABSOR} {func[3]} {N_1, N_2, ..., N_n} [fname] [subrgn]`

ABSOR

The absorptivity for radiation is specified. It is to be noted that all 5-characters of the modifier `ABSOR` must be present, since the 4 character modifier `ABSO` is used to denote the absolute value of the function (see Section 4.3). By default gas absorptivity is computed from the built-in formulae, which take account of gas and soot constituents.

`func`

One of the modifiers listed in Table 4.2.1 that denotes the functional form of gas absorptivity. If no function is specified then the value is assumed to be constant.

`ξ`

One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

`N_1,...,N_n`

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

`fname`

The name of the file containing the numerical values `N_2` through `N_n` This option is available only for selected functions. See Section 3.3 for additional information.

`subrgn`

The sub region for which the input is specified. See Section 3.4. If no sub region is specified, the entire computational domain is selected.

COMMENTS

The absorptivity is denoted by the symbol “ARAD” in ACRI software. The `SET` command with `ARAD` modifier may also be used to set the value of gas absorptivity. This symbol can also be used to obtain output of gas absorptivity.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (`RADI`) with modifier `ABSOR` must replace the keyword used in these examples.
Keyword Commands

MODE 4: Specification of Surface Emissivity

SYNTAX

RADI {EMIS} {func[ξ]} {N₁, N₂, ..., Nₙ.fname} [[subrgn] [dir][[WALL]] [EXTE|INTE|BLOC]

EMIS
The emissivity of a surface is specified. By default the emissivity for all surfaces is set to unity. However if this command is present, and no value is specified, then the default value is set to 0.8.

func
One of the modifiers listed in Table 4.2.1 that denotes the functional form of surface emissivity. If no function is specified then the value is assumed to be constant.

ξ
One of the independent variables listed in Table 4.2.2. If no variable is specified, then the independent variable is assumed to be time.

N₁,...,Nₙ
The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname
The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

subrgn
The sub region for which the input is specified. See Section 3.4. If no sub region is specified, the entire computational domain is selected.

dir
Orientation index for the boundary to which the input is applied. See Section 3.5 for available choices. If dir is omitted, then all surfaces of the selected subrgn are selected.

WALL
If this modifier is present then any specification of subrgn and dir is ignored and the input is applied to walls of the computational domain. The input is applied to all the walls unless one of the modifiers EXTE, INTE or BLOC is present.

EXTE
If this modifier is present along with the WALL modifier, then the input is applied only to the exterior walls of the domain.

INTE
If this modifier is present along with the WALL modifier, then the input is applied only to the interior walls of the domain defined with the WALL command.

BLOC
If this modifier is present along with the WALL modifier, then the input is applied only to the walls of the domain defined with the BLOCK command.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (RADI) with modifier EMIS must replace the keyword used in these examples.
MODE 5: Radiation Constants

SYNTAX  RADI  [SCAT=V_{scatter}] [STEF|BOLT=\sigma]

SCAT   The scattering coefficient for the gas is specified. The default value is 0.01.

V_{scatter} The numerical value for the Scattering coefficient. It must be \geq 0.

STEF   Stefan-Boltzmann constant is specified. The default value is 5.669E-8

BOLT   Stefan-Boltzmann constant is specified. The default value is 5.669E-8

\sigma   The numerical value for the Stefan-Boltzmann constant. It must be > 0.

EXAMPLES

RADIation SCATTERing coefficient is 0.02
RADIation STEFan-Boltzmann constant is 4.76E-13 in fps units.
RADIation SCATTERing coefficient= 0.02; STEFan= 4.76E-13 in fps units.
Keyword Commands

COMMAND  REACTION
PURPOSE To select the nature and mode of control of chemical reaction for reactive flows.

MODE 1: The Built-In 2 or 4-Step, 8 Species Reaction Mechanism.

SYNTAX REAC [TWO] [KINE] [PROD] [HYDR] [USER] [OFF]

TWO By default, the reaction mechanism is composed of four steps:

\[ C_n H_m \rightarrow C_n H_{m-2} + H_2 \]  
\[ C_n H_{m-2} + 1/2 n O_2 \rightarrow n CO + 1/2 (m - 2) H_2 \]  
\[ CO + 1/2 O_2 \rightarrow CO_2 \]  
\[ H_2 + 1/2 O_2 \rightarrow H_2O \]

If this modifier is present, then the reaction mechanism is assumed to be:

\[ C_n H_m + 1/2 n O_2 \rightarrow n CO + 1/2 m H_2 \]  
\[ CO + 1/2 O_2 \rightarrow CO_2 \]

See Section 3.5 and comments below for further details.

KINE By default, the reaction rate for the built-in reaction mechanism is taken to be the smaller of the chemical kinetics (Arrhenius) reaction rate and the eddy break up (EBU) rate to account for turbulence. If this modifier is present, then the EBU model is deactivated and the reaction rate is that given by the chemical kinetics.

PROD This modifier is used if the user selects the explicit reaction mode (Mode 2) but still wants to employ the equilibrium algebraic relations to determine the mass concentrations of \( O_2 \), \( H_2O \), \( CO_2 \), and \( N_2 \) from the solved species and conserved variables. This option assumes the reactants are only pure hydrocarbons and oxygen or air.

HYDR The reaction is for a hydrocarbon fuel but the user explicitly specifies the equilibrium relations for those chemical species for which a transport equation is not solved.

USER Reaction is assumed to be explicitly specified by the user (see Mode 2). The default 4-step reaction is switched off.

OFF Same as the USER modifier.

COMMENTS

The default reaction systems consist of the 2 steps and 7 species or 4 steps and 8 species described in ANSWER™ Theory Manual. The 2 step system, the gas phase consists of 7 chemical species: \( C_n H_m \), \( CO \), \( H_2 \), \( O_2 \), \( H_2O \), \( CO_2 \), and \( N_2 \). For the 4-step system, an 8th species, \( C_n H_{m-2} \), is added. The default fuel is \( C_{10}H_{19} \). This can be changed with the FUEL command. The default Arrhenius reaction constants are given in Table 3.5.1; these can be changed by the ARRHENIUS command. The EBU constants can be changed by the EBU command.

EXAMPLES

REACTIVE flow with default options
REACTIVEtion with TWO-step mechanism default options
REACTIVEtion process is KINEtically controlled
REACTIVEtion process; use default PRODuct relations; explicit reactions supplied later
REACTIVEtion for HYDRocarbon fuel; next commands explicitly supply the reaction details
REACTIVEtion specified by USER. Explicit reactions of Mode 2 will be specified.
MODE 2: User-Specified Chemical Reaction Rate.

SYNTAX

REAC {idreac} {Φ} [EBU] [TEMP] [subrgn] [option] {Z₀, E, α, β, γ} [θ]

idreac
A unique identifier for the reaction rate. The reaction rate is computed as:

\[
\text{Rate} = Z₀ \exp \left( -\frac{E}{R_u T} \right) \Phi_1^α \Phi_2^β \Phi_3^γ T^θ
\]

where \( Z₀ \) is the pre-exponential constant, \( E \) is the activation energy, \( R_u \) is the universal gas constant, \( (E/R_u) \) is the activation temperature, \( T \) is the temperature in absolute units, \( α, β, γ \) and \( θ \) are exponents and \( Φ \)'s are the reactant concentrations. The \( Z₀ \) is generally reported in the literature in molar units where the \( Φ \)'s are molar concentrations. The actual computed \( Φ \)'s in ACRi Software may be in mass, molar, volumetric or user specified units. Therefore the specified value of \( Z₀ \) may need to be converted to appropriate units internally.

Φ
One or more symbols that specify the chemical species participating in the reaction as reactants. A maximum of three species can be specified.

EBU
The reaction is limited by the eddy breakup (EBU) rate (see EBU command).

TEMP
By default \( N₂ \) specifies the activation energy, \( E \) (e.g. J/kg-mole). If this modifier is present, then \( N₂ \) is the activation temperature \( (E/R_u) \) in units of Kelvin.

subrgn
The subregion for which the idreac reaction is computed. If no subregion is specified, the reaction is computed for the entire computational domain. See Section 3.4.

option
The modifier for interpretation of numerical input

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>MASS</td>
<td>By default it is assumed that the computed ( Φ )'s are in mass units and that ( Z₀ ) is given in molar units. Therefore ( Z₀ ) is internally converted to appropriate mass units. If this modifier is present, then no unit conversion is performed. It is assumed that ( Z₀ ) is specified in appropriate units for the computed ( Φ )'s.</td>
</tr>
<tr>
<td>CGS</td>
<td>By default, ( Z₀ ) and ( E ) are assumed to be in specified SI ((\text{kg-mole} \cdot \text{m}^3 \cdot \text{J} \cdot \text{K})) units. If this modifier is present, then ( Z₀ ) and ( E ) are assumed to be in the cgs ((\text{gm-mole} \cdot \text{cm}^3 \cdot \text{cal} \cdot \text{K})) units and the activation energy in calories. The specified values are converted to SI units on the assumption that the computed ( Φ )'s are mass concentrations.</td>
</tr>
<tr>
<td>LIFE</td>
<td>( Z₀ ) is in units of time ([t]) representing the half-life of the reaction. In this case ( E ) must be the activation temperature ([T]).</td>
</tr>
<tr>
<td>DECA</td>
<td>( Z₀ ) is in units of inverse of time ([t^{-1}]) representing the decay rate of the reaction. In this case ( E ) must be the activation temperature ([T]).</td>
</tr>
</tbody>
</table>

\( Z₀ \)
The pre-exponential constant, \( Z₀ \). The specified value may be internally converted to appropriate units based on the option modifier. For example, in the CGS system, units are \( \text{cm}^{3n-3} / \text{moles}^{n-1} \cdot \text{s} \), where \( n = α + β + γ \).

\( E \)
Activation energy, \( E \) (J/kg-mole or cal/gm-mole) or activation temperature, \( E/R_u \) (Kelvin).

\( α, β, γ \)
Stoichiometric coefficients or exponents \( α, β, γ \) and \( θ \) for the species specified by \( Φ \)'s. There is no default value. One value must be specified for each identified reactant.

\( θ \)
Exponent of the temperature, \( θ \), in the reaction rate equation; it is the 4th, 5th or 6th numerical value depending on the order of the reaction (1, 2, or 3 reactants). The default value is 0.
EXAMPLES

REACION R1 preexp=1.960E+18, activ_e=2.48E+04 FU ^ 0 and O2 ^ 0.5
REACION R1 FU, O2 1.960E21 2.062E8 0.0 0.5 1.07 CGS EBU TEMP SELECTed subregion
REACION R2 CH, O2, FU: 5.395E16, 2.50E04 0.0 0.9 1.18 -0.57 TEMP for ID=RGN1 active
REACION R1 MASS based preexp=1.50, activ_T= 600 FU ^ 1 and O2 ^ 1
REACION R1 MASS FU, O2 1.50 0. 1 0.5 1.07 EBU! No effect of temperature
REACION R2 DECAy frequency FU: 2.00, 1000 1.0 for SELECTed region
REACION R2 between C1 & C2 Half Life = 0.01 Active_T=0., exponents: 1 & 1 ID=RGN1
MODE 3: Fast-Chemistry Reaction Mechanism

SYNTAX

REAC {FAST} \{N_1, N_2 \} \{N_3, \ldots, N_n\} \{fname\}

FAST

The two-parameter PDF fast-chemistry reaction model is used. In this mode, two differential equations are solved for the mean and variance of the mixture fraction. The values of the mean mixture fraction and variance at each node are then used to determine the properties (temperature, species concentrations, and density) at the node by a lookup table procedure. The lookup table consists of the properties as a function of the mixture fraction mean and variance. The table is constructed by assuming that the mean and variance describe the PDF (usually a beta-function) of the properties at each point of the domain. The properties for each mean and variance value in the table are then determined by convoluting the corresponding PDF with the properties, which are assumed to be a function of the mixture fraction and are determined by chemical equilibrium considerations. This model is based on the approach described by Jones and Whitelaw (1982).

fname

The name of the file containing the fast-chemistry lookup table. The total number of values in the table must equal $N_1$ times $N_2$.

$N_1$

The number of rows of data in the fast-chemistry lookup table. Each row represents the properties (temperature and species concentrations) for a given value of the mean and the variance. There is no default value.

$N_2$

The number of columns of data in the fast-chemistry lookup table. The first column represents the mean, the second column the variance, and each of the others represents a property. There is no default value.

$N_3, \ldots, N_5$

These represent the numerical values in the table. If the file name is specified, then these values are read from the file; otherwise $N_1$ times $N_2$ values must be specified with the command. There is no default value.

EXAMPLES

REAC\{ion\} FAST chemistry; lookup table has 1000 rows and 5 columns on file 'FAST_CHEM'
REAC\{ion\} FAST chemistry 1000 rows & 5 columns values!!!! 5000 values must be specified)
Keyword Commands

MODE 4: Empirical Constants for Fast-Chemistry Reaction

SYNTAX REAC {FAST} {CONS} {N₁, N₂}

FAST The two-parameter PDF fast-chemistry reaction model is used.

CONS The empirical constants required for the fast-chemistry reaction are specified.

N₁ The constant C₉₁ (>0) for fast-chemistry reaction (see Jones and Whitelaw, 1982). The default value is 2.

N₂ The constant C₉₂ (>0) for fast-chemistry reaction (see Jones and Whitelaw, 1982). The default value is 2.

EXAMPLES

REAC:ion FAST chemistry CONStants: cg1 = 3.0
REAC:ion FAST chemistry CONStants: cg1 = 2.0 and cg2 = 3.0
REAC:ion FAST chemistry CONStants: cg1 = 2.0 and cg2 = 3.0
MODE 5: Disable Previously Specified Reaction

SYNTAX

REAC \{idreac\} \{subrgn\} \{OFF\}

idreac A unique identifier for the reaction rate.
subrgn Same as Mode 2.
OFF Any previously specified reaction with idreac identifier for the specified subregion is disabled. A new specification may follow.

EXAMPLES

REACtion R1 for subdomain ID=R1DMn switched OFF
REACtion R2 for SELECTed subdomain OFF
COMMAND  READ

PURPOSE  To read the archive file for basic problem information and initial conditions.

MODE 1:  Read a Generic Archive File

SYNTAX  READ  {fname} [fmt] [SKIP[ONLY=Φ] [STAR] [N1]

fname  The name of the file from which the input is obtained. There is no default file name; a file name must be specified.

fmt  The modifier "FORMATTED" or "UNFORMATTED" that define the nature of the data in the restart file. If this specification is omitted, the file is assumed to be formatted (see Section 2.10).

SKIP  If this modifier is present then any explicitly specified variables, if present on the file, are ignored at time of reading of the file. If this modifier is present, then the ONLY modifier must not be present on the command.

ONLY  If this modifier is present then only the explicitly specified variables, if present on the file, are read from the file. If this modifier is present, then the SKIP modifier must not be present on the command.

Φ  One or more of the character strings listed in Table 2.8.1 that represent the corresponding variables on the file that is not to be read from the file. This input is ignored if the SKIP modifier is not present.

STAR  If this modifier is present, the calculation step number for the current simulation is set to 0; otherwise, it is computed by reference to the step number at which the data was archived.

N1  The data set number (≥0) to be read from the archive file. If no data-set number is specified, then the first set is read from the archive file. As explained in Section 2.9, a data set in this context consists of several records. The default value is 1.

COMMENTS

If no simulation time has been explicitly set (such as by the TIME command) and a file is read at the start of the computations, then the starting simulation time is set to be the value read from the file. This ensures a continuity of time from the previous record read from the file. In this case, for transient simulations, the time specified on the SOLVE command must account for that the starting time is that read from the file.

EXAMPLES

READ from archive file ‘PROBLEM.SAV’
READ record number 3 from file ‘PROBLEM.SAV’
READ from ‘EXAMPLE1.SAV’
READ record number 5 from ‘EXAMPLE2.SAV’ in FORMatted mode
READ record # 5 from ‘EXAMPLE2.SAV’ and STARt step count from now
READ record # 5 from ‘EXAMPLE2.SAV’ but SKIP variables U and MTYP
**MODE 2:** Read a Restart File

**SYNTAX**

```
READ {REST} [fname] [STAR]
```

**REST**
A restart file is read in “unformatted” mode to continue the computations from a previous simulation. This file must have been generated previously by a **SAVE** command with **RESTART** modifier. If this restart option is used, then it is recommended that the input command file must be identical to the file that generated this particular restart file except for changes in, or presence of, **READ, SAVE, OUTPUT** and **SOLVE** commands. Any other changes in, say, boundary conditions or geometry may lead to unpredictable results.

**fname**
The name of the file from which the input is obtained. See Sections 2.4 and 3.3 for more information. The default file name is the output file name (see **OUTPUT** Command) but with the extension “_RESTART.TMP” attached to the file name. For example if the standard output file name is “MYCASE” or “MYCASE.OUT”, then the default file name will be “MYCASE_RESTART.TMP”.

**STAR**
If this modifier is present, the calculation step number for the current simulation is set to 0; otherwise, it is computed by reference to the step number at which the data was archived.

**EXAMPLES**

```
READ RESTart data from ‘STAGE_1.FIL
READ RESTart file with default file name
READ RESTart data from file ‘STAGE_1.FIL’; START step count again
```
COMMAND: REFERENCE

PURPOSE: To specify the reference values of selected constants and variables.

MODE 1: Specify Reference Value for a Variable

SYNTAX: REFERENCE {Φ|TEMP} [ABSO|FREEZ] [N1]

Φ: The symbol for the variable to which the specified input applies. The valid symbols are listed in Table 2.8.1-3

TEMP: The reference value for temperature, \( T^* \), is specified. The default value is 0.

ABSO: The absolute base for the temperature scale, \( T_a \), is specified. This modifier is effective only if the modifier \( T \) or TEMP is also simultaneously present. The default value is 273.15.

FREEZ: The freezing point for the fluid is specified for phase change operations. The modifier is effective only if the modifier \( T \) or TEMP is also simultaneously present. Only the PORFLOW™ Software Tool currently uses this input. The default value is 0.

N1: The reference value of the corresponding variable specified by \( \Phi \) or another modifier.

EXAMPLES:

REFERENCE P is 2.5E5 N/m^2
REFERENCE T = 30 deg C
REFERENCE T = 60 F
REFERENCE T ABSOLUTE base = 459.67 R
REFERENCE ABSOLUTE TEMPERATURE base = 459.67 R
REFERENCE FREEZE TEMPERATURE is = 0.0 C
MODE 2: Specify Absolute Pressure mode for PORFLOW™

SYNTAX REFE {P} {ABSO}

ABSO In the PORFLOW™ Software Tool, by default the governing equation for \( P_n \), pressure for the \( n^{th} \) fluid phase, is solved for the normalized form of pressure;

\[
P_n = \frac{p - p^*}{\rho \ g}
\]

The pressure is therefore in units of length (also called Head). If this modifier is present then the governing equation for pressure is solved with the normalizing denominator set to unity. Thus pressure is now in absolute thermodynamic units (such as N/m²) with reference to the datum pressure, \( p^* \). In this form of the equations, all the initial and boundary conditions must be specified with reference to the datum pressure in absolute thermodynamic units. The sources and fluxes are then in mass units and input for hydraulic conductivity (HYDRAULIC command) must be replaced by that for hydraulic permeability divided by viscosity.

In the ANSWER™ Software Tool, by default for incompressible flow, the computed pressure is modified by subtracting the computed pressure at a reference node; that is (See REFE P NODE mode of command):

\[
P = p_{\text{computed}} - p_{\text{reference node}}
\]

If this modifier is present then the reference node pressure is not subtracted. This mode is also automatically invoked for the compressible (COMP Command) mode is used or if P is explicitly specified through one or more BOUN commands.

EXAMPLES

REFErence P in ABSOlute mode
MODE 3: Specify Constants and Options for Pressure Related Choices

SYNTAX  REFE {P} [VALU|NORM] {N1}

P The specified input pertains to the pressure equation.

VALU In both ANSWER™ and PORFLOW™ Software Tool, the pressure is computed with reference to a datum, p*. In the presence of this modifier, N1 is the reference datum pressure. This is the default option. This input can also be provided by the GAS P or GAS PRES command.

NORM The normalizing pressure is specified. By default the normalizing pressure is unity except for PORFLOW™ where it is equal to p*g (see REFE P ABSO command).

N1 The datum or normalizing pressure value.

EXAMPLES

REFERENCE P = 10000 for this case.
REFERENCE NORMalizing P = 1
REFERENCE NORMalizing P = 10
MODE 4: Location of Reference Pressure

SYNTAX

```
REFE {P} {NODE|COEF} {N1, ..., Nn}
```

**P**
The specified input pertains to the pressure equation.

**NODE**
In the ANSWER™ Software Tool, for incompressible flow, the absolute value of pressure does not appear in the governing equations. Only relative pressure is computed from the continuity constraint. By default, the computed pressure is chosen to be relative to the pressure at the first inlet node or the first open node in the computational domain. This means that the computed pressure at the selected node is set equal to zero. If NODE modifier is present then pressure is set to zero at the grid node or element specified by N1 through Nn.

For compressible mode of the ANSWER™ software and for the other ACRi software packages (PORFLOW™, TIDAL™, etc.), this information is ignored unless pressure coefficient is computed and the COEF mode of this command is not invoked to explicitly specify the reference pressure location.

**COEF**
The location of the reference value for computation of the pressure coefficient is specified. The pressure coefficient, $C_p$, is defined as:

\[
C_p = \frac{P - P_{\text{ref}}}{0.5 \rho V^2}
\]

In the equation above, $P$ is the computed pressure, $P_{\text{ref}}$ is the pressure at the specified location, $\rho$ is the density and $V$ is the fluid speed. By default the location of the reference pressure is assumed to be the same as that of the datum (see NODE).

**N1, ..., Nn**
The location of the reference pressure in terms of grid indices for structured grid or element number for unstructured grid.

EXAMPLES

```
REFErence NODE for P at (I=5, J=10, K=3)
REFErence location for P COEFFicient is (I=1, J=5, K=2)
```
COMMAND REGENERATION

PURPOSE To specify regeneration rate of one species from another in the decay chain. This command is effective only for the PORFLOW™ Software Tool.

SYNTAX REGE {Φ} {Ψ} [V_{reg}]

Φ The symbol for the species that is generated by the decay of another species (denoted by Ψ) in the decay chain. The valid symbols are listed in Table 2.7.1.

Ψ The symbol for the species that is decaying to generate the species denoted by Φ. The valid symbols are listed in Table 2.7.1.

V_{reg} The factor to convert the decay rate of Ψ to the source for the decay product Φ. For species in mass units this number is between 0 and 1. However if the species are in user-defined units (such as curies) then this number may take on any value. The user must ensure that the value supplied is consistent with the defined units of Φ and Ψ. If no value is specified, then the factor is assumed to be equal to 1.

APPLICABILITY This command is available only for the PORFLOW™ Software Tool.

EXAMPLES

REGENeration of C2 from decay of species C; converted fraction is 1.0 (total conversion)
REGENeration of C2 from C; conversion factor = 1000!! (C1 in kg but C2 in g units)
REGENeration of C2 from C; conversion factor = 60!! To account for different units of C1 and C2
COMMAND RELAX

PURPOSE To specify relaxation factors for iterative solution of the matrix of equations.

SYNTAX RELA [{Φ=N₁, Φ=N₂, ..., Φ=Nₙ} | OFF]

Φ One or more of the symbols for which the relaxation parameters are specified. The valid symbols are those listed in Table 2.7.1 plus RHO and VIS.

OFF All relaxation parameters are set to unity. Any other input in the command is ignored. In essence, the relaxation feature is disabled.

N₁, .., Nₙ Θ is the relaxation factor as shown in the equation below for the variable denoted by the symbol immediately preceding the value. The numerical value must be larger than 0 and less than 2.

\[ \Phi^{k+1} = \Theta \Phi^{\text{computed}} + (1 - \Theta) \Phi^k \]

Where:
- \( \Phi^k \) is the value at the k\text{th} step (most recent previous value)
- \( \Phi^{\text{computed}} \) is the value computed from the numerical process at the k+1\text{st} step, and
- \( \Phi^{k+1} \) is the value stored as the new value at the k+1\text{th} step.

COMMENTS This command is effective in both steady state and transient modes of solution. The relaxation factor affects the convergence of the numerical solution. If the solution shows instability, a relaxation factor with a value less than unity may help obtain a stable solution. Alternatively, if the convergence rate is too slow, a value greater than unity may result in more rapid convergence. A value larger than 2 will lead to exponentially unstable growth of the solution.

In the steady state modes the relaxation factor affects the values of the variable during outer-loop step-to-step iterations. In the transient mode, a relaxation factor is used during execution of the inner loop in which multiple iterations (N2 on CONVERGENCE command) are used at each time step. A more complete discussion of the role of the relaxation parameter is given in standard textbooks (for example, Varga, 1962).

where
- The subscript P denotes the node point at which the discrete equation is derived.
- \( \delta V \) is the volume of the element at P
- K is the grid node values at E,W,N,S,U and D respectively.
- A’s in the above equation are the functions of grid size, fluid velocity and properties of the fluid.
- The superscripts k and k+1 denotes the value of the variable Φ at two successive time steps.
- θ determines whether the numerical scheme is explicit, implicit or semi-implicit.

EXAMPLES

RELAXation factor for P = 0.7
RELAXation factors: T = 1.2, C = 0.9
RELAXation factors: T = 0.7, C = 0.9, C₂ = 0.7
RELAXation factors: P = 0.1, P₂ = 0.1, T = 0.1, S = 0.5
RELAXation OFF
**COMMAND**  
RENAME

**PURPOSE**  
To rename the output variables listed in Table 2.8.1-3.

**SYNTAX**  
RENA \{Φ=name\}

Φ  
The current symbol for the output variable that is to be renamed.

name  
A character string that defines the new symbol and name for the variable currently denoted by the symbol, Φ. The name must be enclosed in single or double quotes and must be a character string no longer than 64 characters. **The first four characters of this name will be used as the new symbol for all subsequent references to this renamed variable.**

**EXAMPLES**

// Rename "U" to "XDIR Velocity of Fluid Flow" for all future reference
RENAme U = 'XDIR Velocity of fluid flow'

// Rename "T" to "TEMPERATURE (THERMODYNAMIC)"
RENAme T = 'TEMPERATURE (THERMODYNAMIC)'

// Rename "FF" to "TC99 Technetium 99 in solution"
RENAme FF = "TC99 Technetium 99 in solution"
COMMAND  RETARDATION

PURPOSE  To specify the retardation coefficient for the governing differential equations. This command is effective only for the PORFLOW™ Software Tool.

APPLICABILITY
This command is available only for the PORFLOW™ Software Tool.

COMMENTS
This command has been replaced by the more general STORAGE command. The term “retardation” is normally applied only to the transport of chemical species whereas the term “storage coefficient” applies to any of the governing transport equations.

EXAMPLES
See the STORAGE command
Keyword Commands

**COMMAND**  SAVE

**PURPOSE**  To write the archival and post-processing file for restart, plotting and archiving purposes.

**MODE 1:**  Archival and Post-Processing Data in ACRi Block Format

**SYNTAX**  SAVE [Φ] [BLOC|TABL] [ADD] [fname] [fmt] [GEOM|COMP] [DATA] [REPL|SEQU] [subrgn] [TIME] [Vfrq] [IMME|NOW|ONLY|OFF]

**Φ**  One or more of the symbols that represent the variables for which output is desired. The valid symbols are listed in Table 2.8.1-3. The output for listed variables is produced in the order of specification. If no symbols are specified, and the ADD modifier is not present, then a suitable default set is automatically selected after the 1st SOLVE command is encountered. The default set includes the variables for which equations are solved, and some important supporting variables based on the nature of the problem.

**BLOC**  The output for each variable is written in a block format. One record is written for each variable. The variables are written in the order in which they appear on the command. If the grid is structured then the variable is written in the manner of a FORTRAN DO loop (over the grid indices I, J, K). If the grid is unstructured, then the record for the variable is sequential over element numbers starting with the 1st element. This is the default mode.

**TABL**  The file is written as a columnar table of values with one record per element. Each record contains the element number, the element material type, and its node coordinates (x and y for 2D and x, y and z for 3D) followed by the specified variables. If there are more than 7 total values (including node coordinates but excluding element number and material type) then the record wraps to the next line of output with 7 variable values per line.

**ADD**  One SAVE command is activated by default. If the ADD modifier is present, then the specified command is added to the list of active SAVE commands. On the other hand, if the ADD modifier is not specified, then the default command is modified or replaced by user specified command.

**fname**  The name of the file to which the output is directed. See Section 3.3 for additional information. The default file name is the Standard Output Unit name (see OUTPUT Command) but with the extension changed to “SAV” for the BLOCK and “_TABLE.SAV” for the TABLE format file.
For example, if the Standard Output Unit file name is “MYCASE” or “MYCASE.OUT”, then the default file names will be “MYCASE.SAV” and “MYCASE_TABLE.SAV”, respectively.

If a file name is specified on an SAVE command with an ADD modifier, then this file is uniquely attached to a unit for output from that command and any subsequent SAVE command that specifies the same file name. The file name specification is case sensitive and the case must be consistent, otherwise some operating systems may report an error. See Section 3.3 for additional information.

Output from all SAVE command without an ADD modifier is directed to a single common file (with a default name as stated above). If any such command specifies a file name, then that file becomes the common output file for all commands without the ADD modifier. If a new file name is subsequently specified, then the previous file is closed and all subsequent output from all SAVE commands without an ADD modifier is directed to the new file.

**fmt**  The modifier “FORMATTED” or “UNFORMATTED”, which defines the nature of the data in the archive file. By default, the file is formatted.

**GEOM**  By default the archive file contains problem geometry and grid connectivity variables plus variables specified by the user or active default variables (see Φ above). If GEOMETRY modifier is present, then only the problem geometry and grid connectivity information is written to the file; the Φ variables are omitted.

**COMP**  If this modifier is present, then the problem geometry and grid connectivity information is not written to the file; only the Φ variables are written. If both modifiers are specified, then COMPACT modifier takes precedence over the GEOMETRY modifier.

**DATA**  By default standard ACRi file header containing information about the problem and nature of data appears at the start of the file. If DATA modifier is present then the file header information is omitted.
<table>
<thead>
<tr>
<th>Modifier</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>REPL</strong></td>
<td>If multiple records are written due to the ( V_{frq} ) input or the <strong>NOW</strong> modifier, then by default each new record is appended to the existing file. If this modifier is present, then the old records are replaced by the new record.</td>
</tr>
<tr>
<td><strong>SEQU</strong></td>
<td>If <strong>SEQU</strong> modifier is present, then sequential files are written at a frequency determined by the ( V_{frq} ) input and the <strong>NOW</strong> modifier. A 4 digit numerical index (from 0001 to 9999) is appended to the file name for each file written in the order determined by ( V_{frq} ) and <strong>NOW</strong> input. Any extension specified for each file written in the order is retained without change. For example if the file name is “MYDATA.SAV”, then the names for sequential files, in order, will be: “MYDATA0001.SAV”, “MYDATA0002.SAV”, and so on. If more than 9999 files are generated, then the subsequent data will be appended at the end of the 9999th file.</td>
</tr>
<tr>
<td><strong>subrgn</strong></td>
<td>This modifier is effective only for the <strong>TABLE</strong> mode of the command. It specifies the subregion for which the output is required. If no subregion is specified, then entire computational domain is selected. See Section 3.4.</td>
</tr>
<tr>
<td><strong>TIME</strong></td>
<td>By default, ( V_{frq} ) is the frequency of output in terms of number of steps. If this modifier is present, then ( V_{frq} ) is interpreted to be time interval between successive outputs.</td>
</tr>
<tr>
<td><strong>V_{frq}</strong></td>
<td>The frequency (step or time interval) at which the output is written to the output device. See Section 3.7 for further details. The specified value is ignored if it is zero or negative. The default value is set so that output is obtained only at the end of simulations.</td>
</tr>
<tr>
<td><strong>IMME</strong></td>
<td>The output is produced immediately. This modifier is necessary only before the 1st <strong>SOLVE</strong> command is given. It then enables the output of the current value of specified variable(s) immediately. After the 1st <strong>SOLVE</strong> command, the output is always produced as soon as the command is encountered and this modifier is redundant. The symbol(s) for the output variable(s) must be specified with this modifier since the default output symbols are not available till after the 1st <strong>SOLVE</strong> command.</td>
</tr>
<tr>
<td><strong>NOW</strong></td>
<td>If this modifier is specified before the 1st <strong>SOLVE</strong> command, then the output is produced just before the 1st step of the solution but after all the initial and boundary conditions have been processed. Thus, this modifier provides the output of the initial conditions for the variable(s) at the start of the solution process. After the 1st <strong>SOLVE</strong> command, the output is always produced as soon as the command is encountered; this modifier is redundant.</td>
</tr>
<tr>
<td><strong>ONLY</strong></td>
<td>If this modifier is specified then the output is produced only once at the step number or time specified by the ( V_{frq} ). This modifier is ignored if <strong>NOW</strong> or <strong>IMMEDIATE</strong> modifier is present.</td>
</tr>
<tr>
<td><strong>OFF</strong></td>
<td>Output for any previous command(s) for the same <strong>subrgn</strong> and type (<strong>BLOCK</strong> or <strong>TABLE</strong>) is subsequently suppressed.</td>
</tr>
</tbody>
</table>

**COMMENTS**

If no **SAVE** command is specified then a command is automatically invoked to produce output for active variables at the end of simulations. The active variables consist of all variables for which the equations are solved plus other variables that are of interest to the problem being solved. Successive commands may be used to accommodate changing output requirements.

Any modifiers or numerical input specified on an **SAVE** command without the **ADD** modifier stay active for all commands without the **ADD** modifier unless changed by a subsequent command. For example, any output frequency specified on one such command will stay in effect till it is replaced by new value on a subsequent command. The fmt, GEOM, COMP and DATA modifiers can only be specified before the actual writing of the file has started.

**EXAMPLES**

- **SAVE** every 20 steps
- **SAVE** U, V, W on file ‘DEMO.PLT’ in UNIFORMatted mode
- **SAVE** U, V, P IMMEDIATEly on file ‘PRESOLVE.SAV’
- **SAVE** U, V, P, K and L every 100 steps
- **SAVE** U, V, P, K and L every 100 steps by REPLacing old records
- **SAVE** U, V, P at TIME interval = 0.2 units
- **SAVE** U, T and K **NOW** and every 20 steps
- **SAVE** **ADD** output of GEOMETRY data to file ‘GEOM.SAV’
SAVE in COMPact form only on file 'VARIABLES.SAV'
SAVE in COMP form with DATA file 'DATAONLY.SAV'
SAVE in COMP only on file 'DATA.SAV' in SEQUential mode every 100 steps
SAVE OFF for all variables
SAVE TABLE of U, V, W on file 'TABLE.ARC'
SAVE U, V, P, K and L in TABLE format every 100 steps
SAVE in TABLE format at TIME interval of 1.25 years
SAVE in TABLE format at TIME interval of 1.25 years and REPLACE every time
SAVE TABLE of U, V, P for subregion on most recent LOCATE command
SAVE TABLE of T NOW at TIME interval of 20 years
SAVE OFF for TABLE option
SAVE TABLES SEQUentially every 100 steps on file 'SEQUENCE.TBL'
MODE 2: Output of Properties and Coefficients for the Differential Equations

SYNTAX

SAVE \{Φ\} \{(COND|DIFF|STOR|SOUR|MATR|RESI)\} [BLOC|TABL] [ADD] \{fname\} \{fmt\} \{GEOM|COMP|DATA|REPL|SEQU\} \{subrgn\} \{TIME\} \{Vfrq\} \{IMME|NOW|ONLY|OFF\}

Φ One, and only one, of the symbols that denotes the dependent variable for which a differential equation is solved. The valid symbols are listed in Table 2.7.1. There is no default value; a valid symbol must be specified.

COND The conduction or diffusion coefficient for the variable is printed to the output file. If the conduction or diffusion coefficient is a tensor, then the output is produced for each component of the tensor.

DIFF Same as COND.

STOR The storage coefficient for the variable is printed to the output file.

SOUR The net source (algebraic sum of source and sink) for the variable is printed to the output file.

MATR The matrix coefficients for the variable are printed to the output file. The coefficients are printed in the order of the forcing function (rhs of the matrix), the diagonal coefficient and the influence coefficients for each of the neighboring elements.

RESI The residue of the matrix equation or the governing differential equation is printed to the output device. If the output is requested at an intermediate stage of computation, then the matrix residue (B_j - A_ij X_i) is printed. If the output is requested at the final stage of computations, then the residue of the governing differential equation is printed.

BLOC See Mode 1 specification.

TABL See Mode 1 specification.

ADD This modifier is assumed by default. Each command in this mode, unless an OFF modifier is present, is treated as an additional command that adds to the active commands.

fname The file name to which the output is directed. Since the ADD modifier is assumed by default, the filename, if specified, is considered unique for the command and any subsequent SAVE command that specifies the same file name. By default, the output is directed to the same file that is used for Mode 1 output of SAVE commands without the ADD modifier. See Section 3.3 for additional information.

fmt See Mode 1 specification.

GEOM See Mode 1 specification.

COMP See Mode 1 specification.

DATA See Mode 1 specification.

REPL See Mode 1 specification.

SEQU See Mode 1 specification.

subrgn See Mode 1 specification.

TIME See Mode 1 specification.

Vfrq The frequency (step or time interval) at which the output is written to the output device. In this mode of the command, there is no default value. A value must be specified or the modifiers NOW or IMMEDIATE must be present for an output to be obtained. See COMMENTS below.

IMME The output is produced at the start of computations. In this mode of input, this modifier is equivalent to the NOW modifier because the coefficients and components of the transport equation are not available till the 1st SOLVE command is given and the computation process has started.

NOW See Mode 1 specification.

ONLY See Mode 1 specification.

OFF Output for any previous command(s) for the same subrgn, same type (BLOCK or TABLE).
and same combination of COND, DIFF, STOR, SOUR, MATR, and RESI modifiers is subsequently suppressed.

**COMMENTS**

This mode of the SAVE command provides the ability to monitor the coefficients and contribution of the various components of the transport equation. Any combination of the modifiers COND, DIFF, STOR, SOUR, MATR, and RESI may be specified. **At least one** of these must be specified to trigger this mode of the command.

This command mode triggers output for quantities which are computed (and needed) only during the solution of the equations. Most of these quantities are not allocated permanent storage but are computed on as needed basis. Therefore this output is possible only during the solution of the equation for the corresponding variable. **This command must therefore be given before the last SOLVE command.** Also a frequency (Vfrq with or without the ONLY modifier) or NOW modifier must be specified for the output to be generated.

Multiple commands may be used to obtain output for different variables. Output is generated after all the coefficients for the solution matrix have been computed. These commands essentially form a queue and are executed for each variable in order as the solution for that variable at the specified step is initiated.

**EXAMPLES**

SAVE: for U and P of DIFFusion coefficients at the final stage
SAVE: for T DIFFusion, coefficients NOW and the end to file = ‘DIFFUSION.T’
SAVE: for T STORage and MATRix coefficients NOW (at the next step)
SAVE: for T CONDuction, STORage, SOURce, MATRIx and RESIDUe at step number 52 ONLY
SAVE: for C: SOURce at step number every 52 steps
SAVE: in TABLE format of MATRIX for T and P at frequency of 75 steps
SAVE: of RESIdue for T at the end
MODE 3:  Output of Convective, Diffusive and Total Flux for each Element

SYNTAX  
SAVE  {Φ} {FLUX} {CONV} {DIFF} {TOTA} {AREA} {BLOC|TABL} {ADD} {fname} {fmt}  
{GEOM|COMP} {DATA} {REPL|SEQU} {subrgn} {TIME} [V_{frq}]  
{IMME|NOW|ONLY|OFF}

Φ  One, and only one, of the symbols that denotes the dependent variable for which a differential equation is solved. The valid symbols are listed in Table 2.7.1. There is no default value; a valid symbol must be specified.

FLUX  The total flux for each face of the elements of the computational domain is printed. The total flux is the sum of the convective and diffusive components.

CONV  The convective flux for each face of the elements of the computational domain is printed.

DIFF  The diffusive flux for each face of the elements of the computational domain is printed.

TOTA  The sum total of the convective and diffusive fluxes for each face of the elements of the computational domain is printed. This modifier is assumed by default if the CONV or DIFF modifiers are not present.

AREA  The computed flux is divided by the projected area of the face for output.

BLOC  See Mode 1 specification.

TABL  See Mode 1 specification.

ADD  This modifier is assumed by default. Each command in this mode, unless an OFF modifier is present, is treated as an additional command that adds to the active commands.

fname  The file name to which the output is directed. Since the ADD modifier is assumed by default, the filename, if specified, is considered unique for the command and any subsequent SAVE command that specifies the same file name. By default, the output is directed to the same file that is used for Mode 1 output of SAVE commands without the ADD modifier. See Section 3.3 for additional information.

fmt  See Mode 1 specification.

GEOM  See Mode 1 specification.

COMP  See Mode 1 specification.

DATA  See Mode 1 specification.

REPL  See Mode 1 specification.

SEQU  See Mode 1 specification.

subrgn  See Mode 1 specification.

TIME  See Mode 1 specification.

V_{frq}  The frequency (step or time interval) at which the output is written to the output device. In this mode of the command, there is no default value. A value must be specified or the modifiers NOW or IMMEDIATE must be present for an output to be obtained. See COMMENTS below.

IMME  The output is produced at the start of computations. In this mode of input, this modifier is equivalent to the NOW modifier because the coefficients and components of the transport equation are not available till the 1st SOLVE command is given and the computation process has started.

NOW  See Mode 1 specification.

ONLY  See Mode 1 specification.

OFF  Output for any previous command(s) for the same subrgn, same type (BLOCK or TABLE) and same combination of FLUX, CONV, DIFF and TOTAL modifiers is subsequently suppressed.
This mode of the SAVE command provides the output of the convective, diffusive and total fluxes at the faces of the elements. Any combination of the choice of fluxes may be specified. **At least one** of these must be specified to trigger this mode of the command.

This command mode triggers output for quantities which are computed (and needed) only during the solution of the equations. These quantities are not allocated permanent storage but are computed on as needed basis. Therefore this output is possible only during the solution of the equation for the corresponding variable. **This command must therefore be given before the last SOLVE command.** Also a frequency ($V_{frq}$ with or without the ONLY modifier) or NOW modifier must be specified for the output to be generated.

Multiple commands may be used to obtain output for different variables. Output is generated after all the fluxes required for solution of the transport equation have been computed. These commands essentially form a queue and are executed for each variable in order as the solution for that variable at the specified step is initiated.

**This mode of the SAVE command may be combined with Mode 2 of the command. That is, the modifiers of Mode 2 may be simultaneously specified with those of Mode 3 on the same command.** Also, if the output of both the diffusion coefficients and the diffusive fluxes is desired through such a single command, then the modifier DIFF must be specified twice or both the COND and DIFF modifiers must appear simultaneously on such a command.

**EXAMPLES**

SAVE: FLUX for T for each element at the final stage! Output to default Mode 1 file
SAVE: CONVective FLUX for T NOW (at the next step) to file ‘CFLUX.TMP’
SAVE: CONVective and DIFFusive FLUX for T at step number 50 ONLY on ‘CD_File.50’
SAVE: CONVective, DIFFusive and TOTAL FLUX divided by AREA for T every 50 steps
SAVE: FLUX divided by AREA for T at step# 52 ONLY for ID=SUBREGION
SAVE: in TABLE mode FLUX for T for ID=SUBREGION at end of simulations to ‘FLUX.TBL’
MODE 4: Output of Special Derived Flow Based Variables

SYNTAX
SAVE {(GRAD) [VORT] [STRUCTURE] [STRAIN] [STRESS] [LIGHTHILL]} {BLOC|TABL}
{[ADD] [fname] [fmt]} [GEOM] [COMP] [DATA] [REPL] [SEQU] [subrgn] [TIME] [Vfrq]
{[IMME|NOW|ONLY|OFF]}

GRAD
The tensor components of the gradients of velocity, $\varphi_{ij}$, are output, where:
$$\varphi_{ij} = \frac{\partial u_i}{\partial x_j}$$
Here $u_i$ is the $i^{th}$ component of velocity and $x_j$ is the $j^{th}$ coordinate. The gradient consists of 4 components for 2D and 9 for 3D.

VORT
Output of the components of vorticity vector, $\omega$, is obtained, where:
$$\omega_1 = \frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_3}; \quad \omega_2 = \frac{\partial u_1}{\partial x_3} - \frac{\partial u_3}{\partial x_1}; \quad \omega_3 = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}$$
There are 3 components of vorticity for 3D flow but only one for 2D flow.

STRUCTURE
Output of a “vorticity” structure variable, $\Omega$, is obtained. It is defined as:
$$\Omega = -\frac{\partial u_1}{\partial x_2} \frac{\partial u_2}{\partial x_1}$$
for 2D
$$\Omega = \frac{\partial u_1}{\partial x_2} \frac{\partial u_2}{\partial x_1} - \frac{\partial u_2}{\partial x_3} \frac{\partial u_3}{\partial x_2} - \frac{\partial u_3}{\partial x_1} \frac{\partial u_1}{\partial x_3}$$
for 3D

STRAIN
Output of the components of strain tensor, $S_{ij}$, is obtained, where:
$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$
There are 3 components for 2D and 6 for 3D flow.

STRESS
Output of the components of stress tensor, $\tau_{ij}$, is obtained, where:
$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \sum_k \frac{\partial u_k}{\partial x_k} \right) - \delta_{ij} \rho$$
Here $\mu$ is viscosity and $\rho$ is the pressure. There are 3 components for 2D and 6 for 3D flow.

LIGHTHILL
Output of the components of “lighthill” stress tensor, $L_{ij}$, is obtained, where:
$$L_{ij} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \sum_k \frac{\partial u_k}{\partial x_k} \right) + \rho u_i u_j$$
Here $\mu$ is the viscosity and $\rho$ is the density. There are 3 components for 2D and 6 for 3D flow.

BLOC
See Mode 1 specification.

TABL
See Mode 1 specification.

ADD
This modifier is assumed by default. Each command in this mode, unless an OFF modifier is present, is treated as an additional command that adds to the active commands.

fname
The file name to which the output is directed. Since the ADD modifier is assumed by default, the filename, if specified, is considered unique for the command and any subsequent SAVE command that specifies the same file name. By default, the output is directed to the same file that is used for Mode 1 output of SAVE commands without the ADD modifier. See Section 3.3 for additional information.

fmt
See Mode 1 specification.

GEOM
See Mode 1 specification.

COMP
See Mode 1 specification.

DATA
See Mode 1 specification.
Keyword Commands

REPL  See Mode 1 specification.
SEQU  See Mode 1 specification.
subrgn See Mode 1 specification.
TIME  See Mode 1 specification.
$\nu$ See Mode 1 specification.
IMME  See Mode 1 specification.
NOW  See Mode 1 specification.
ONLY  See Mode 1 specification.
OFF  Output for any previous command(s) for the same subrgn, same type (plane or TABLE) and same combination of GRAD, VORT, STRUCTURE, STRAIN, STRESS and LIGHTHILL modifiers is subsequently suppressed.

EXAMPLES

SAVE: VORTICITY and GRADients of velocity at the final stage to file ‘VORTGRAD.FIL’
SAVE: VORTICITY STRUCTure, STRESS and LIGHTHILL stress every 100 steps to ‘VFLOW.FIL’
SAVE: in TABLE mode VORTICITY STRUCTure, STRESS and LIGHTHILL every 100 steps
**MODE 5:** Output of Partitioning for Species Variables

**SYNTAX**

```
SAVE  {SECO} {PHAS} {Φ} [plane] [TABL] [ADD] [STAN] [fname] [subrgn] [STAT] [NOST] [NARR] [WIDE] [TIME] [Vfrq] [IMME] [NOW] [ONLY] [OFF]
```

**SECO**
The output for the inventory (amount in storage at an element) of a species in phases other than the primary phase is generated. The output is computed as:

\[ Q_{ΦS} = Q_Φ - Q_Ι \]

Here \( Q_{ΦS} \) is the inventory of property in an element in phases other than the primary phase, \( Q_Φ \) is the total inventory and \( Φ \) is the species concentration in the primary phase for the element.

**PHAS**
A companion modifier that must be present to invoke this mode of the command.

**Φ**
**One or more** of the symbols that represent the variables for which output is desired. The valid symbols are the species symbols listed in Table 2.7.1. This output can only be obtained for species variables for which a transport equation is solved. There is no default value; a valid symbol must be specified.

**plane**
See Mode 1 specification.

**TABL**
See Mode 1 specification.

**ADD**
**This modifier is assumed by default.** Each command in this mode, unless an **OFF** modifier is present, is treated as an additional command that adds to the active commands.

**STAN**
See Mode 1 specification.

**fname**
See Mode 2 specification.

**plane**
See Mode 1 specification.

**subrgn**
See Mode 1 specification.

**NARR**
See Mode 1 specification.

**WIDE**
See Mode 1 specification.

**TIME**
See Mode 1 specification.

**Vfrq**
See Mode 1 specification.

**IMME**
See Mode 1 specification.

**NOW**
See Mode 1 specification.

**ONLY**
See Mode 1 specification.

**OFF**
Output for any previous command(s) for the same **subrgn**, same type (**plane** or **TABLE**) and same combination variable is subsequently suppressed.

**COMMENTS**

This mode of the command is currently active only for the **PORFLOW™** Software Tool where some of the property may be present in secondary phases (solid and gas components of the porous matrix). The partitioning between different phases is specified by the **TRANSPORT, DISTRIBUTION** or **RETARDATION** commands.

The output from this mode of the command can be generated **only after** the start of the solution process. At the initial stage, before the solution process starts, the meaningful values of the inventory of variables may not be available. **This mode of the command operates independently of any other modes of the command and essentially adds to any other commands that are specified.**

**EXAMPLIES**

```
SAVE: SECOndary PHASe partitioning for variables C and C2.to file ‘SOLIDC.FIL’
SAVE: SECO PHAS for C and C2.to file ‘SOLIDC.FIL’ every 100 steps
```
MODE 6: Restart File for Later Continuation of Simulations

SYNTAX: SAVE (REST) [fname] [TIME] [Vfrq] [NOW]

REST A special file is generated to restart the computations at a later time. It is always in machine-specific "unformatted" mode. This file is generated in addition to other archive files that may be generated by other SAVE commands.

This file can be read only by a READ command with RESTART modifier to restart the computations for the same identical problem. Only the SOLVE command may be modified for the new simulations; all other input data must be identical to the run that generated the file. RESTART file should not be used to start a different problem or to restart the same problem with different input commands. In these latter cases, the required variables should be explicitly saved by Mode 1 of the SAVE command. If multiple commands are given, and a new file name is not specified, then any previous data on the file is replaced by the new data.

fname The name of the file to which the output is directed. See Section 3.3 for additional information. The default file name is the output file name (see OUTPUT Command) but with the extension "_RESTART.TMP" attached to the file name. For example if the standard output file name is "MYCASE" or "MYCASE.OUT", then the default file name will be "MYCASE_RESTART.TMP".

TIME By default, the Vfrq is interpreted to be the frequency in terms of number of steps. If this modifier is present, then Vfrq is interpreted to be time interval between successive outputs.

Vfrq The frequency (step or time interval) at which the restart file specified by 'fname' is written. See Section 3.7 for further details. If no value is specified and if NOW modifier is not present, then the output is obtained only at the end of simulations. If a value (> 0) is specified, then the file is written at the specified frequency and also at the end of simulations. The restart file always contains only one data record. The data on the file is replaced each time the file is written.

NOW A restart file is immediately written. If Vfrq modifier is not present, then the file is written only once, otherwise the file is replaced at the specified frequency.

EXAMPLES

SAVE REST
SAVE RESTART file! acr_RESTART.TMP file will be generated at end of simulations
SAVE RESTART file as ‘STAGE_1.FILE’! File STAGE_1.FILE will be generated at end of simulations
SAVE RESTART NOW! acr_RESTART.TMP file will be immediately generated.
SAVE RESTART every 10 steps on file named ‘REST.FIL’! Above command will generate REST.FIL every 10 steps and also at the end of simulations.
SAVE RESTART NOW and replace every 10 steps on file named ‘REST.FIL’! Above command will generate REST.FIL file immediately, and then replace it every 10 steps and also at the end of simulations.
**COMMAND**  SCALE

**PURPOSE**  To allow internal scaling of the specified input according to the equation:

\[ Q_{in} = a_1 \cdot Q + a_2 \]

where \( Q_{in} \) is the internal representation of a quantity, \( Q \) is the value specified by the user, and \( a_1 \) and \( a_2 \) are user-specified constants.

**SYNTAX**  SCAL \( \{N1\} \[N2\] \)

- **N1**  Multiplier, \( a_1 \), in the scaling equation automatically set to 1 at the end of each application. The default value is 1.
- **N2**  Addend, \( a_2 \), in the scaling equation automatically set to 0 at the end of each application. The default value is 0.

**COMMENTS**

This command must be used immediately before the command that contains the data to be scaled. It can be used for internal scaling in conjunction with some of the modes of the COORDINATE, LOCATE, SET and SOURCE commands. See those commands for further details.

**EXAMPLES**

SCALe multiply by 3.3 and add 10.
SCALe multiply by 0.3048
**COMMAND**

**SCHMIDT NUMBER**

**PURPOSE**

To specify the Schmidt number for the fluid. This command is effective only for the **ANSWER™** Software Tool.

**SYNTAX**

SCHM [EFFE] [Φ = V1, Φ = V2, ..., Φ = Vn]

**EFFE**

If the modifier **EFFECTIVE** is present then the input is assumed to be for the effective Schmidt number; otherwise it is assumed to be the molecular Schmidt number for the fluid.

**Φ**

One or more symbols to denote the variables for which the Schmidt numbers are specified. The valid symbols are those listed in Table 2.7.1 with the exception of the U, V, W and P. If no symbol is specified, then the input is assumed to be for the first mass transfer variable in the system of equations.

**V1, ..., Vn**

Schmidt numbers for the dependent variables denoted by the symbol immediately preceding the value. The numerical value must be greater than 0. The default value is 0.7.

**COMMENTS**

This input is only effective for the **ANSWER™** Software Tool.

**EXAMPLES**

SCHM idt number for fluid = 1.
SCHM idt number for FF = 0.5, FU = 0.7, CH = 0.7
SCHM idt number EFFEctive value for FF = 0.5
ACRi™ Software Tools  Keyword Commands

COMMAND      SCREEN

PURPOSE      To control the echo of diagnostic output obtained from the DIAGNOSTIC command to the CRT device.

SYNTAX       SCRE [OFF | ON] [WIDE]

OFF          The diagnostic output to the CRT device is turned off.

ON           The diagnostic output to the CRT device is turned on. This is the default option. This option may also be used to turn on the CRT output, which was previously turned off.

WIDE         By default a maximum of 5 selected diagnostic variables (DIAGNOSTIC command) are echoed to the CRT device. If this modifier is present, then the maximum is set to 9.

COMMENTS

This command allows the user to monitor progress of the numerical simulation on the CRT device. It does not affect the diagnostic output to the standard output device.

EXAMPLES

SCREen echo for diagnostic output to be turned OFF
SCREen ON! This is the default option
SCREen in WIDE format
SCREen ON in WIDE format! Turn on previously off screen output
<table>
<thead>
<tr>
<th>COMMAND</th>
<th>SELECT</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To locate and identify a subregion or material type in the domain of computation for later input by one of the other commands.</td>
</tr>
</tbody>
</table>

**COMMENTS**

This command is identical in all respects to the **LOCATE** command.

**EXAMPLES**

See **LOCATE** command
COMMAND: SET

PURPOSE: To set the value of a field variable as a function of space, time or other variables.

MODE 1: Specification of Field Variable

SYNTAX: 

```
SET {Φ} [func[ξ]] {N₁, N₂, ..., Nₙ} [fname] [operation] [mod] [ALWA] [subrgn] [STAC]
```

Φ: One, and only one, symbol that denotes the variable for which the values are specified. The valid symbols include those listed in Table 2.8.1-3 plus the user defined variables (ALLOCATE command) and the real type variables defined in the initialization file (xxxINIT.ACR). There is no default value; a symbol must be specified.

func: One of the modifiers listed in Table 4.2.1, which denotes the functional form of the dependent variable. If no function is specified, the value is assumed to be constant.

ξ: One of the independent variables listed in Table 4.2.2. If no variable is specified, the independent variable is assumed to be time.

N₁,...,Nₙ: The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname: The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

operation: Available modifiers are REPLACE, ADD, SUBTRACT, MULTIPLY, DIVIDE, ABS, ABSOLUTE, POSITIVE and NEGATIVE. See Section 4.3 for further details.

ALWA: By default the SET command is implemented immediately and only once – as soon as the command is encountered. If this modifier is present then the command is executed immediately as well as repeatedly at the beginning of each time step (or iterative step in steady state mode) of the solution procedure.

subrgn: The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected. Subregion may be specified with the FIEL or dir modifiers. See Section 3.4 for further details.

STAC: By default Φ is computed from the value of ξ at the same location. If this modifier is present, then Φ is computed from ξ at a location previously specified by the STACK LOCATE command.

COMMENTS:

The primary purpose of the SET command is to specify the value of a dependent variable. Combinations of ALLOCATE and SET commands can be used to define complex multi-variate functions by specifying the appropriate operation to be performed during each intervening step.

If the subrgn is specified with a dir modifier (see Section 3.4) then the SET command may be effectively used as an alternative to the BOUNDARY command.

EXAMPLES:

Generic examples for this command are given in Section 4.4. The keyword SET must replace the keyword used in these examples.

SYNTAX

\[
\text{SET } \{ \Phi \} \{ \text{NODE} | \text{STRU} | \text{UNST} | \text{fname} \} \{ V_1, \ldots, V_m \} \{ \text{subrgn} \}
\]

**Φ**

A symbol to denote the variable for which the values are specified. The valid symbols include those listed in Table 2.8.1-3 plus the supplementary integer or real type field variables that are defined in the initialization file (xxxINIT.ACR). A symbol must be specified.

**NODE**

The input is specified in a node-by-node manner. By default if is assumed that the input values are given in the **STRUCTURED** mode if the **subrgn** was defined with a **LOCATE** command in terms of grid indices or in the **UNSTRUCTURED** mode otherwise.

**STRU**

The input is read in the manner of nested implied FORTRAN DO loops:

\[
\text{Read (NUNIT, *) } (((\text{VAR (I, J, K), I = ILO, IHI), J = JLO, JHI, K = KLO, KHI})
\]

Where **NUNIT** is an internally assigned unit number, **VAR** is the variable denoted by **Φ**, and **ILO, IHI, JLO, JHI, KLO, KHI** define, respectively, the starting and ending grid index values for the **subrgn** for a structured grid. For 2D grid, **KLO** and **KHI** are set to unity.

**UNST**

The input is read in the manner of a simple implied FORTRAN DO loop:

\[
\text{Read (NUNIT, *) (VAR (M), M = MLO, MHI)}
\]

Where **NUNIT** is an internally assigned unit number, **VAR** is the variable denoted by **Φ**, and **MLO and MHI** are the starting and ending element numbers for the **subrgn**. The order of the elements is the same as the one specified (or implied) by the corresponding **LOCATE** command which can be examined by including a file name on the **LOCATE** command.

**fname**

The name of the file for numerical values unless the values are directly specified by **V_1, \ldots, V_m** below. See Section 3.3 for additional information.

**V_1, \ldots, V_m**

The values of the variable at each node selected by the **subrgn** and **dir** modifiers. These values must be present unless **fname** is present. In this case, one of the modifiers, **NODE, STRU, or UNST** must also be specified.

**subrgn**

The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected. This input is ignored for the supplementary variables. For these, the number of values specified on the file must match the total number of elements in the selected variable.

**FIEL**

See Mode 1 specification.

**dir**

See Mode 1 specification.

**COMMENTS**

It is highly recommended that the user examine the input data (for example by running the data set with **SOLVE OFF** command) to make sure that the input has been properly interpreted.

**EXAMPLES**

- **SET T** from file ‘ALLVAL’ input for the entire domain of computation
- **SET T** for SELected region from ‘ACTIVAL’ input for active subregion
- **SET T** in ID=RGN1 region ‘RGN1VAL’ input for identified subregion
- **SET FC** – a supplementary flux variable for the entire field from file: ‘VALUES.FC’
- **SET MTYP** – a supplementary material type index (integer) for the entire field from file: ‘VALUES.IZ’
MODE 3: Specification of a Variable on a Node by Node Basis as a Function of Time

SYNTAX

```
SET {Φ} {NODE|STRU|UNST} {TIME} fname} [LINE|STEP] [subrgn] [FIEL] [dir]
```

Φ — A symbol to denote the variable for which the values are specified. The valid symbols include those listed in Table 2.8.1 plus the supplementary integer or real type field variables that are defined in the initialization file (xxxINIT.ACR). A symbol must be specified.

NODE — The input is specified in a node-by-node manner. By default if is assumed that the input values are given in the STRUCTURED mode if the subrgn was defined with a LOCATE command in terms of grid indices or in the UNSTRUCTURED mode otherwise.

STRU — The input is read in the manner of nested implied FORTRAN DO loops:

```
Read (NUNIT, *) (((VAR (I, J, K), I = ILO, IHI), J = JLO, JHI), K = KLO, KHI)
```

Where NUNIT is an internally assigned unit number, VAR is the variable denoted by Φ, and ILO, IHI, JLO, JHI, KLO, KHI define, respectively, the starting and ending grid index values for the subrgn for a structured grid. For 2D grid, KLO and KHI are set to unity.

UNST — The input is read in the manner of a simple implied FORTRAN DO loop:

```
Read (NUNIT, *) (VAR (M), M = MLO, MHI)
```

Where NUNIT is an internally assigned unit number, VAR is the variable denoted by Φ, and MLO and MIHI are the starting and ending element numbers for the subrgn. The order of the elements is the same as the one specified (or implied) by the corresponding LOCATE command which can be examined by including a file name on the LOCATE command.

fname — The name of the file for numerical values. See Section A.1.1 for file format. A file name must be specified; the input cannot be read directly from the command. The number of values for each record at each time step must equal the number of elements for the subdomain; any extra values present in the record are ignored.

LINE — The time step interpolation is linear; this is the default option.

STEP — The time step interpolation is step function (Equation 4.1.4).

subrgn — The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected. This input is ignored for the supplementary variables. For these, the number of values specified on the file must match the total number of elements in the selected variable.

FIEL — See Mode 1 specification.

dir — See Mode 1 specification.

COMMENTS

It is highly recommended that the user examine the input data (for example by running the data set with SOLVE OFF command) to make sure that the input has been properly interpreted.

EXAMPLES

```
SET T from file ‘ALLVAL’ input for the entire domain of computation
SET T for SELECTed region from ‘ACTIVAL’ input for active subregion
SET T in ID=RGN1 region ‘RGN1VAL’ input for identified subregion
SET FC – a supplementary flux variable for the entire field from file: ‘VALUES.FC’
SET MTYP – a supplementary material type index (integer) for the entire field from file: ‘VALUES.IZ’
```
MODE 4: Specification of Multiple Variables on a Node-by-Node Basis from a Table

SYNTAX

\[ \text{SET} \ \{ \Phi_1, \ldots, \Phi_n \} \ \{(\text{MODE}|\text{STRU}|\text{UNST}) \ | \text{fname}\} \ \{V_1,\ldots,V_{nm}\} \ \{\text{subrgn}\} \ \{\text{FIEL}\} \ \{\text{dir}\} \]

\(\Phi_1, \ldots, \Phi_n\) Symbols to denote the variables that are to be set by the command. The symbols include all those listed in Table 2.8.1-3 plus the user defined variables (ALLOCATE command) and the real type variables defined in the initialization file. In addition a special symbol “SKIP” can be specified to by-pass the input of any of the columns. Any symbol may occur multiple times. There is no default value appropriate symbols must be specified.

\text{NODE} The \(\Phi\) variables are set individually for each of the nodes of a subregion. It is assumed that the input is in a tabular format with \(n\) columns (1 for each variable) and \(m\) rows (1 for each node of the subregion). By default if is assumed that the input values are given in the STRUCTURED mode if the subrgn was defined with a LOCATE command in terms of grid indices or in the UNSTRUCTURED mode otherwise.

\text{STRU} The input is read in the manner of nested implied FORTRAN DO loops:

\[
\text{Read} (\text{NUNIT, } \*) (((\text{VAR} (L, I, J, K), L=1,n), I=ILO, IHI), J=JLO, JHI), K=KLO, KHI)
\]

Where \text{NUNIT} is an internally assigned unit number, \text{VAR} is the set of variables denoted by \(\Phi\)’s, \(n\) denotes the number of variables, and \(ILO, IHI, JLO, JHI, KLO, KHI\) define, respectively, the starting and ending grid index values for the \text{subrgn} for a structured grid. For 2D grid, \(KLO\) and \(KHI\) are set to unity.

\text{UNST} The input is read in the manner of a simple implied FORTRAN DO loop:

\[
\text{Read} (\text{NUNIT, } \*) (\text{VAR} (L, M), L=1,n), M = MLO, MHI)
\]

Where \text{NUNIT} is an internally assigned unit number, \text{VAR} is the set of variables denoted by \(\Phi\)’s, \(n\) denotes the number of variables, and \(MLO\) and \(MIHI\) are the starting and ending element numbers for the \text{subrgn}. The order of the elements is the same as the one specified (or implied) by the corresponding LOCATE command which can be examined by including a file name on the LOCATE command.

\text{fname} The name of the file (see Section 3.3) from which \(V_1\) through \(V_{nm}\) are read.

\(V_1,\ldots,V_{nm}\) The table of values that pertains to the variable values at each node selected by the \text{subrgn} and \text{dir} modifiers. If \(n\) symbols are specified on the command and there are \(m\) nodes in the subregion, then \(n\) times \(m\) values must be specified in \(n\) columns and \(m\) rows.

\text{subrgn} See Mode 1 specification.

\text{FIEL} See Mode 1 specification.

\text{dir} See Mode 1 specification.

EXAMPLES

\text{SET} by \text{NODE} following variables for ID=SUBRGN1! There are 3 nodes in this region)

\[
\begin{align*}
U & \quad V & \quad T \\
10 & \quad -5 & \quad 100 \\
-10 & \quad +5 & \quad 150 \\
-10 & \quad +10 & \quad 200
\end{align*}
\]

\text{SET} by \text{NODE} following variables for ID=SUBRGN1! There are 3 nodes in this region)

\[
\begin{align*}
\text{SKIP} & \quad \text{SKIP} & \quad U & \quad V & \quad \text{SKIP} & \quad T \\
0.2 & \quad 0.2 & \quad 10 & \quad -5 & \quad 10.20 & \quad 100 \\
3.5 & \quad 0.6 & \quad -10 & \quad +5 & \quad 12.50 & \quad 150 \\
10 & \quad 1.0 & \quad -10 & \quad +10 & \quad 2.00 & \quad 200
\end{align*}
\]

\text{SET} by \text{NODE} for ID=MIDDLE at X-boundary! 3 boundary nodes

\[
\begin{align*}
(\text{SKIP}, \text{SKIP}, \text{SKIP}) & \quad U & \quad V & \quad T \\
(0.2, 0.2, 0.2) & \quad 10 & \quad -5 & \quad 100 \\
(3.5, 0.6, 1.0) & \quad -10 & \quad +5 & \quad 150 \\
(10., 1.0, 2.0) & \quad -10 & \quad +10 & \quad 200
\end{align*}
\]

\text{SET} by \text{NODE} ID=MIDDLE T, U, V \text{SKIP} from file ‘SPATIAL’! File with 4 x #of nodes values
MODE 5: Specification of a Variable as a Linear Sum of other Variables

SYNTAX

SET \{ \Phi \} \{ SUM|LINE | MASS \} \{ \xi_1, \ldots, \xi_n \} \{ a_1, \ldots, a_n \} \{ a_0 \} \{ option \} \{ mod \} \{ ALWA \} \{ subrgn \} \{ FIEL \}

\Phi 

See Mode 1 specification.

SUM

The variable \( \Phi \) is computed from:

\[ \Phi = \sum \xi_n \]

LINE

The variable \( \Phi \) is computed from:

\[ \Phi = \sum a_n \xi_n + a_0 \]

MASS

By default, the \( \xi \)'s (see definition below) on the right hand side of the defining equation are assumed to be the field variables. If this modifier is present, then \( \xi \)'s are replaced by the total mass of the corresponding \( \xi \) variable. The total mass is equal to the quantity that appears in the accumulation term of the governing differential equation for \( \xi \) (see Chapter 2) multiplied by the volume of the element. In the presence of this modifier only those \( \xi \)'s can appear on the right hand side for which differential equations are solved.

\( \xi_1, \ldots, \xi_n \)

Symbols to denote the variables, or their masses, which contribute to the linear sum as in the above equation. The valid symbols include those listed in Table 2.8.1-3 plus the variables defined by the user (ALLOCATE command) or the real type variables defined in the initialization file (xxxINIT.ACR). There is no default value; appropriate symbols must be specified. No more than 10 symbols can be specified.

\( a_1, \ldots, a_n \)

The numerical constants and coefficients for the linear function. These values must be specified if the LINEAR modifier is present. With the SUM modifier these values must not be specified. There is no default value; appropriate number of values must be specified.

\( a_0 \)

The datum for the linear function if LINEAR modifier is specified. The default value is 0.

option

See Mode 1 specification.

mod

See Mode 1 specification.

ALWA

See Mode 1 specification.

subrgn

See Mode 1 specification.

FIEL

See Mode 1 specification.

EXAMPLES

SET T as SUM of X + Y + U
SET T as SUM of X + Y + U ALWAYS for ID=T1DOMAIN
SET T as LINEAR function 1. * X + 2. * Y -0.5 * U + 5. ALWAYS for ID=T1DOMAIN
MODE 6: Specification of a Variable as a Square or Square Root Sum of other Variables

SYNTAX

SET \{ \Phi \} \{ \text{SQUA|ROOT} \} \{ \xi_1, \ldots, \xi_n \} \{ a_1, \ldots, a_n \} \{ a_0 \} \{ \text{option} \} \{ \text{mod} \} \{ \text{ALWA} \} \{ \text{subrgn} \} \{ \text{FIEL} \}

\Phi 
See Mode 1 specification.

SQUA
The variable \( \Phi \) is computed from:

\[
\Phi = \sum_n \xi_n^2 \quad \text{or} \quad \Phi = \sum_n a_n \xi_n^2 + a_0
\]

ROOT
The variable \( \Phi \) is computed from:

\[
\Phi = \sqrt{\sum_n \xi_n^2} \quad \text{or} \quad \Phi = \sqrt{\max\left( \sum_n a_n \xi_n^2 + a_0 \right), 0}
\]

\( \xi_1, \ldots, \xi_n \)
Symbols to denote the variables that contribute to the linear sum as in the above equation. The valid symbols include those listed in Table 2.8.1-3 plus the variables defined by the user (ALLOCATE command) or the real type variables defined in the initialization file (xxxINIT.ACR). There is no default value; appropriate symbols must be specified. No more than 10 symbols can be specified.

\( a_1, \ldots, a_n \)
The numerical constants and coefficients for the function. Either all coefficients must be omitted (in which case the function without coefficients is used) or all must be specified.

\( a_0 \)
The datum for the function. The default value is 0.

option
See Mode 1 specification.

mod
See Mode 1 specification.

ALWA
See Mode 1 specification.

subrgn
See Mode 1 specification.

FIEL
See Mode 1 specification.

EXAMPLES

SET T as SQUARE sum of X, Y and Z

SET T as ROOT of sum of SQUAREs of X, Y and U ALWAYS for ID=T1DOMAIN

SET T as SQUARE sum of 1.* X -1.* Y and 5.* Z

SET T as ROOT of sum of SQUAREs of 1.* X, 2.* Y and 3.* U + 4. ALWAYS for ID=T1DOMAIN
MODE 7: Specification of Variables as Distance-based Interpolated Function from a Table

SYNTAX
SET {DIST} [LINE|SQUA|CUBE|FOUR|EIGH} {Φ₁, ..., Φₙ} {Nsets} {V₁,...,Vₘ|fname} 
[DOMA=V_domain|NEAR=V_near] [option] [mod] [ALWA] [subrgn] [FIEL]

DIST
The Φₙ variables are computed from an inverse distance based interpolation function (here ξᵢ is the iᵗʰ value in the specified table for the corresponding variable, xₖ,i are its coordinates and N is the power to which the distance is raised):

\[ Φ = \sum \frac{ξᵢ}{rᵢ^N} \; ; \; rᵢ^2 = \sum (x_k - xₖ,i)^2 \]

LINE
The inverse distance based interpolation is used (N=1).

SQUA
The inverse distance squared interpolation is used (N=2). This is the default option.

CUBE
Interpolation is based on distance raised to the 3ʳᵈ power (N=3).

FOUR
Interpolation is based on distance raised to the 4ᵗʰ power (N=4).

EIGH
Interpolation is based on distance raised to the 8ᵗʰ power (N=8).

Φ₁, ..., Φₙ
Symbols to denote the variables that are to be computed from the distance-based interpolation. There is no default value; appropriate symbols must be specified. No more than 7 symbols can be specified.

Nsets
The number of sets of values in the table. Each set must consist of (x, y; for 2D) or (x, y, z; for 3D) and as many values as the symbols specified above. There is no default value.

V₁,...Vₘ
The table of values that pertains to the coordinates of the locations and the variable values at those locations. If the table is viewed to consist of a n number of columns and rows, then each row must contain, in order, (x, y; for 2D) or (x, y, z; for 3D) and n values for Φ₁ through Φₙ. The number of rows of the table must equal Nsets.

fname
The name of the file (see Section 3.3) from which V₁,...,Vₘ are read.

DOMA
The interpolation is restricted to the specified ξᵢ that lie within the distance specified by V_domain. In the formula above any values where rᵢ > V_domain are excluded from the formula. If no values within the specified domain are found, then the nearest value is selected.

V_domain
The maximum distance that specifies the extent of the domain of influence in the interpolation formula. V_domain must be the last numerical value on the command.

NEAR
The interpolation is restricted to the nearest V_near number of ξᵢ determined by rᵢ. If this modifier is present and V_near is omitted or is < 1, then the nearest specified ξᵢ is selected.

V_near
The number of nearest values to be included in the above interpolation formula. Default value is 1. V_near must be the last numerical value on the command.

option
See Mode 1 specification.

mod
See Mode 1 specification.

ALWA
See Mode 1 specification.

subrgn
See Mode 1 specification.

FIEL
See Mode 1 specification.

EXAMPLES

SET by DISTANCE interpolation from specified values at 3 stations (Two-dimensional)
(X, Y) U V T
(0.2, 0.2)  10  -5  100
(3.5, 0.6) -10  +5  150
(10, 1.0)  -10  +10 200

SET by LINEAR DISTANCE interpolation for ID=MIDDLE from values at 3 stations (Three-dimensional)
(X, Y, Z) U V T
(0.2, 0.2, 0.2) 10  -5  100
SET by DISTANCE interpolation for ID=MIDDLE from values at 3 stations (Three-dimensional)

\begin{align*}
(3.5, 0.6, 1.0) & \quad -10 & +5 & 150 \\
(10, 1.0, 2.0) & \quad -10 & +10 & 200
\end{align*}

\begin{itemize}
\setlength\itemsep{0em}
\item \(X, Y, Z\) \quad U \quad V \quad T
\item (0.2, 0.2, 0.2) \quad -10 & -5 & 100
\item (3.5, 0.6, 1.0) \quad -10 & +5 & 150
\item (10, 1.0, 2.0) \quad -10 & +10 & 200 \quad \text{DOMAIN of influence=0.5}
\end{itemize}

SET by DISTANCE interpolation for ID=MIDDLE from 5 values

\begin{align*}
(3.5, 0.6, 1.0) & \quad -10 & +5 & 150 \\
(10, 1.0, 2.0) & \quad -10 & +10 & 200
\end{align*}

\begin{itemize}
\setlength\itemsep{0em}
\item \(X, Y, Z\) \quad U \quad V \quad T
\item (0.2, 0.2, 0.2) \quad 10 & -5 & 100
\item (3.5, 0.6, 1.0) \quad -10 & +5 & 150
\item (10, 1.0, 2.0) \quad -15 & +10 & 200
\item (10, 2.0, 2.0) \quad -20 & +15 & 250
\item (10, 5.0, 2.0) \quad -10 & +10 & 300 \quad \text{interpolate from NEAREST 3}
\end{itemize}

SET by DISTANCE interpolation for ID=MIDDLE from 5 sets for U V T on file='INTER.FIL', NEAR=3

SET by DISTANCE ID=MIDDLE 3 sets of U V T file 'SPATIAL' \text{ ALWAYS ADD POSITIVE} to existing
MODE 8: Specification of Values from Total Inventory

SYNTAX

SET \{ \Phi \} \{ \text{INVENT} \} \{ \text{subrgn} \} \{ Q \} \{ \text{VOLU} \} \{ \text{UNIF} \} \{ \text{SCAL} \} \{ \text{ADD} \}

\Phi

A symbol that denotes the variable for which the values are specified. This input mode can only be used for the mass species and heat transfer variables for which a differential equation is solved. The valid symbols include those listed in Table 2.7.1, except the pressure variables, plus the user defined variables (ALLOCATE command) for which a differential equations a solved. There is no default value; a symbol must be specified.

INVENT

The total inventory or amount of the property, \( \Phi \), is specified. The inventory, \( Q \), for a subregion is defined as:

\[
Q = \sum_{\text{subrgn}} \alpha_i \Phi_i \delta V_i
\]

Here \( Q \) the subscript “i” denotes the values for an element, \( \alpha \) is the accumulation coefficient for the transport equation, and \( \delta V \) is the volume of the element. The summation is taken over all elements of the subregion.

subrgn

The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected.

Q

The specified inventory (> 0) of the property, \( \Phi \).

VOLU

The inventory is distributed so that the amount added to each element is proportional to the volume of the element. This is the default option. The new value is computed as:

\[
\Phi_i = \theta \Phi_i^0 + \frac{1}{\alpha_i} \frac{Q}{\sum_{\text{subrgn}} \delta V_i}
\]

Here \( \Phi_i^0 \) is the existing value of variable, and \( \theta = 0 \) by default but is set to 1 if modifier \text{ADD} \ is present.

UNIF

The inventory is distributed so that the increment in \( \Phi \) is uniform and constant:

\[
\Phi_i = \theta \Phi_i^0 + \frac{Q}{\sum_{\text{subrgn}} \alpha_i \delta V_i}
\]

SCAL

The inventory is distributed proportional to the existing value of \( \Phi \):

\[
\Phi_i = \theta \Phi_i^0 + \frac{Q \Phi_i^0}{\sum_{\text{subrgn}} \alpha_i \Phi_i^0 \delta V_i}
\]

Since the old value of \( \Phi \) appears in the denominator, this modifier should be used only if the variable is positive definite; that is all values are greater than zero.

ADD

By default the specified inventory replaces any existing value; that is the constant \( \theta = 0 \) in the above equation. If this modifier is present, then the inventory is added to the existing value; that is \( \theta = 1 \).

COMMENTS

This command can be used to set the values only in the interior elements of the computational domain. The external boundary nodes are excluded. If this command is used in the middle of a solution in progress, it net effect is to inject (or withdraw, if replaced amount is greater than the existing amount) property into the domain. The balance for the property will then show a net flux disparity.

EXAMPLES

SET INVENTORY of mass species \( C \) to 10 kg
SET INVENTORY of FF to 10 kg; distribute UNIFORMly over SELECTed region
SET T INVENTORY in ID=RGN1 is 1.E6 units; SCALE with existing value
MODE 9: Transfer of Inventory From One Subregion to Another

SYNTAX

SET \{Φ\} \{INVE\} \{ID=subrgn1\} \{ID=subrgn2\} \{VOLU\} \{UNIF\} \{SCAL\} \{β\} \{FRAC\} \{TIME\} \{ALWA\} \{OFF\}

Φ

A symbol that denotes the variable for which the values are specified. This input mode can only be used for the mass species and heat transfer variables for which a differential equation is solved. The valid symbols include those listed in Table 2.7.1, except the pressure variables, plus the user defined variables (ALLOCATE command) for which a differential equation is solved. There is no default value; a symbol must be specified.

INVE

The inventory of the property is transferred from a donor to a receptor region. See the previous mode of the command for a more complete definition.

ID=subrgn1

The donor region from which the inventory is transferred to the receptor region. There is no default value. A valid subregion name with an ID modifier must be specified. The total amount of inventory, Q, which is transferred from the donor region, is computed as:

\[ Q = \lambda \sum_{i=Donor}^{s} \alpha_i \Phi_i^o \delta V_i \]

Here superscript ‘o’ denotes the existing value of the variable Φ, subscript ‘i’ denotes the value for an element, α is the accumulation coefficient for the transport equation, δV is the volume of the element, and λ is a constant. The summation is taken over all elements of the donor subregion. The constant, λ, is determined as follows:

\[ \lambda = 1 \text{ by default if } \beta \text{ is not specified.} \]

\[ \lambda = \min(\beta, 1) \text{ if } \beta \text{ is specified but } \text{TIME is not specified} \]

\[ \lambda = \min(\beta \delta t, 1) \text{ where } \delta t \text{ is the time step if } \beta \text{ and } \text{TIME are specified} \]

Values of the variable for all elements in the donor region are decreased to preserve mass balance for the variable. The modified value, i.e. the remaining property, for element ‘i’ is computed as:

\[ \Phi_i = (1-\lambda) \Phi_i^o \]

ID=subrgn2

The receptor region to which the inventory is transferred. There is no default value. A valid subregion name with an ID modifier must be specified.

VOLU

The donor inventory is distributed so that the amount added to each receptor element is proportional to the volume of the element. This is the default option. The new value is computed as

\[ \Phi_i = \Phi_i^o + \frac{1}{\alpha_i} \frac{Q}{\sum_{i=Receptor}^{s} \delta V_i} \]

UNIF

The inventory is distributed so that the increment in Φ is uniform and constant:

\[ \Phi_i = \Phi_i^o + \frac{Q}{\sum_{i=Receptor}^{s} \alpha_i \delta V_i} \]

SCAL

The inventory is distributed proportional to the existing value of Φ:

\[ \Phi_i = \Phi_i^o + \frac{Q \Phi_i^o}{\sum_{i=Receptor}^{s} \alpha_i \delta V_i} \]

Since the old value of Φ appears in the denominator, this modifier should be used only if the variable is positive definite; that is all values are greater than zero.
\( \beta \) is a constant \(( \beta \geq 0 \)\) that determines how much of the current inventory is transferred from the donor to the receptor region. The specified value must not be negative. If no value is specified, then the total amount is transferred.

**FRAC**\( \beta \) specifies the fraction of the current inventory in the donor region that is transferred. Limits are imposed so that \((0 \leq \beta \leq 1)\); that is the minimum transferred amount is zero and the maximum is equal to the total amount in the donor region at any time. This is the default interpretation of \( \beta \).

**TIME**\( \beta \) specifies the fraction per unit time of the current inventory that is transferred. The actual fraction transferred is equal to \( \beta \delta t \) where \( \delta t \) is the time step. Limits are imposed dynamically so that \((0 \leq \beta \delta t \leq 1)\).

**ALWA** By default, the specified amount is transferred only once, that is, the first time the command is encountered. If the **TIME** modifier is present then the specified amount is transferred at each step starting with the first time the command is encountered.

**OFF** If this modifier is present then any previous **SET INVE** command that was specified by the **ALWAYS** modifier for the same \( \Phi \), and the same donor and receptor subregions is disabled.

**COMMENTS**

Inventory can be transferred only between interior elements of the computational domain. The external boundary nodes are excluded. Since the command essentially transfers the property from one region to another, there is no net effect on the total amount of property in the domain. If total inventory is transferred from one region to another, then the variable in the donor region will instantaneously fall to zero.

This command can be used, for example, to approximate the transfer of a contaminant from an originally un-collapsed containment area (such as a vault) to a smaller area after collapse without revising the mesh. It provides an approximate method of simulating the settling of a contaminated region without having to deal with the additional complexity of the physics of consolidation.

Another example of its use is that of leakage of a contaminant from one region to another through a structure (such as a duct or pipe) that is not explicitly modeled by the grid but the leakage rate is determined from other considerations.

**EXAMPLES**

- **SET INVE**ntory of C from ID=DONOR to ID=RECEPTOR! Total amount transferred
- **SET INVE**ntory of C from ID=DONOR to ID=RECEPTOR **FRAC**tion=0.5| 50% transferred
- **SET INVE**ntory of C from ID=DONOR to ID=RECEPTOR 0.1 **TIME** ALWAYS| 0.1*dt every time step
- **SET INVE**ntory of C from ID=DONOR to ID=RECEPTOR OFF| previous command off
MODE 10: Computation of Gradient of a Variable

SYNTAX

```
SET {GRAD} {Ψ} {Φ} {ξ} [fnc] [BLOC] [FIEL] [ALWA|OFF]
```

**GRAD**
The Gradient of the specified variable is computed as:

\[
\Psi = \frac{\partial \Phi}{\partial \xi} \quad \text{or} \quad \Psi = \text{function}\left(\frac{\partial \Phi}{\partial \xi}\right)
\]

The function, if any, is defined by the fnc modifier as given below.

**Ψ**
The symbol for the variable where the computed gradient values are stored. This must be a valid symbol for one of the default field variables of ACRi Software or it must be allocated through the ALLOCATE command.

**Φ**
Symbol for one of the previously defined field variables listed in Table 2.7.1. There is no default value; a variable must be specified.

**ξ**
One of the symbols: X, Y, r or Z that denotes the coordinate with respect to which the gradient is computed. The symbol r can only be used if the specified coordinate system is cylindrical. There is no default value; a value must be specified.

**fnc**
The modifier for function evaluation

<table>
<thead>
<tr>
<th>fnc</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABS or ABSO</td>
<td>The absolute value for the computed gradient is taken.</td>
</tr>
<tr>
<td>POSI</td>
<td>The negative values for the computed gradient are set to zero</td>
</tr>
<tr>
<td>NEGA</td>
<td>The positive values for the computed gradient are set to zero</td>
</tr>
<tr>
<td>SQUA</td>
<td>The function is computed as the square of the gradient</td>
</tr>
<tr>
<td>ROOT</td>
<td>The function is computed as the square root of the gradient; negative values are set to 0.</td>
</tr>
</tbody>
</table>

**BLOC**
If this modifier is present then the value of the gradient at the blocked nodes see (BLOC command) is set to zero. Otherwise the computed value is retained.

**FIEL**
By default the gradient is computed throughout the computational domain including the field and the boundary nodes. If this modifier is present, then only the field values are computed.

**ALWA**
By default the SET command is implemented immediately and only once – as soon as the command is encountered. If this modifier is present then the command is implemented immediately as well as repeatedly at the beginning of every time step (or iterative step in steady state mode) of the solution procedure.

**OFF**
Any previous SET command with GRAD modifier for the specified variable is deactivated.

**EXAMPLES**

```
SET DTDX = GRAD of T with respect to X
SET DTDR = ABSOLUTE value of GRAD of T with respect to R compute ALWAYs
SET PHIR = GRAD of T with respect to R only once
SET DTDY = GRAD of T with respect to Y for FIELD nodes only with BLOC value set to zero
SET DTDY = POSITIVE values of GRAD of T with Y with BLOC = 0
SET DTDY = SQUARE ROOT of GRAD of T with Y with BLOC = 0
SET DTDY OFF
```
MODE 11: Specification of Multiple Variables from Table of Values at Vertices

SYNTAX

```
SET {VERT}{Φ1, ..., Φn} {V1,..V (n+1)m|fname} [subrgn] [FIEL] {dir|BOUN}
```

**VERT**
The Φ_n variables are set individually for each of the external boundary nodes of a computational domain from a given set of values at the vertices. It is assumed that the input is in a tabular format with n columns (1 for each variable) and m rows (1 row for each boundary vertex). The input for the variables must be provided for all the vertices required to set the values for the identified sub domain. However, additional vertices of the domain may be present in the input file.

**Φ1, ..., Φn** Symbols to denote the variables that are to be set by the command. The symbols include all those listed in Table 2.8.1-3 plus the user defined variables (ALLOCATE command) and the real type variables defined in the initialization file. In addition a special symbol “SKIP” can be specified to by-pass the input of any of the columns. Any symbol may occur multiple times. There is no default value; appropriate symbols must be specified.

**V1,..Vnm** The table of values in the format of columns and rows. Each row consists of a vertex number followed by n values – one for each of the specified symbols. If n symbols are specified on the command and there are m boundary vertices, then (n+1) times m values must be specified in n+1 columns and m rows.

**fname** The name of the file (see Section 3.3) from which V1 through V(n+1)m are read.

**subrgn** The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected.

**FIEL** See Mode 1 specification.

**dir** The input is applied only to the nodes at the subregion boundary where the outward normal matches the specified modifier. See Section 3.5 for available choices.

**BOUN** If this modifier is present then the values at all boundary nodes of the specified subregion are set by this command.

**EXAMPLES**

```
SET boundary from VERTex locations! 12 boundary vertices for a 4 by 3 by 3 grid
  #   SKIP  P  T  SKIP  C
  1   0.2   1.0 -5  10.20 100
  2   0.6   0.0  +5  12.50 150
  3   1.0   -1.0 +10  2.00  200
  4   0.2   1.0 -5  10.20 100
  5   0.6   0.0  +5  12.50 150
  6   1.0   -1.0 +10  2.00  200
  7   0.2   1.0 -5  10.20 100
  8   0.6   0.0  +5  12.50 150
  9   1.0   -1.0 +10  2.00  200
 10   0.2   1.0 -5  10.20 100
 11   0.6   0.0  +5  12.50 150
 12   1.0   -1.0 +10  2.00  200
```

SET boundary P T SKIP C from VERTex data on file 'VERTEX.VAL'! Table of vertex values on file
**MODE 12: Special User Empirical Function for Colloidal Settling**

**SYNTAX**

\[
\text{SET} \{ \text{ZALU} \} \{ \Phi \} \{ \xi \} \{ x_0, y_0, [z_0] \} \{ q_0 \} \{ t_{\text{start}}, t_{\text{end}} \} \{ C_0, C_1, C_2, C_3 \} \{ \text{LIMIT} \} \{ \text{subrgn} \} \{ \text{FIEL} \} \{ \text{ALWA} \} \{ \text{FREQ} \} \{ \text{NOW} \} \{ \text{ONLY} \} \{ \text{TIME} \} = V_{frq}
\]

**ZALU**

This modifier indicates that a special user function is invoked. This function was developed by Dr. Zaluski for the deposition rate of a specific iron colloidal solution. It expresses the deposition rate, \(q\), (in kg/kg of soil) of the colloids in terms of multi-variate function of time, \(t\) (seconds), distance, \(d\) (m) and modulus of the Darcy velocity, \(U\) (m/s). The specific function is:

\[
q = \xi \max \left[ (C_0 + C_1 t + C_2 d + C_3 U), 0.0 \right] \quad \text{if} \quad t_{\text{start}} < t \leq t_{\text{end}} \quad \text{and} \quad S_t \geq 0.99
\]

\[
q = 0 \quad \text{otherwise}
\]

The default values of the constants are: \(C_0 = 4.0581 \times 10^{-2}\), \(C_1 = 2.88 \times 10^{-7}\), \(C_2 = -2.294 \times 10^{-2}\), \(C_3 = 19.6801\). The \(q\) is further modified to ensure that the total amount present in the field does not exceed the total released up to that point. The total amount in the field and the total injected are computed as:

\[
Q_{\text{total}} = \sum q (1 - \theta) \rho_s dV;
Q_{\text{inj}} = q_0 \min(t - t_{\text{start}}, (t_{\text{end}} - t_{\text{start}})); \quad t > t_{\text{start}}
\]

In these relations, \(\rho_s\) is the particle density of solid, \(\theta\) is the porosity and \(dV\) is the volume of the element; the summation is carried out over all elements of the sub-domain if the modifier \text{LIMIT} is present then \(q\) is corrected according to:

\[
q_{\text{final}} = q \min \left[ \frac{Q_{\text{inj}}}{Q_{\text{total}}}, 1.0 \right]
\]

If the modifier \text{LIMIT} is not present, then full correction is applied so that:

\[
q_{\text{final}} = q \frac{Q_{\text{inj}}}{Q_{\text{total}}}
\]

**\(\Phi\)**

Symbol for one of the previously defined field variables that will contain the computed deposition rate. There is no default value; a variable must be specified.

**\(\xi\)**

The independent variable that multiplies the computed value of \(q\). The variable \(\xi\) can be computed from an equation or specified by other means. If the symbol \(\xi\) is not specified, then it is replaced by unity.

**\(x_0, y_0, [z_0]\)**

The coordinates of the point of injection of the colloid. Two numerical values must be specified for 2D and 3 for 3D geometry. There is no default value

**\(q_0\)**

The injection rate of the colloids. The units must be consistent with the units of the correlation equation given above.

**\(t_{\text{start}}, t_{\text{end}}\)**

The start and end time for the injection of the colloids.

**\(C_0, C_1, C_2, C_3\)**

The constants of the deposition relation. Default values are given above.

**\text{LIMIT}\)**

If this modified is present, then the computed \(q\) is corrected only if the total computed amount exceeds the injected amount. See the equations above.

**\text{subrgn}\)**

The subregion for which the colloidal deposition is computed. If no subregion is specified, then entire computational domain is selected.

**\text{FIEL}\)**

See Mode 1 specification.

**\text{ALWA}\)**

By default the computation is performed only once when the command is given. If this modifier is present, then the computation is performed at every step.

**\text{FREQ}\)**

The computation is performed at the frequency specified by \(V_{frq}\).

**\text{NOW}\)**

The computation is performed immediately and at the frequency specified by \(V_{frq}\).
ONLY The computation is performed only once at the step number or time specified by the \( V_{frq} \).

TIME By default, \( V_{frq} \) is the frequency of output in terms of number of steps. If this modifier is present, then \( V_{frq} \) is interpreted to be time interval between successive outputs.

\( V_{frq} \) The frequency (step or time interval) at which the computation is performed.

COMMENTS

This is a very specific and limited-applicability empirical function developed by Dr. Marek Zaluski (marek.zaluski@mse-ta.com) and his colleagues for the deposition rate of an iron colloidal solution. It should only be used for type of application for which it was developed, and then only within the range of conditions for which it was developed.

EXAMPLES

SET ZALUSKI function for COLLIOD at (0.1,0.5) \( q=0.55, t_{start}=10, t_{end}=500 \) ALWAYS
SET ZALUSKI COLLIOD at (0.1,0.5,0.4) \( q=0.55, t_{start}=10, t_{end}=500 \) FREQ=5 in TIME units
SET ZALU CO (0.1,0.5,0.4) \( q=0.55, ts=10, te=50, c0=0.1, c1=0.005, c2=0.1, c3=1.2 \) FREQ=5 TIME
SET ZALU CO multiply by C (0.1,0.5,0.4) \( q=0.55, ts=10, te=50 \) ALWAYS
MODE 13: Disable Previously Specified SET Commands

SYNTAX

\texttt{SET \{\Phi\} \{OFF\} [\text{subrgn}]}

\texttt{\Phi} \quad \text{See Mode 1 specification.}

\texttt{OFF} \quad \text{Previous \texttt{SET} commands for the specified variable in the identified subregion are deactivated. A new specification may follow.}

\texttt{\text{subrgn}} \quad \text{Identifier for the subregion that appeared previously in a \texttt{SET} command for the current variable, \texttt{\Phi}.}

**EXAMPLES**

\texttt{SET commands for T for OFF for currently SELECTed subregion}

\texttt{SET commands OFF for T for ID=MIDDle}
COMMAND  SOLID

PURPOSE  To specify the conjugate heat transfer mode for the ANSWER™ Software Tool.

SYNTAX  SOLI

APPLICABILITY

This command is available only for the ANSWER™ Software Tool.

COMMENTS

By default the thermal transport in the solid is ignored in the ANSWER™ Software Tool. If this command is present, the thermal equation accounts for both the fluid and the solid phases. The properties of the solid must be specified with the appropriate CONDUCTIVITY, DENSITY, POROSITY and SPECIFIC HEAT commands.

EXAMPLES

SOLId: thermal transport to be accounted for.
COMMAND: SOLVE

PURPOSE: To initiate solution of the governing equations and to select the transient or steady state mode of solution.

MODE 1: Transient Solution Mode With Manual Time Step

SYNTAX: SOLV [\(\Phi\)] [ADD] [MANU] [N1, N2, N3, N4, N5]

\(\Phi\): By default, an appropriate set of governing equations is solved based on the user-specified input. The default selection includes any variable that occurs on a BOUNDARY or SOURCE command and the basic flow and thermal variables that occur on a SET command.

The user may override the default selection by explicitly specifying one or more \(\Phi\) symbols to select the corresponding dependent variable for which the governing equations are solved. The valid symbols are listed in Table 2.7.1. See the ADD modifier for more details.

ADD: If this modifier is present, then the variables specified by \(\Phi\) are added to the list of default variables for which a governing equation is solved. In the absence of the ADD modifier, the governing equations are solved ONLY for the variables specified by \(\Phi\).

MANU: The time step is determined according to the user-specified input of \(N2\) through \(N4\). This is the default mode.

N1: The incremental time period (> 0) for solution of the governing equations that are added to any previously specified value. The default value is 0.

N2: The time step (> 0) at the start of the current segment of calculations. The time step may be changed during the calculations or by a subsequent SOLVE command. The default value is \(N1/1000\).

N3: The geometric ratio multiplier (> 0) for the time step. Each successive time step is multiplied by this value until a maximum value specified by \(N4\) is reached. The default value is 1.

N4: The maximum permissible time step. The default value is \(10^{30}\).

N5: The maximum number of time steps. The default value is 999999999.

EXAMPLES

SOLVe for 50 years in steps of 2
SOLVe for 50 hours, initial step=0.2 hr, increase by 1.1, max=10 hr
SOLVe 1.6E6 yrs, DT=1, fac=1.1, max=1000, min=1, dfac=1.1, max steps=1000
SOLVe for 10 days, MANUal mode from now on! Previously an AUTO mode was used.
SOLVe for T only for 10 days in steps of 0.2
SOLVe for P2, T and C3 only for 10 days in steps of 0.2
MODE 2: Transient Solution Mode with Flux Based Automatic Time Step

SYNTAX

\[ \text{SOLV } [\Phi] [\text{ADD}] [\text{AUTO}] [\text{PASS}] [N_1, N_2, N_3, N_4, N_5, N_6, N_7] \]

\(\Phi\)
See Mode 1.

\(\text{ADD}\)
See Mode 1.

\(\text{AUTO}\)
The time step is automatically determined so that the specified primary convergence constraint is achieved for each time step (See CONVERGENCE command with FLOW modifier). The time step is increased if the number of iterations to converge is less than 1/2 of the maximum number of iterations specified on the CONVERGENCE command with FLOW modifier and decreased if it is larger than 4/5\textsuperscript{th} of the maximum number of iterations.

\(\text{PASS}\)
With the AUTO modifier, the time step may be adjusted either dynamically or passively. This modifier disables the dynamic mode; only passive adjustment takes place. In the dynamic adjustment mode, if the solution fails to converge to a specified tolerance in the specified number of iterations (see above), the time step is decreased and the solution process is repeated from the previous time. In the passive adjustment mode, the time step is adjusted only from the next time step; the currently computed values are retained.

\(N_1\)
See Mode 1.

\(N_2\)
See Mode 1.

\(N_3\)
The geometric ratio multiplier (>0) for the time step. Each successive time step is multiplied by this value until a maximum value specified by \(N_4\) is reached. The default value is 1.01.

\(N_4\)
The maximum permissible time step. The default value is 10\textsuperscript{30}.

\(N_5\)
The minimum permissible time step. With the AUTO modifier, it is very important to specify a reasonable lower bound for the time step. If too low a value is specified, computer resources may be wasted. Alternatively, too high a value may lead to unacceptable numerical errors. The default value is 10\textsuperscript{-10}.

\(N_6\)
The geometric ratio divisor (>0) for the time step. Each successive time step is decreased by this factor if the number of iterations to convergence is larger than the threshold specified in the CONVERGENCE command. The default value is 2.

\(N_7\)
The maximum number of time steps. The default value is 99 999 999.

COMMENTS

The AUTOMATIC solution mode is currently available only with the PORFLOW™ Software Tool. It works quite efficiently for single phase (saturated mode) flow problems. However, with multiphase problems, this mode may lead to excessive computation time unless the residual convergence criterion has been properly set. It is recommended that for such problems initially a manual time step be employed till a satisfactory solution behavior has been established.

EXAMPLES

\[ \text{SOLVe for 10 days in AUTOMATIC mode} \]
\[ \text{SOLVe AUTO 10 days DT=0.2, fac=1.3, mx=1, mn=1.E-5, df=1.1, Nmax=1000} \]
\[ \text{SOLVe for T only for 10 days in AUTO mode} \]
MODE 3: Transient Solution Mode with Automatic Time Step Based on CFL-Type of Limit

SYNTAX

SOLV [Φ] [ADD] {CFL} [N₁, N₂, N₃, N₄, N₅, N₆, N₇, N₈]

Φ
See Mode 1.
ADD
See Mode 1.
CFL
The time step is automatically determined so that largest normalized matrix coefficient for any of equations is smaller than the prescribed threshold value (Runchal 2004); that is:

\[
R = \max_i \left( \frac{\max_j |A_{ij}|}{A_{jj}} \right) \leq R_{\text{max}}
\]

where \(A_{ij}\) are the coefficients of the solution matrix: \(A_{ij} X_j = B_i\)

This criterion is numerically equivalent to the CFL criterion except that the matrix terms also include the contribution from the diffusion terms. For the same reason, it is also more versatile than the CFL criterion in that it incorporates the elements of both the CFL and the "diffusion" limit in a single criterion, which is numerically convenient to compute. It essentially complies with the oft-stated heuristic limit for matrix stability so that none of the errors for a linear system shall grow with an iterative process.

N₁
See Mode 1 of command.
N₂
See Mode 1 of command.
N₃
See Mode 1 of command.
N₄
The maximum permissible time step. The default value is 10\(^{30}\).
N₅
The minimum permissible time step. It is very important to specify a reasonable lower bound. If too low a value is specified, computer resources may be wasted. Alternatively, too high a value may lead to unacceptable numerical errors. The default value is 10\(^{-7}\).
N₆
The cut-off threshold value, \(R_{\text{max}}\), for the CFL parameter. If the computed value of \(R\) exceeds the threshold value then new time step is computed from:

\[
dt_{\text{new}} = \frac{dt_{\text{old}}}{dt_{\text{fac}}} \quad \text{and} \quad dt_{\text{fac}} = \max(\frac{R}{N_6}, N_7)
\]

where \(N_7\) is defined below. The default value is 0.8
N₇
The minimum geometric ratio divisor (>0) for the time step. The default value is 1.1.
N₈
The maximum number of time steps. The default value is 99 999 999.

COMMENTS

The CFL solution mode is currently available only with the ANSWER™ Software Tool. It works quite efficiently for most flow problems. However, due to non-linearity of the governing equations, complex sources and boundary conditions, there is no guarantee that any automatic procedure will prove economic under all circumstances. It is recommended that in case of doubt, initially a manual time step be employed till a satisfactory solution behavior has been established.

EXAMPLES

SOLVe for 10 days in CFL mode
SOLVe CFL 10 sec DT=0.2, factor=1.0, max=1, min=1.E-5, Rmax=0.5 DTfac_min=1.5 Nmax=1000
SOLVe for T only for 10 seconds in CFL automatic mode with DT=0.2
MODE 4: Transient Solution with Automatic Time Step for TIDAL Software Tool

SYNTAX

SOLV [Φ] [ADD] {AUTO} [N₁, N₂, N₃, N₄, N₅, N₆, N₇]

Φ
See Mode 1.

ADD
See Mode 1.

AUTO
The time step is automatically determined so that the time step stays within the computed value of the CFL limit for the flow.

N₁
See Mode 1.

N₂
The starting value of the time step which will be replaced by the computed value if it is larger than the computed value.

N₃
The geometric ratio multiplier (> 0) for the time step. Each successive time step is multiplied by this value until a maximum value specified by N₄ is reached. The default value is 1.01

N₄
The maximum permissible time step. The default value is 10³⁰.

N₅
The minimum permissible time step. With the AUTO modifier, it is very important to specify a reasonable lower bound for the time step. If too low a value is specified, computer resources may be wasted. Alternatively, too high a value may lead to unacceptable numerical errors. The default value is 10⁻¹⁰.

N₆
This input is ignored in this mode of the command; it is retained for compatibility with other mode in case the maximum number of time steps is specified (N₇ below).

N₇
The maximum number of time steps. The default value is 99 999 999.

COMMENTS

The AUTOmatic solution mode is currently available only with the TIDAL™ Software Tool. It works quite efficiently for most flow problems. However, often, for problems without run-up and draw-down, larger time can be used. In the case, the multiplier (N₃ above) can be larger than unity. For such problem the multipliers of 2 to 5 can be used for most problems.

EXAMPLES

SOLVe for 3.E7 seconds in AUTOmatic mode
SOLVe AUTO 3.E7 seconds  DT=100, Factor =2.0
MODE 5: Steady State Solution Mode

SYNTAX

SOLV \{STEÅ\} [Φ] [ADD] [N₁, N₂]

STEÅ

The equations are solved in their steady state mode. That is, the storage or accumulation term in the governing transport equation is set to zero.

Φ

See Mode 1.

ADD

See Mode 1.

N₁

The maximum number of iterative steps for solution of the matrix. The default value in this instance is 99999999.

N₂

The minimum number of iterative steps to be performed on the matrix. The default value is 100.

EXAMPLES

SOLVe in STEAdy state mode: maximum steps 200
SOLVe in STEAdy mode: maximum steps 500; minimum steps 20
**MODE 6:** Frequency of Computation for Selected Variables

**SYNTAX**  
SOLV \{FREQ\} [Φ] [N₁]

**FREQ**  
By default all variables are solved at every step of the solution process. Any exceptions to this are noted in the relevant sections. This modifier may be used to set a frequency for the computation of selected variables.

**Φ**  
One or more symbols to specify the variables for which the solution frequency is explicitly specified. Valid symbols are listed in Table 2.7.1. There is no default value.

**N₁**  
The frequency, in terms of number of steps of the solution process, for the solution of the variables identified on the command.

**EXAMPLES**

SOLVe FREQency for C₁ is every 10 steps  
SOLVe FREQency for FU, CO and C₂ every 20 steps
MODE 7: Dummy Run Initial Condition Mode

SYNTAX SOLV \{OFF\}

OFF The actual solution of the equations is disabled; however, a dummy run through the solution process is made to compute values of derived variables for the specified initial and boundary conditions. This mode is useful to check initial conditions and to create output or archive files of initial data and problem geometry for checking and verification of input.

COMMENTS

The Mode 1 and 2 of the SOLVE command immediately initiate solution of the governing differential equations. Therefore, these commands should be specified only after input has been supplied that is complete to initiate solution. However, the sequence of calculations may be sub-divided into as many segments as desired and a SOLVE command specified for each segment. See Section 2.10 for more information.

EXAMPLES

SOLVe OFF
SOLVe OFF now to obtain initial output for problem verification.
COMMAND  SOOT

PURPOSE  To activate soot computation and specify soot constants and parameters.

MODE 1:  Soot Particle Constants

SYNTAX  SOOT [N₁, N₂, N₃, N₄]

N₁  Soot particle density. The default value is 2000 (kg/m³).
N₂  Diameter of the smaller soot particles in microns. The default value is 1/40 micron.
N₃  Diameter of the larger soot particles in microns. If this value is ≥ 0 or is omitted, then the computations are performed with only one soot particle size specified by N₂. The default value is 1 micron.
N₄  Percentage of the smaller soot particles in the total. This input is ignored if N₃ is zero or is omitted. The default is 90 percent.

APPLICABILITY

This command is available only for the ANSWER™ Software Tool.

EXAMPLES

SOOT rho= 2200, d₁ = 0.05
SOOT rho= 2200, d₁ = 0.05, d₂= 2., fraction 50 %
MODE 2: Soot Nuclei Constants

SYNTAX

SOOT \{NUCL\} [N_1, N_2, ..., N_6]

NUCL

Soot nuclei constants are specified.

N_1

The Arrhenius prefactor \((>0)\) for the soot nuclei equation. The default value is \(1.16 \times 10^{31}\).

N_2

The Arrhenius activation energy constant divided by the universal gas constant \((>0)\) for the soot nuclei equation. The default value is \(9.00 \times 10^{4}\).

N_3

The 1\(^{st}\) exponent \((\geq 0)\) of the soot nuclei equation. The default value is 1,000.

N_4

The 2\(^{nd}\) exponent of the soot nuclei equation. The default value is 8.00 \times 10^{-16}.

N_5

The 3\(^{rd}\) exponent of the soot nuclei equation. The default value is 1.00 \times 10^{15}.

N_6

The constant \((\geq 0)\) in the soot nuclei equation. The default value is 100.

EXAMPLES


SOOT NUMLei constants: 5.00E31, 1.0E4, 900, 8.E-15, 1.E-14, 100.
MODE 3: Soot Formation Constants

SYNTAX  
SOOT {FORM} [N₁, N₂, , N₇]

FORM  Soot formation constants are specified.

N₁  The Arrhenius prefactor (>0) for the soot formation equation. The default value is 1.5626 x 10¹³.

N₂  The Arrhenius activation energy constant divided by the universal gas constant (>0) for the soot nuclei equation. The default value is 1.60 x 10⁴.

N₃  The 1ˢᵗ exponent (≥0) of the soot formation equation. The default value is 1.81.

N₄  The 2ⁿᵈ exponent of the soot formation equation. The default value is −0.50.

N₅  The 3ʳᵈ exponent of the soot formation equation. The default value is −1.94.

N₆  The incipient carbon-to-oxygen ratio at which the soot formation starts. The default value is 0.1.

N₇  The incipient temperature (in absolute units) at which soot formation starts. The default value is 400.

EXAMPLES

SOOT FORMation constants are 1.90E13, 1.50E4, 2.0, -0.5, -2.0, 0.1, 500.

SOOT FORMation constants: 1.90E13, 1.50E4, 2.0, -0.5, -2.0, 0.1, 500.
MODE 4: Soot Computation Frequency

SYNTAX

SOOT {FREQ} [N₁]

FREQ Frequency of soot computations is specified.

N₁ The frequency of soot computations in terms of number of steps of the solution process. If the value specified is <1 or the input is omitted, then the soot computations are triggered at the default or previously specified frequency. The default value is 10.

EXAMPLES

SOOT FREQuency of calculations every 20 steps
SOOT computation FREQency by default.
Keyword Commands

ACRi™ Software Tools

COMMAND  SOURCE

PURPOSE  To specify the sources (or sinks) of fluid, heat or chemical species.

MODE 1:  Direct Source or Sink for a Single Selected Variable

SYNTAX  SOUR {Φ} [TOTA] [func{ξ}] {N1, N2, ..., Nn} [fname] [option] [subrgn] [dir] [Nn+1, Nk] [ρB]

Φ  The symbol for the dependent variable for which the source is specified. Valid symbols are listed in Table 2.7.1. A symbol must be specified.

TOTA  By default, the amount of source specified, or computed from func (ξ), is applied to each element of the subrgn. If this modifier is present then the amount is assumed to be the total amount over whole of the subrgn. In this case, the amount is distributed equally to all the elements of the subrgn unless the VOLUME or AREA modifiers are present.

func  One of the modifiers listed in Table 4.2.1 that denotes the functional form of the source. If no function is specified, the value is assumed to be constant.

ξ  One of the independent variables listed in Table 4.2.2. If no independent variable is specified, the variable is assumed to be time.

N1,...,Nn  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  The name of the file containing the numerical values Nk through Nn. This option is available only for selected functions. See Section 3.3 for additional information.

option  Options selected for implementation of the source.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>VOLU</td>
<td>If the TOTAL modifier is not present, the source for each element is computed as: ( Q = \delta V ). Here q is the amount specified by the user and ( \delta V ) is the volume of the element. The q, in turn, is computed from func(ξ) and N1 through Nn. If the TOTAL modifier is present, the amount for each element is computed as: ( Q = q \delta V / V ), where V is the volume of the total subrgn.</td>
</tr>
<tr>
<td>AREA</td>
<td>If the TOTAL modifier is not present, the source for each element is computed as: ( Q = \delta A ), where ( \delta A ) is the area of the element boundary indicated by dir. If the TOTAL modifier is present, the source for each element is computed as: ( Q = q \delta A / A ), where A is the total area of the subrgn in the dir direction.</td>
</tr>
<tr>
<td>INTE</td>
<td>By default, if dir points to a boundary wall, then any special treatment for the wall is deactivated and the diffusive flux at the wall is set to zero. If the INTERNAL modifier is present then the wall treatment and wall diffusive flux are retained.</td>
</tr>
<tr>
<td>NORM</td>
<td>In the absence of the TOTAL modifier, the source, Q, is computed as: ( Q = q \sum A_i \cdot V_i ) where ( A_i ) is the ( i^{th} ) direction component of the element boundary area specified by dir. ( V_i ) are the values specified by Nn+1 through Nk (2 for 2D, and 3 for 3D). In the presence of the TOTAL modifier, Q is computed in a manner identical to that for the AREA modifier.</td>
</tr>
<tr>
<td>DENS</td>
<td>The computed source, Q, is further multiplied by density. The density may be specified as the last value, ( \rho_B ), on the command. If this value is omitted, then the boundary value at the node indicated by the dir direction is used if the AREA or NORMAL modifier is present, otherwise the local density for the element is used. If the dir modifier is present, then the boundary value of density is overwritten by the specified value.</td>
</tr>
<tr>
<td>subrgn</td>
<td>The subregion for which the input is specified. If no subregion is specified, then entire computational domain is selected.</td>
</tr>
</tbody>
</table>
| dir    | The orientation index for the element boundary associated with the source if AREA or
NORMAL modifier is present. See Section 3.5 for available choices. There is no default value for this input.

\( N_{n+1}, \ldots, N_k \) The normalizing vector components, \( V_i \), if the NORMAL modifier is present. Two values must be specified for 2D and 3 for 3D flows. There are no default values for this input.

\( \rho_B \) The density value that multiplies the computed source. It can only be specified if the DENSITY modifier is present and then it must be the last value on the command. If no value is specified but the modifier DENSITY is present, then default value is the boundary value at the node indicated by the dir direction if the AREA or NORMAL modifier is present, otherwise the default value is the local density for the element.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (SOURCE) must replace the keyword used in these examples. Some additional examples that illustrate the use of the attributes specific to this command are given below.

- **SOURCE** for \( T = 10 \) W/per unit by VOLUME for SELECTed region
- **SOURCE** \( T \) is TABLE per unit AREA in X- direction: 3 sets (TIME, value) \( (0., 0.01), (100., 0.10), (200, -0.20) \)
- **SOURCE** for \( T \) 10 per unit AREA in X- direction for SELECTed region
- **SOURCE** for \( T \) 10 per unit area in X- direction with NORMALized of 0, 1.5, 2.5 ID=VSOURCE
- **SOURCE** for \( T \) 10 in X- dir with NORMALized vel 1, 1.5, 2.5 and DENSITY for ID=VSOURCE
- **SOURCE** for \( T \) 10 X- dir INTERNAL with NORMALized vel 1., 1.5, 2.5 and DENSITY = 5 for ID=VSOURCE
- **SOURCE** for \( T \) 10 in per unit VOLUME multiply by DENSITY = 5 for SELECTed region
MODE 2: Flow Injection with Fixed Variable Values

SYNTAX

SOUR {FLOW} [TOTA] [func[ξ]] {N₁, N₂, .., Nₙ |fname} [option] [subrgn] [dir] [Φ =Nₙ₊₁, .., Nₘ] [Nₘ₊₁, Nₖ] [ρ₈]

FLOW

The source (or sink) for a variable is created due to direct fluid injection or withdrawal. The amount of the property of interest (momentum, heat, chemical species etc.) of the injected (or withdrawn) fluid acts as the source or sink for each of the relevant properties.

TOTA

See Mode 1 specification

func

See Mode 1 specification.

ξ

See Mode 1 specification.

option

See Mode 1 specification.

subrgn

See Mode 1 specification.

dir

See Mode 1 specification.

fname

See Mode 1 specification.

Φ

The symbols that denote the dependent variables injected with the fluid. If no dependent variable is specified, all properties in the injected fluid are assumed to be zero. This specification is ignored if the fluid is being withdrawn because the amount of property withdrawn is equal to the local value of that property.

N₁, .., Nₙ

See Mode 1 specification.

Nₙ₊₁, .., Nₘ

Each of these represents the value of injected variable denoted by the symbol immediately preceding the value.

Nₘ₊₁, .., Nₖ

The normalizing vector components, Vᵢ, if the NORMAL modifier is present. Two values must be specified for 2D and 3 for 3D flows. There are no default values for this input.

ρ₈

See Mode 1 specification.

COMMENTS

The SOURCE FLOW command is designed to allow injection of fluid through a solid boundary (or blocked region) inside the domain of computation. Its use is most appropriate when the scale of injection is smaller than the grid size. If the scale of injection is comparable to the grid size, then the FLOW command may be more appropriate. The injection at an exterior domain boundary is often better accounted for by the INLET command.

In implementing this command it is assumed that at the point of injection, the boundary wall is essentially removed. The computational treatment is akin to that for inflow such as through an INLET boundary. If the injection occurs through a blocked element or at an exterior boundary of the domain, then the injected values are also assumed to be the boundary values of the variables. If the wall needs to be retained, such as for flow percolating through a solid matrix or through holes much smaller than the boundary area of the inflow element, then the INTERNAL modifier should be used with the command.
EXAMPLES

All examples cited for Mode 1 are applicable provided that the modifier \texttt{FLOW} is added. Some illustrative examples of the use of attributes specific to this mode are given below.

\texttt{SOUR}ce with \texttt{FLOW} injection: amount = 0.001 with T=50, C=1.
\texttt{SOUR}ce with \texttt{FLOW} per unit AREA of X- face: = 0.001 with T=50, C=1.
\texttt{SOUR}ce with \texttt{FLOW} withdrawal: amount =-0.001 per second
\texttt{SOUR}ce \texttt{FLOW}: \texttt{TABLE} 3 sets \texttt{SELE}cted (0, 0), (100, 1), (200, 0) U=1, V=0.1, W=0., T=10, K=0.001, L=1
\texttt{SOUR}ce for \texttt{FLOW}: \texttt{EXPOnential} series with \texttt{TIME} 7 sets from 'SOURCE' T=100, C=0.
\texttt{SOUR}ce \texttt{FLOW} q=10 X- direction T=100, U=20. \texttt{NORMa}lized velocity 0., 1.5, 2.5 ID=VSOURce;
\texttt{SOUR}ce \texttt{FLOW} \texttt{q}=-10 in X- dir with \texttt{NORMa}lized vel 1., 1.5, 2.5 and \texttt{DENSity} for ID=VSOURce
\texttt{SOUR}ce \texttt{FLOW} \texttt{q}=10 X- dir \texttt{v}ariable values: U=10, V=0, W=-20, T=100, K=0.03, L=0.5 \texttt{INTErnal} with \texttt{NORMa}lized vel 1., 1.5, 2.5 and \texttt{DENSity} for ID=VSOURce;
\texttt{SOUR}ce \texttt{FLOW} \texttt{q}=10 per unit \texttt{VOLUme} injected variables: U=10, V=0, W=-20, T=100, K=0.03, L=0.5 multiply by \texttt{DENSity} = 5 for \texttt{SELE}cted region
MODE 3:  Flow Injection with Fixed Variable Values and Computed Momentum Components

SYNTAX  SOUR  {MOME} {func[ξ]} {N1, N2, .., Nn, fname} [TOTA] [option] [Φ=Nn+1, .., Φ=Nm, Nm+1, Nk] [ρB] [subrgn] {dir}

MOME  The source (or sink) for a variable is created due to direct fluid injection or withdrawal. The amount of the property of interest of the injected (or withdrawn) fluid acts as the source or sink for each of the relevant properties. In addition, the velocity components of the injected flow are computed from the source flow rate for the element, Q, as:

\[ V_j = \frac{Q}{\rho_B A} n_j, \]

where \( V_j \) are the computed velocity components of the injected flow in the \( j^{th} \) direction, \( \rho_B \) is the density, \( A \) is the area of the element boundary specified by the \( \text{dir} \) modifier, and \( n_j \) is a normalizing vector. If the \text{NORM}al modifier is present, then \( n_j \) is obtained from the user input, otherwise the area unit vector (\( A_j/A \); where \( A_j \) is the component in the \( j^{th} \) direction) is used as the normalizing vector. By default the density is the fluid density at the boundary, unless the user specifies a value. Any velocity input given by the user is ignored.

func  See Mode 1 specification.

ξ  See Mode 1 specification.

N1, .., Nn  See Mode 1 specification.

fname  See Mode 1 specification.

TOTA  See Mode 1 specification

option  See Mode 1 specification. Unless the \text{NORM}al modifier is present, it is assumed that the \text{AREA} modifier is in effect. Any specification of the \text{VOLU}me modifier is ignored. All other modifiers can be used as for Mode 1 Specification.

Φ  See Mode 1 specification.

Nn+1, .., Nm  These values represent the value of injected variable denoted by the symbol immediately preceding the value.

Nm+1, .., Nk  The normalizing vector components, \( V_i \), if the \text{NORM}al modifier is present. Two values must be specified for 2D and 3 for 3D flows. There are no default values for this input.

ρB  The density value to compute the velocity components. It can only be specified if the \text{DENS}ity modifier is present and then it must be the last value on the command. If no value is specified, then boundary value at the node indicated by the \text{dir} is used.

subrgn  See Mode 1 specification.

dir  See Mode 1 specification. This modifier must be present for this mode of command.

COMMENTS

The \text{SOURCE MOMETUM} command is similar to the \text{SOURCE FLOW} command except that the momentum (or velocity) of the incoming flow is computed on the assumption that the direction of injected mass is normal to the boundary and that the mass is uniformly distributed at the boundary. All other details of its implementation are identical to those for the \text{SOURCE FLOW} command.
EXAMPLES

All the examples cited for Mode 2, except those with `VOLUME` modifier, are applicable provided that the modifier `MOMENTUM` is added. Some illustrative examples specific to this mode are given below.

**SOUrce with MOMEntum q=10 X- direction with ID=VSOURce; T=100, K=0.05, L=0.02**

**SOUrce MOMEntum q=10 X- direction with ID=VSOURce; T=100, K=0.05, L=0.02, DENSity 5**

**SOUrce MOMEntum q=10 X- direction with ID=VSOURce; T=100, K=0.05, L=0.02, NORMAL 1. -1, 0**

**SOUrce MOMEntum q=10 X- ID=VSOURce; T=100, K=0.05, L=0.02, NORMAL 1. -1, 0, DENSity=5.**

**SOUrce MOMEntum: TABLE 2 sets SELECT (0, 0), (100, 1) T=10, K=0.001, L=1**

**SOUrce MOMEntum EXPOnential SERies TIME 7 sets ‘SOURCE’ T=100, C=0. NORMAL 1. -1 SELECTe**

**SOUrce MOMEntum q=10 X- dir INTErnal for ID=VSOURce: injected variables: T=100, K=0.03, L=0.5 NORMALized vel 1., 1.5, -0.7 and DENSity as exists**
**MODE 4:** Flow Injection at Fixed Spherical Angles with Computed Momentum Components

**SYNTAX**

```
SOUR {ANGL} [func[ξ]] {N1, N2, ..., Nn | fname} [TOTA] [Φ =Nn+1, ..., Φ =Nm] [Nm+1, ..., Nm+5] [DENS | SPEE] [ρB | VS] [subrgn] {dir}
```

**ANGL**

Fluid is injected or withdrawn. The amount of the property of the injected (or withdrawn) fluid acts as the source or sink for each of the relevant properties. If the flow is injected, then the velocity component of the injected flow, \( U_i \) in the \( i^{th} \) direction, is either computed from the source flow rate, \( Q \), or determined from a specified injection speed, \( V_S \), as:

\[
U_i = \frac{Q}{\rho_B A} n_i \quad \text{or} \quad U_i = V_S n_i
\]

where \( \rho_B \) is the density at the neighboring element and A is the area of the element boundary specified by the `dir` modifier. The local direction vector, \( n_i \), for each segment of the surface is obtained from the user input of two spherical angles and a reference axis.

**func**

See Mode 1 specification.

**ξ**

See Mode 1 specification.

**N1, .., Nn**

See Mode 1 specification.

**fname**

See Mode 1 specification.

**TOTA**

See Mode 1 specification.

**Φ**

See Mode 1 specification.

**Nm+1, .., Nm**

The values of injected variables denoted by the symbols immediately preceding the values.

**Nm+2**

The spherical angle, \( \Theta \) in degrees measured as the deflection of the injection vector from the face normal. The magnitude of the angle must be less than 180 degrees.

**Nm+3, Nm+5**

The direction cosines of the axis vector used to measure the angle \( \phi \); 3 values must be specified since this option is only available for 3D flows.

**DENS**

The density, \( \rho_B \), is specified as the last value on the command.

**ρB**

See Mode 3 specification.

**SPEE**

The injection speed, \( V_S \), is specified as the last value on the command.

**VS**

The value \( V_S \) if the `SPEED` modifier is present. There is no default value for this input.

**subrgn**

See Mode 1 specification.

**dir**

See Mode 1 specification. This modifier must be present for this mode of command.

**EXAMPLES**

All examples cited for Mode 1 are applicable provided that the modifier `ANGL` is added and appropriate input for spherical angles is appended. Some illustrative examples of the use of attributes specific to this mode are given below.

```
SOURce q=10, X- direction with ID=VSOURce; T=100, K=0.05, L=0.02, Theta=45, phi=20, axis=1., 0, 0
SOURce q=10, X- ID=VSOURce; T=100, K=0.05, L=0.02, Theta=45, phi=20, axis=1., 0, 0, SPEEd=120
SOURce q=10, X- ID=VSOURce; T=100, K=0.05, L=0.02, Theta=45, phi=20, axis=1., 0, 0, DENSity=2.5
```
MODE 5: Flow Injection with Multiple Tabular Functions

SYNTAX SOUR \{FLOW\} \{Φ\} \{TABL\} \{MULT\} \{option\} \{subrgn\} \{N_{sets}\} \{N_1, \ldots, N_n\} \{fname\}

FLOW The source (or sink) for a variable is created due to direct fluid injection or withdrawal. The amount of the property of interest (momentum, heat, chemical species etc.) of the injected (or withdrawn) fluid acts as the source or sink for each of the relevant properties.

Φ One or more of the symbols that denote the dependent variables, which are specified as functions of time. There is no default value; at least one symbol must be specified.

TABL The variables are specified as tabular functions of time. This is the only available option in this mode.

MULT Multiple variables are tabular functions of time.

option See Mode 1 specification.

subrgn See Mode 1 specification.

N_{sets} The number of sets of data for the tabular functions.

N_1, \ldots, N_n The N_{sets} sets of data for the flow rate and variables as tabular functions of time. Each set must consist of time, flow rate, and one value for each variable specified by the symbol Φ on the command, in that order. Thus if 4 variables are selected, then each data set must consist of 6 values. There is no default value; the correct number of values must be specified. If the flow rate is negative (withdrawal of fluid), then specified value of the property is ignored since it is assumed that the fluid is being withdrawn with an amount of property equal to the local value of that property.

fname See Mode 1 specification.

EXAMPLES

SOURce with MULTiple TABLe functions: 4 sets

<table>
<thead>
<tr>
<th>Time</th>
<th>Flow</th>
<th>U</th>
<th>V</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.</td>
<td>0.001</td>
<td>1.00</td>
<td>0.02</td>
<td>100</td>
</tr>
<tr>
<td>1.</td>
<td>0.002</td>
<td>0.50</td>
<td>0.01</td>
<td>200</td>
</tr>
<tr>
<td>2.</td>
<td>0.004</td>
<td>2.00</td>
<td>0.01</td>
<td>500</td>
</tr>
<tr>
<td>5.</td>
<td>0.010</td>
<td>5.00</td>
<td>0.02</td>
<td>600</td>
</tr>
</tbody>
</table>

SOURce with FLOW MULTiple TABLe: 4 sets per unit VOLUme

<table>
<thead>
<tr>
<th>Time</th>
<th>Flow</th>
<th>U</th>
<th>V</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.</td>
<td>0.001</td>
<td>1.00</td>
<td>0.02</td>
<td>100</td>
</tr>
<tr>
<td>1.</td>
<td>0.002</td>
<td>0.50</td>
<td>0.01</td>
<td>200</td>
</tr>
<tr>
<td>2.</td>
<td>0.004</td>
<td>2.00</td>
<td>0.01</td>
<td>500</td>
</tr>
<tr>
<td>5.</td>
<td>0.010</td>
<td>5.00</td>
<td>0.02</td>
<td>600</td>
</tr>
</tbody>
</table>
MODE 6: Solubility-Limited Source for a Chemical Species

SYNTAX

SOUR \{Φ\} {SOLU} {\{func[ξ]\}} {N_1, N_2, .., N_n} {fname} {Q_{total}} {T_{start}} {subrgn}

Φ
A symbol that denotes the dependent variable for one of the chemical species. A symbol must be specified.

SOLU
The source is solubility-limited. That is, the source is specified as the total initial mass of a chemical species and the solubility of the species in the fluid phase is limited to a maximum saturation value that is defined by the rate of dissolution equation as shown below

\[
S_C = f_S (C_S - C)
\]

where
- \( S \) is the rate of species dissolution,
- \( f_S \) is a dissolution frequency,
- \( C_S \) is the solubility limit (maximum concentration) of the species in the fluid,
- \( C \) is the concentration of the species in the fluid

func
The function that specifies the solubility limit, \( C_s \), for the species.

ξ
See Mode 1 specification.

N_1, .., N_n
See Mode 1 specification.

fname
See Mode 1 specification.

Q_{total}
Total amount of material to be dissolved. The default value is 0.

T_{start}
Time at which release begins. The default value is 0.

subrgn
See Mode 1 specification.

EXAMPLES

All examples cited for Mode 1 are applicable provided that the modifier "SOLU" is added and the values for the variables (N_{n+1} and N_{n+2}) are appended at the end of the command, as necessary. Some illustrative examples of the use of attributes specific to this mode are given below.

SOURce for FF: SOLUbility limited: Cs=0.05, S=100 kg, t=0 for selected zone.
SOURce for FU: SOLUbility: 75 sets file 'SOURCE.DAT', S=75., t_start = 20.
MODE 7: Radiation Type of Source For a Variable

SYNTAX: SOUR {Φ} {RADI} [COEF] [VARI] {H, Φ_eq} [POSI | NEGA] [option] [subrgn]

Φ: A symbol to denote the dependent variable for which the source is specified. A symbol must be specified; otherwise, a fatal error will occur.

RADI: The radiation type of source is specified. This source is defined as:

\[ Q = H (\Phi_{eq} - \Phi) \]

In the above equation, \( Q \) is the source for \( \Phi \) in appropriate units, \( H \) is a transfer coefficient and \( \Phi_{eq} \) is an equilibrium value of \( \Phi \). The \( H \) and \( \Phi_{eq} \) may be constants or symbols for previously defined variables.

COEF: By default it is assumed that \( h \) is a constant (with its value specified as a numerical constant on the command). However, if this modifier, along with the VARI modifier, is present, then \( h \) must be a symbol for a previously defined variable.

VARI: This modifier must be present with the COEF modifier if \( H \) is specified as a symbol for a variable. Otherwise it is ignored.

H: The transfer coefficient, \( H \), of the radiation source. A numerical value must be specified unless the modifiers COEF and VARI are present. In this case, a valid symbol for a previously defined variable must be specified.

\( \Phi_{eq} \): The equilibrium value for the radiation source. A numerical value or a valid symbol for a previously defined variable must be specified.

POSI: The source is implemented only if \( Q > 0 \).

NEGA: The source is implemented only if \( Q < 0 \).

option: See Mode 1 specification. NORMAL and DENSITY options are not available with this type of source.

subrgn: See Mode 1 specification.

EXAMPLES:

SOURce for T: Radiation type coefficient 0.001, equilibrium value = 15 degrees.

SOURce for T: Radiation hcoef = 0.001 value from variable EQVA! EQVA is a symbol

SOURce for T: Radiation VARI COEF as function HVALu, value=15! HVAL is a symbol

SOURce for T: RADIA VARI COEF HCOE & HVALu! HCOE & EQVA are symbols
MODE 8: Source Term as a Linear Decay or Half-Life.

SYNTAX SOUR {Φ} {DECA} [HALF] [subrgn] {λ|σ}

Φ A symbol to denote the variable for which the source is specified.

DECA The decay rate of the variable is specified; it is equivalent to introducing a source term in the corresponding governing equation for Φ as:

\[ Q = -\lambda \rho \Phi. \]

In this equation, \( Q \) is the source rate for \( \Phi \), \( \lambda \) is the decay rate and \( \Psi \) is the fluid density if the variable \( \Phi \) is defined in terms of mass units and unity if it is defined in terms of volumetric units.

LIFE Half-life of the property \( \Phi \) is specified. The decay rate is computed from the half life, \( \sigma \):

\[ \lambda = -\frac{\log(0.5)}{\sigma}. \]

subrgn See Mode 1 specification.

λ The decay rate, \( \lambda \), for the variable \( \Phi \).

σ The half-life, \( \sigma \), for the variable \( \Phi \).

EXAMPLES SOURce DECAy rate for \( C = 0.001 \)
SOURce DECAy rate for \( C = 0.001 \) in the SELEcted subregion
SOURce DECAy rate for \( C = 0.001 \) in the subregion ID=DRGN
SOURce DECAy rate for half LIFE of 29 years in subregion ID=DRGN
MODE 9: Source as a Linear Function of User-Defined Reaction Rates

SYNTAX

```
SOUR {Φ} {REAC} {id_1, . . ., id_n} {N_{i1}, .., N_{in}}[subrgn]
```

Φ
A symbol to denote the chemical species for which the source is specified.

REAC
Modifier specifying the source term as a linear combination of reaction rates for a given chemical species according to the equation:

\[
Q = \sum_n C_n R_n,
\]

In this equation, \( Q \) is the source for \( Φ \), \( C_n \) are the scaling constants and \( R_n \) are the previously specified reactions.

Id_1,.., id_n
Identifiers for the reactions, \( R_n \), described by Mode 2 of REACTION command, which comprise the source. Up to 9 reactions may be specified.

N_{i1}, .., N_{in}
The scaling constants, \( C_n \), for linear combination of the selected reaction rates. These must include the stoichiometric coefficients and the conversion factors to ensure that the source term is expressed in the proper units (kg of specie \( Φ \) per second). The number of constants must match the number of reactions specified.

subrgn
See Mode 1 specification.

EXAMPLES

```
SOURce REAc tion type FU LINEar -1. * R1
SOURce REAc tion type CH LINEar -1. * R2 + 0.9586 * R1 in SELEc ted subdomain.
SOURce REAc tion type CH LINEar -1. * R2 + 0.9586 * R1 for ID=RRGN
```
MODE 10: Flux Transfer between Adjacent Elements

SYNTAX

SOUR {FLUX} {VALU|DIFF|GRAD} [AREA|NORM|VOLU] {dir} [subrgn] [func[ξ]] \{N_1, N_2, .., N_n, fname\} [N_{n+1}, N_k] [DENS] [ρ_b]

Φ
A symbol to denote the dependent variable for which the flux transfer is specified. A symbol must be specified.

FLUX
The flux, Q, is transferred from a donor to a receptor element across an interface between the two elements according to the relation:

Q = q F_Φ F_V F_ρ

Here, q is the amount specified by the user (func (ξ) and N_1 through N_n). The factors F_Φ, F_V and F_ρ are functions of other modifiers as described below. The quantity Q is algebraically added to the source for the receptor cell and subtracted from the source term of the donor cell. There is no net source for the system.

VALU
F_Φ = Φ_0, where Φ_0 is the value of Φ in the donor cell (that lies upstream with respect to direction of the computed Q). The source acts essentially as a convective flux across the interface between the donor and the receptor cells. This type of source can be used to implement processes such as settling of particulate material or droplets due to body forces. This is the default option.

DIFF
F_Φ = Φ_B - Φ_F, where Φ_B and Φ_F are the values of Φ in the “boundary” and “field” cells, respectively. The field cell is that defined by the subrgn modifier; the boundary cell is selected in reference to the field cell by the dir modifier. The source acts as a diffusive flux and enhances equilibrium between neighboring elements. For this type of source, the boundary cell acts as the donor cell and the field cell as the receptor cell. This option can be used to incorporate supplementary equilibrium, diffusive or radiative processes.

GRAD
F_Φ = (Φ_B - Φ_F)/L, where L is the eulerian distance between the donor and receptor cell nodes. This type of source allows simulation of a diffusive process that depends on the gradient of the variable across an interface.

AREA
The factor F_V is set equal to the area of the receptor cell boundary indicated by the dir modifier. If the AREA, NORM and VOLU modifiers are all absent, then F_V is set to unity.

NORM
F_V = \sum A_i V_i, where A_i is the projected area of the interface in the direction of the i^{th} coordinate denoted by dir modifier, and V_i are the user inputs, N_{n+1} through N_k. The summation is over 2 terms for 2D, and 3 for 3D simulations.

VOLU
The factor F_V is set equal to the volume of the receptor cell.

subrgn
See Mode 1 specification.

func
See Mode 1 specification.

ξ
See Mode 1 specification.

N_1, .., N_n
See Mode 1 specification.

fname
See Mode 1 specification.

N_{n+1}, .., N_k
See Mode 1 specification.

DENS
F_ρ is equal to ρ_b. In the absence of this modifier, F_ρ is equal to unity.

ρ_b
The density value that multiplies the computed source. It can only be specified if the DENSITY modifier is present and then it must be the last value on the command. If no value is specified but the modifier DENSITY is present, then default value is the boundary value at the node indicated by the dir direction if the AREA or NORM modifier is present, otherwise the default value is the local density for the element.

EXAMPLES

All examples cited for Mode 1 are applicable provided that the modifier FLUX is added. Some illustrative examples of the use of attributes specific to this mode are given below.
SOURce FLUX type for T: \( q=0.1 \) for X- direction of currently active subregion.
SOURce FLUX type for C1: \( q=1.5 \) multiply by AREA of X- direction interface for ID=RGN1.
SOURce FLUX for C2: \( q=1.5 \) NORMalized velocities 0, 0, 0.25 for X- direction of ID=RGN1.
SOURce FLUX C2: \( q=1.5 \) NORM 0.12., 0, 0.25 multiply by DENSity; X- direction ID=RGN1.
SOURce FLUX C2: DIFFerence. \( q=1.5 \) NORM 0.12., 0, 0.25 DENSity = 5; X- ID=RGN1.
SOURce FLUX C2: GRADient. \( q=1.5 \) VOLUmetric DENS; X- ID=RGN1.
Keyword Commands

MODE 11: Disable Previously Specified SOURce commands

SYNTAX SOUR {OFF} {Φ} {subrgn}

Φ See Mode 1 specification.

OFF Previous SOURCE commands for the identified subregion are deactivated for the specified variable. A new specification may follow.

subrgn See Mode 1 specification.

EXAMPLES

SOURce OFF for T for most recently SELECTed region
SOURce OFF for T for ID=MIDDle
COMMAND SPECIFIC HEAT

PURPOSE To specify the specific heat of the fluid.

MODE 1: Generic Functional Form for Specific Heat

SYNTAX SPEC {func[ξ]} {N₁, N₂, ..., Nₙ | fname} [phase] [subrgn]

func One of the modifiers listed in Table 4.2.1 that denotes the functional form of the specific heat. If no function is specified, the value is assumed to be constant.

ξ One of the independent variables listed in Table 4.2.2. If no independent variable is specified, the variable is assumed to be time.

N₁,...,Nₙ The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

phase The phase for which the input is specified. See Section 3.6 for available options. By default the input pertains to the 1st phase of the fluid. This modifier is available only for the multi-phase versions of the PORFLOW™ and ANSWER™ Software Tools.

subrgn The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

EXAMPLES

SPECific heat = 1234

Generic examples for this command are given in Section 4.4. The command keyword (SPECIFIC) must replace the keyword used in these examples and the dependent variable (φ) must be omitted. Only the functional form, the independent variable and the numerical values need to be specified.
Keyword Commands

MODE 2: Pre-Defined Specific Heat Function

SYNTAX SPEC {GORD} [fname]


fname The name of the file containing the numerical values to define the Gordon and McBride relations. The file format must be consistent with the format required by the Gordon-McBride specification. If no file name is then the default data is obtained from the initialization file. Any numerical input on the command is ignored.

EXAMPLES SPECific heat from GORDon-McBride formulae with default library values SPECific heat by GORDon-McBride on file called ‘CPHTDATA.JP4’
COMMAND STACK

PURPOSE To store some information or variable on the stack for later use.

MODE 1: Store Location of an Element for Later Use

SYNTAX STAC {LOCA} [ELEM|IJ|IJK] {N₁, ..Nₙ}

LOCA A grid location is stored in the stack. Only a single location can be stored; this may be replaced as often as needed. Only the internal elements can be specified. The boundary nodes, if specified, are ignored.

ELEM The numerical input specifies the grid element number that is stored in the stack.

IJK The numerical input specifies the grid indices of elements (I, J) for 2D or (I, J, K) for 3D geometry. This option can be used only for structured grids.

N₁, .., Nₙ The element number or grid indices for a structured grid. There is no default value; appropriate input must be supplied.

EXAMPLES

STACK LOCATION of ELEMENT number 2978 for later use.
STACK LOCATION of IJK indices: (2, 5) for a two-dimensional structured grid
STACK LOCATION of IJK indices: (2, 5, 2) for three-dimensional structured grid
MODE 2: Store A Local Grid Transformation for Later Use

SYNTAX

\[ \text{STAC \{TRAN\} [MATR|PLAN|POIN] \{N_1, .., N_n\} \{N_{n+1}, .., N_m\} \{N_7, .., N_9\}} \]

TRAN

A local grid transformation is stored for later use. Only a single transformation can be stored; this may be replaced as often as needed. The transformation may be later used by specific FREEFORM™ commands that allow the use of the STACk modifier.

MATR

The 9-component transformation matrix \((T)\) between the local \((x)\) and the global \((X)\) coordinate systems is specified directly. The transformation maps the global system to the local system as \(x_i = T_{ji} X_j\). The index \(j\) varies the fastest. Each row of the transformation matrix is interpreted as a unit vector directed along the \(x_i\) direction. This is the default option.

PLAN

The plane of transformation is specified by the coordinates of a point on the plane and the direction cosines normal to the plane. The transformation is then computed by taking \(x_1\) to be the unit normal to the plane, \(x_2\) is computed by intersecting the plane with the bounding box of the domain, and \(x_3\) is computed as the cross product of \(x_1\) and \(x_2\). The user has no control over the directions of \(x_1\) and \(x_2\). However, they are guaranteed to be in the specified plane and mutually perpendicular.

POIN

The plane of transformation is specified by the coordinates of 2 points. The plane is assumed to pass through the 2\(^{nd}\) point and the normal points from the 1\(^{st}\) to the 2\(^{nd}\) point. The transformation is computed in the same way as the previous option.

\(N_1, .., N_n\)

The 1\(^{st}\) through 3\(^{rd}\) components of the transformation matrix if the MATRIX modifier is present, the \((x, y;\) for 2D\) or \((x, y, z;\) for 3D\) coordinates of the point on the plane of transformation if the PLANE modifier is present and the coordinates of the 1\(^{st}\) point if the POINT modifier is present. There is no default value.

\(N_{n+1}, .., N_m\)

The 4\(^{th}\) through 6\(^{th}\) components of the transformation matrix if the MATRIX modifier is present, a vector (or direction cosines) to specify the normal to the plane of transformation if the PLANE modifier is present and the coordinates of the 2\(^{nd}\) point (on the plane of transformation) if the POINT modifier is present. There is no default value.

\(N_7, .., N_9\)

The 7\(^{th}\) through 9\(^{th}\) components of the transformation matrix if the MATRIX modifier is present; otherwise this input is ignored. There is no default value.

EXAMPLES

\[ \text{STACk TRANsformation between local & global grid is:} \]
\[ 1 \ 0 \ 0 \]
\[ 0 \ 0 \ -1 \]
\[ 0 \ 1 \ 0 \]

\[ \text{STACk TRANsformation between local & global grid is:} \]
\[ 1.0 \ \ 0.0 \ \ 0.0 \]
\[ 0.0 \ \ 0.9950040 \ \ -0.0998334 \]
\[ 0.0 \ \ 0.0998334 \ \ 0.9950040 \]

\[ \text{STACk TRANsformation for PLANE at (0.12, 0.55) normal vector as: (1, -1)} \]

\[ \text{STACk TRANsformation for PLANE at (0.12, 0.55, 0.012) normal vector as: (1, -1, 0)} \]

\[ \text{STACk TRANsformation between POINTS (0.12, 0.55, 0.012) (0.15, 0.47, 0.012)} \]
MODE 3: Store Scaling Factors to Normalize Output of Variables

SYNTAX

STAC  \{WRIT\} \{\Phi|OFF\} \{a\} [b]

WRIT

The output produced by the \texttt{WRITE} command for the specified variable is scaled by \(a\) and \(b\) according to:

\[
\Phi_{\text{out}} = a \cdot \Phi + b
\]

\(\Phi\)

A symbol that denotes the variable for which the output is required. The valid symbols include those listed in Table 2.8.1-3 plus the user defined variables (\texttt{ALLOCATE} command) and the real type variables defined in the initialization file (\texttt{xxxINIT.ACR}). There is no default value; a symbol must be specified.

OFF

Any previous \texttt{STACK WRITE} commands are deactivated; new commands may follow.

\(a\)

The multiplier factor for the variable. There is no default value.

\(b\)

The additive constant for scaling the variable. The default value is 0.

COMMENTS

Up to 10 \texttt{STACK WRITE} commands each with its own \(\Phi\) may be active at any given time.

EXAMPLES

\texttt{STACk WRITE T} by scaling with 1.8 and add 32 to convert deg Celsius to Fahrenheit.

\texttt{STACk WRITE P} by scaling with 1.00E5 and add 0.
Keyword Commands

COMMAND    STATISTICS

PURPOSE    To compute and obtain output of the statistics for a dependent variable for a selected
            subregion.

SYNTAX    STAT  {Φ} [MAXI] [subrgn] [OFF] [fname] [TABL] [Vfrq] [TIME]

Φ    A symbol for the dependent variable for which the statistics are required. By default, the
     computed statistics consist of the minimum, maximum, mean and standard deviation, and the
     location of the minimum and the maximum. If the modifier MAXI is present then only the
     maximum and its location is computed. The valid symbols are listed in Table 2.8.1-3. One and
     only one character string must be specified for each command.

MAXI    Only the maximum value and its location is computed.

subrgn    The subregion for computation of statistics. If no subregion is specified, the entire domain is
          selected.

OFF    Computation of statistics for the specified variable and subregion is deactivated.

fname    The file name for output. A different output file may be specified for each command. If no file
          name is specified then the output is directed to the most recent previously specified file. If no
          previous file was specified, then the output is directed to a file with the same name as the
          Standard Output file but with the extension removed and replaced by “_STATS.TMP”. For
          example, if the Standard Output file is “PROBLEM.OUT”, then the file is named “PROBLEM_
          STATS.TMP”. A summary of output is also printed to the standard output device at the end of
          simulations.

TABL    If this modifier is specified, then a tabulated summary of the computed statistics appears in the
          standard output file at the end of simulations.

Vfrq    The frequency (step or time interval) of output. See Section 3.7 for further details. The default
          value is set so that output is obtained at every step of simulations.

TIME    By default, Vfrq is interpreted to be the frequency of computations in terms of number of steps.
          If this modifier is present, then Vfrq is interpreted to be the time interval between successive
          computations.

COMMENTS    The user should perform these computations only at the required frequency since frequent computations will
             results in increased computation time.

EXAMPLES    STATistics for U for the entire domain
            STATistics for T MAXImum for SELEcted region every 20 steps !Compute only maximum
            STATistics for T for SELEcted region every 20 steps with TABLEs of output
            STATistics for T for subregion defined by ID=VAULT every TIME=0.50 units
            STATistics for T for iD=VAULT OFF !!! Switch off previously specified STAT command
            STATistics for U to ‘FLUX.OUT’ for SELEcted region at TIME interval of 0.4
COMMAND  STORAGE COEFFICIENT

PURPOSE  To specify the STORage coefficient for the governing differential equations. This command is effective only for the PORFLOW™ Software Tool.

MODE 1:  STORage Coefficient as a General Function

SYNTAX  STOR  \{Φ\} \{func[ξ]\} \{N₁, N₂, ..., Nₙ\}fname \{TOTA\} \{subrgn\}

Φ  A symbol for the dependent variable for which the storage coefficient is specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified. The typical storage or accumulation term for a transport equation is represented as:

\[ \frac{\partial}{\partial t}(\alpha \rho \Phi) \]

where \(\alpha\) is the storage coefficient, \(\rho\) is the fluid density and \(\Phi\) is dependent variable.

func  One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. For this input, the function specifies the value of the appropriate storage coefficient for the corresponding \(\Phi\) variable. If no function is specified then the value is assumed to be constant.

ξ  One of the independent variables listed in Table 4.2.2. If no independent variable is specified, the variable is assumed to be time.

\(N₁, ..., Nₙ\)  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

fname  The name of the file containing the numerical values \(N₂\) through \(Nₙ\). This option is available only for selected functions. See Section 3.3 for additional information.

TOTA  This modifier is effective only for the PORFLOW™ Software Tool. By default it is assumed that any chemical species is adsorbed only in the wetted part to the solid; in this case the effective retardation coefficient (\(R_D\)) is defined by Equation (6) below.

However if the TOTA modifier is present, then the species is assumed to be stored in the total solid and the effective retardation coefficient is defined by Equation (7) below:

\(\text{subrgn}\)  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

COMMENTS

The term "storage coefficient" is normally applied only to the transport of chemical species. However, this command may be used to specify the "storage coefficient" for any of the governing transport equations. This mode of the command is currently implemented only for the PORFLOW™ Software Tool and then only for the pressure and species equations.

In a fluid-solid matrix the total mass of a species per unit volume is given by:

\[ C^k_e = \theta_E S^n C^k + (1 - \theta_E) S_s \rho_s C^k_s. \]  \hspace{1cm} (1)

In this equation the superscript \(k\) denotes the \(k\)th component of a group of species and:

- \(C_e\) is the equivalent concentration of the species in units of \([\text{M/L}^3]\) (e.g. kg/m³),
- \(C\) is the concentration of the species in the fluid phase in units of \([\text{M/L}^3]\) (e.g. kg/m³),
- \(C_s\) is the concentration of the species in the solid phase in units of \([\text{M/M}]\) (e.g. kg/kg of solid),
- \(\theta_E\) is the effective porosity of the host matrix,
- \(S\) is the phase saturation,
- \(S_s\) is fraction of solid that contains the species; it is equal to 1 if species is present throughout the solid and is equal to \(S^n\) if only the ‘wet’ component of the solid contains the species,
- \(\rho_s\) is the particle (not bulk) density of the solid, and

The PORFLOW™ provide for non-linear equilibrium between phases as well as explicit solution of the concentration of each chemical species in different fluid and solid phases with full accounting of phase exchange and geochemistry of species (see PRECIPITATION and TRANSPORT commands). However, a
The common assumption in environmental applications is that a chemical equilibrium exists between the fluid and the solid constituents of the porous matrix. The concentrations in the fluid and the solid are then related through a linear or non-linear isotherm (Freeze and Cherry 1979). With \( k_d \) as the sorption or partitioning coefficient for the species, the concentrations in the solid and the fluid are related by:

\[
C_s^k = k_d^k C^k. \tag{2}
\]

In this equation, \( C \) is in units of \([M/L^3]\), \( C_s \) in units of \([M/M]\) and \( k_d \) in units of \([L^3/M]\). Consequently Equations 1 and 2 combine to yield:

\[
C_e^k = \varphi_E \left( 1 + \frac{S_s}{S^n} \frac{1 - \theta_E}{\theta_E} \rho_s k_d^k \right) C^k.
\]

The saturated porosity, \( \varphi_E \), and the retardation coefficient, \( R_D \), are defined by:

\[
\varphi_E = S^n \theta_E. \tag{4}
\]

\[
R_D^k = 1 + \frac{S_s}{S^n} \frac{1 - \theta_E}{\theta_E} \rho_s k_d^k. \tag{5}
\]

**PORFLOW™** provides for \( S_s \) to be set equal to fluid saturation, \( S^n \) or to unity. The default assumption is the former and then saturation drops out of the retardation relation. In this case:

\[
R_D^k = 1 + \frac{1 - \theta_E}{\theta_E} \rho_s k_d^k. \tag{6}
\]

If it is assumed that \( S_s = 1 \), then it implies that some mechanism is available for the chemical species to move into the dry solid which is not connected by effective porosity. It further implies that even if saturation falls to zero, some concentration may remain in the dry solid matrix. In this limiting case, there is no reason for the solid concentration to be related to a hypothetical fluid concentration and the basic isotherm assumption that the species may move freely between the fluid and the solid phases is no longer valid. This assumption then yields:

\[
R_D^k = 1 + \frac{1 - \theta_E}{\varphi_E} \rho_s k_d^k. \tag{7}
\]

**EXAMPLES**

Generic examples for this command are given in Section 4.4. The command keyword (**STORAGE**) must replace the keyword used in these examples.
MODE 2: Dynamic Computation of Storage or Accumulation Term

SYNTAX  

STOR \{\Phi\} \{DYNA\}

\Phi 
One or more symbols for the dependent variables for which the input is specified. Valid symbols are listed in Table 2.7.1. There is no default value; at least one symbol must be specified.

DYNA 
A typical storage term, \( S_\Phi \), for a transport equation and its numerical representation is given by the relation:

\[
S_\Phi = \frac{\partial}{\partial t} (\alpha \rho \Phi) = \frac{(\alpha \rho \Phi)^{n+1} - (\alpha \rho \Phi)^{n}}{\delta t},
\]

where superscripts \( n \) and \( n+1 \) denote time steps. At the start of a step the total storage for the variable may be computed from the current available values of \( \alpha, \rho \) and \( \Phi \) or the product \( (\alpha \rho \Phi) \) can be stored at the end of \( n^{th} \) time step and re-used at the \( n+1^{th} \) step. When \( \alpha \) and \( \rho \) are constants, the two procedures lead to identical results. However, if \( \alpha \) and \( \rho \) are functions of other variables, then depending on the method and sequence of solution of equations, \( \alpha \) and \( \rho \) may be revised after \( \Phi^n \) was computed. That is the prevailing values of \( \alpha \) and \( \rho \) may have been used to compute \( \Phi^n \) at the \( n^{th} \) time step and then modified by subsequent operations. For strict compliance with balance equations the product of \( (\alpha \rho \Phi) \) used at the \( n^{th} \) time step is stored and used in computing the values at the \( n+1 \) step. This is the default practice in ACRi software tools.

If \( DYNA \) modifier is present, then the required product \( (\alpha \rho \Phi)^n \) is recomputed from the most recent values of the variables at the start of the \( n+1^{th} \) step. This removes the need for storage arrays to store the previous product and also accounts for dynamic changes in \( \alpha \) and \( \rho \). However, the strict mass balance of the \( \Phi \) variables may not be achieved if \( \alpha \) and \( \rho \) change significantly from one step to another.

EXAMPLES

STOR term for C computed DYNamically
STOR term for C, K and E computed DYNamically
MODE 3: Deactivate or Reactivate Storage or Accumulation Term

SYNTAX

 Stark {Φ} {OFF|ON}

Φ One or more symbols for the dependent variables for which the input is specified. Valid symbols are listed in Table 2.7.1. There is no default value; at least one symbol must be specified.

OFF The storage or accumulation term in the governing equation for the variable is deactivated. This is equivalent to solving the steady state form of the equation.

ON Storage term, if previously deactivated, if re-activated.

COMMENTS

This command may be used to explore the effect of the storage on the solution of the transport equation for a selected variable. At any given time at least one of the three (storage, convection and diffusion) terms in the transport equation must stay active, otherwise the transport equation has no solution.

EXAMPLES

STOR term for C is OFF
STOR term for C is now ON again
MODE 4: Minimize Memory Allocation for Storage or Accumulation Term

SYNTAX

STOR \{MINI\MIN\}

MINI

A typical storage term for a transport equation, S, is given by the relation:

\[ S_\Phi = \frac{\partial}{\partial t} (\alpha \rho \Phi) = \frac{(\alpha \rho \Phi)^{n+1} - (\alpha \rho \Phi)^n}{\delta t}, \]

By default if \( \alpha \) and \( \rho \) vary with time, then product \( \alpha \rho \Phi \) must be stored at the end of \( n^{th} \) time step for strict mass balance of the variable. This requires the allocation of memory to store the product for each variable. This is the default practice in ACRi software tools.

However if MINI modifier is present, then the required product \( (\alpha \rho \Phi)^n \) is recomputed from the most recent current values of the variables at the start of the \( n+1^{th} \) step.

MIN

Same as MINI.

EXAMPLES

STOR term allocate MINimum storage
Keyword Commands

COMMAND    SWIRL

PURPOSE    To specify the transformation of the velocity components from an induced swirl. This command is effective only for the ANSWER™ Software Tool.

MODE 1:    Swirl induced by Vanes at Fixed Angles or by Solid Body Rotation

SYNTAX    SWIR {ANGL|SOLI} [LOCA|FLUX|SOUR] {N_1} {N_2, . . . N_n} [R_{swirler}] [subrgn] [dir]

ANGL    Swirl is induced in the manner of the flow passing vanes at a fixed angle. With \( \alpha \) as the vane angle, the tangential (swirling) velocity, \( V_T \), at the swirl plane is computed as:

\[
V_T = V_N \tan (\alpha),
\]

where \( V_N \) is the normal component of velocity at the surface.

SOLI    Swirl is induced in the manner of solid body rotation. With \( \omega \) as the angular velocity, the tangential velocity (swirl component), \( V_T \), at the swirl plane is computed as:

\[
V_T = 2 \pi \omega r,
\]

where \( r \) is the radius from the specified center of rotation.

LOCA    The normal component of velocity at the swirl plane, \( V_N \), is computed as:

\[
V_N = \sum_i n_i U_i
\]

where \( n_i \) is the normal vector and \( U_i \), the velocity vector just upstream of the swirl plane. This is the default option if none is specified.

FLUX    The normal component of velocity at the swirl plane, \( V_N \), is computed as:

\[
V_N = \frac{q}{\rho A}
\]

where \( \rho \) is the fluid density, \( q \) is the flow rate and \( A \) is the area of the surface.

SOUR    The normal component of velocity at the swirl plane, \( V_N \), is computed as:

\[
V_N = \frac{q}{\rho A}
\]

where \( \rho \) is the fluid density, \( q \) is the source and \( A \) is the area of the surface. If this modifier is present, then a TRANSFER command with SOURCE modifier must have been previously specified for the same subrgn.

subrgn    The subregion that defines the surface at which the velocity transformation occurs. If the subregion was previously defined by a LOCATE MATCH command, then the transformation is applied only to the 2nd surface. A subregion must be defined; there is no default value.

dir    The orientation index for the element boundary associated with the input. See Section 3.5 for available choices. There is no default value for this input. A value must be supplied unless the subrgn was defined by a LOCATE PAIR or LOCATE MATCH command.

N_1    The vane angle, \( \alpha \), in degrees if the ANGLE modifier is specified or the angular velocity of rotation, \( \omega \), if the SOLID modifier is specified. The numerical value of \( \alpha \) must be less than 89.9. There is no default value for this input.

N_2, N_n    The (x, y) or (x, y, z) coordinates of the center of the swirl around which the velocity vector is rotated. The center must lie in the plane of the surface defined subrgn and dir. The transformed tangential velocity is assumed to lie in this plane. Two values are needed for 2D and 3 for 3D geometry. There is no default value for this input.
The radius of the swirler. This is radius of the circle (in the plane of the surface) within which the velocity components are transformed. Any velocity components in the surface outside this radius are not transformed. The default value $10^{30}$.

**COMMENTS**

The local Cartesian components of velocity at the swirl plane are computed from the normal and tangential velocity components by transforming from cylindrical to Cartesian components. The global Cartesian components of velocity are obtained by transforming the local components as:

$$ U_j = T_{ij} u_i $$

where $T_{ij}$ is the transformation vector and $u_i$ is the velocity vector.

The transformation is applied only if the computed $V_N > 0$; otherwise the command is ignored. The computed Cartesian velocity components are set at a location just upstream of the swirl surface. A `BLOCK` or `FIX` command must be used to ensure that these values are not overwritten by values computed from the governing momentum equations.

**EXAMPLES**

```plaintext
SWIRL velocity with a vane ANGLE of 50 degrees center at (0.14, 0.22, 0.0) ID=Q_TRANSFER
SWIRL vane ANGLE = 50 degrees VN from LOCAL velocity; center at (0.14, 0.22, 0.0) ID=Q_TRANSFER
SWIRL vane ANGLE = 50 degrees VN from FLUX; center at (0.14, 0.22, 0.0) ID=Q_TRANSFER
SWIRL vane ANGLE = 50 degrees VN from SOURce; center at (0.14, 0.22, 0.0) ID=Q_TRANSFER
SWIRL velocity ANGLE of 50 deg. Center: (0.14, 0.22, 0.0) within radius of 0.25 meters ID=Q_TRANSFER
SWIRL with angular speed of 200 radian/second center at (0.14, 0.22, 0.0) ID=Q_TRANSFER
SWIRL with 200 radians/second; center: (0.14, 0.22, 0.0) within radius of 0.25 meters ID=Q_TRANSFER
```
MODE 2: Swirl from User Specified Value of Function

SYNTAX

SWIR [LOCA|FLUX|SOUR] [subrgn] [dir] {N1} [N2, ..,Nn] [fname] [Nn+1,..,Nm] [Rswirler]

LOCA  See Mode 1 Specification.
FLUX  See Mode 1 Specification.
SOUR  See Mode 1 Specification.
subrgn  See Mode 1 Specification.
dir  See Mode 1 Specification.
N1, .., Nn  The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.
fname  The name of the file from which numerical values N2 through Nn are read. This option can be used only if the selected function is a table or one of the series functions. See Section 3.3 for further information.
Nn+1, ..,Nm  The (x, y) or (x, y, z) coordinates of the center of the swirl around which the velocity vector is rotated. The center must lie in the plane of the surface defined subrgn and dir. The transformed tangential velocity is assumed to lie in this plane. Two values are needed for 2D and 3 for 3D geometry. There is no default value for this input.
Rswirler  The radius of the swirler. This is radius of the circle (in the plane of the surface) within which the velocity components are transformed. Any velocity components in the surface outside this radius are not transformed. The default value 10^3.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (SWIRL) must replace the keyword and the dependent variable (φ ) used in these examples. Some additional examples that illustrate the use of the attributes specific to this command are given below.

SWIRL tangential velocity 0.25; center at (0.14, 0.22, 0.0) ID=SWIRL
SWIRL tangential velocity 0.25; normal from LOCAL; at (0.14, 0.22, 0.0) ID=SWIRL
SWIRL tangential velocity 0.25; normal from FLUX; at (0.14, 0.22, 0.0) ID=SWIRL
SWIRL tangential velocity 0.25; normal from SOUR; at (0.14, 0.22, 0.0) ID=SWIRL
SWIRL factor of 0.25; center: (0.14, 0.22, 0.0) within radius of 0.25 meters ID=SWIRL
Keyword Commands

**MODE 3:** Swirl Profile or Mapping from a data file

**SYNTAX**

```
SWIR [PROFile] [RADial] {subrgn} {dir} {N1,N2,N3,N4} {fname} [SCALE [NONE] N5,N6] [AXIS N7,N8,N9] [ALWA] [FUEL=N10] [DIAG] (Φ1..Φn)
```

**PROF**

Implies that a profile of the velocity components and other specified variables be read in from a data file.

**RADI**

Implies a radial swirler. The default is an axial swirler.

*For an axial swirler, the axial velocity component is scaled to match the mass flow.* The other velocity components are then scaled by the same factor. If the turbulent kinetic energy is listed as one of the dependent variables on this command, then it is scaled by the square of the scale factor. *The velocity profile data is assumed to be a function of the radius.*

*For a radial swirler, the radial velocity component is scaled to match the mass flow.* The other velocity components are scaled by the same factor. If the turbulent kinetic energy is listed as one of the dependent variables on this command, then it is scaled by the square of the scale factor. *The velocity profile data is assumed to be a function of the axial distance.*

**subrgn**

The subregion that defines the surface at which the velocity transformation occurs and also defined to be an inlet or open or dirichlet boundary. A subregion must be defined; there is no default value.

**dir**

The orientation index for the element boundary associated with the input. See Section 3.5 for available choices. There is no default value for this input. A value must be supplied unless the subrgn was defined by a LOCATE PAIR.

**N1**

The mass flow through the subregion. This subregion should be defined as an INLET or an OPEN or DIRICHLET boundary. There are no default values for this input.

**N2, N3, N4**

The (X, Y, Z) coordinates of the origin of the local cylindrical system. This input is mandatory for both axial and radial swirlers. There are no default values for this input.

**fname**

The name of the file from which profile data are read in. This file is mandatory. The file consists of an optional header block ending with a “End Header” string starting from the first column, followed by columns of data, one per variable. The first four data columns are the independent variable (axial distance for radial swirler / radial distance for axial swirler), axial velocity, radial velocity and the swirl velocity. It may also contain additional columns of data for the other variables specified on the command (in the same order). Extra columns of data are ignored.

**SCALE**

Scale factors are specified to normalize the transformed coordinate prior to interpolating the dependent variables from the profile data file. The min and max values of the independent variable should be specified. *In the absence of this modifier, the min value is set to zero and the max value to the actual maximum radial extent of the sub-region for an axial swirler, and to the actual min and max values of the axial extent of the sub-region for a radial swirler.* The independent variable is thus scaled to lie between 0 and 1.

**SCALE NONE**

Turns off all scaling. The independent variable is not scaled prior to doing the interpolation.

**N5, N6**

The min and max scale factors for the transformed coordinate for the SCALE modifier. The coordinate is transformed as \( r = (R - N5) / (N6 - N5) \). **Must be specified if the SCALE modifier is present without the NONE modifier.** In the absence of the SCALE modifier, these values are computed internally as described above.

**AXIS**

The axis of the transformation between the global 3D Cartesian system and the local cylindrical system applicable to the defined subregion. **For an axial swirler, this modifier and the associated data may be omitted,** in which case it is computed as the normal pointing into the mesh from a suitable boundary node. **For a radial swirler this input and the associated data is mandatory.**

**N7, N8, N9**

The three components of direction vector of the axis of the local cylindrical coordinate system. **There are no default values for a radial swirler.** For an axial swirler, in the absence of the AXIS modifier, these are computed as the normal pointing into the mesh from a suitable boundary node.

**FUEL**

This optional input specifies a fuel mass flow rate. The presence of this modifier causes the
Fuel Mass Fraction, $FU$, to be scaled to match the specified fuel mass flow rate.

$N_{10}$
The fuel mass flow rate if the `FUEL` modifier is specified. There is no default.

$\Phi_1..\Phi_n$
Optional list of scalar variables (except pressure) also to be interpolated from the profile data.

ALWA
This modifier causes the command to be executed at every iteration/time step. The default is to execute only once in the startup phase of the next `SOLVE` command. This behavior is analogous to the `SET` vs. `SET ALWAlays` command. This modifier may be used if the density is a function of the dependent variables and an iterative procedure is needed to determine the final boundary conditions.

DIAG
This modifier causes detailed diagnostics to be output. In the absence of the `DIAGnostics` modifier, only a brief summary is output for each swirler.

**COMMENTS**

This command only applies to a 3D Cartesian framework. A global 3D Cartesian to local cylindrical transformation is computed from the center and the axis. Any requested scaling is carried out. The velocity components and other variables are then interpolated from the profile data. The velocity components are then scaled to match the specified mass flux. These velocity components and other variables are then applied to the boundary specified by the sub-region.

If the turbulent kinetic energy, $K$, is also present on the command line, then it is also scaled as the square of the scaling for the velocity variables. However, the turbulent length scale, $L$, is not scaled.

If the fuel mass flow rate is specified, the fuel mass fraction, $FU$, is adjusted to match the specification.

A positive mass flow specification causes the flow to enter the domain whereas a negative mass flow specification causes the flow to leave the domain. If the data in the velocity profile file is not consistent with the mass flow specification, then a negative scale factor is computed. This has the effect of inverting the profile and reversing the sense of the swirl component.
EXAMPLES

**SWIRler PROFile** mdot=50.0 kg/s center= (0.4, 0.5, 1.0)
- FUEL mdotf=5 kg/s file='swirl3.dat'
  additional variables in file: T K L FU at ID=RGN3 Z+ **ALWAYs** detailed DIAGnostics on.

**SWIRler PROFile** mdot=10.0 kg/s center=(1.0,0.5,0.5)
- SCALing (3.53553E-02, 0.1060660) file='swirl3.dat'
  additional variables in file: T K L at ID=RGN2

The contents of file ‘swirl3.dat’:

Swirler mapping file for axial swirler:

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<thead>
<tr>
<th>r</th>
<th>u</th>
<th>Ur</th>
<th>Ut</th>
<th>T</th>
<th>K</th>
<th>L</th>
<th>FU</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-0.1</td>
<td>0</td>
<td>0.1</td>
<td>300</td>
<td>0.001</td>
<td>0.1</td>
<td>0.01</td>
</tr>
<tr>
<td>0.1</td>
<td>-0.2</td>
<td>0</td>
<td>0.2</td>
<td>350</td>
<td>0.002</td>
<td>0.15</td>
<td>0.02</td>
</tr>
<tr>
<td>0.2</td>
<td>-0.3</td>
<td>0</td>
<td>0.3</td>
<td>400</td>
<td>0.003</td>
<td>0.2</td>
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<td>-0.4</td>
<td>0</td>
<td>0.4</td>
<td>450</td>
<td>0.004</td>
<td>0.25</td>
<td>0.04</td>
</tr>
<tr>
<td>0.4</td>
<td>0</td>
<td>0</td>
<td>0.5</td>
<td>500</td>
<td>0.0001</td>
<td>0.3</td>
<td>0.05</td>
</tr>
<tr>
<td>0.5</td>
<td>0.6</td>
<td>0</td>
<td>0.6</td>
<td>550</td>
<td>0.006</td>
<td>0.35</td>
<td>0.06</td>
</tr>
<tr>
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<td>0.7</td>
<td>0</td>
<td>0.7</td>
<td>600</td>
<td>0.007</td>
<td>0.4</td>
<td>0.05</td>
</tr>
<tr>
<td>0.7</td>
<td>0.8</td>
<td>0</td>
<td>0.8</td>
<td>400</td>
<td>0.008</td>
<td>0.45</td>
<td>0.04</td>
</tr>
<tr>
<td>0.8</td>
<td>0.9</td>
<td>0</td>
<td>0.9</td>
<td>300</td>
<td>0.009</td>
<td>0.5</td>
<td>0.03</td>
</tr>
<tr>
<td>0.9</td>
<td>1.0</td>
<td>0</td>
<td>1.0</td>
<td>300</td>
<td>0.01</td>
<td>0.55</td>
<td>0.02</td>
</tr>
<tr>
<td>1.0</td>
<td>1.0</td>
<td>0</td>
<td>0.0</td>
<td>300</td>
<td>0.01</td>
<td>0.6</td>
<td>0.01</td>
</tr>
</tbody>
</table>

**SWIRler PROFile** RADIal mdot=50.0 kg/s center=(0.5,0.5,0.5)
- AXIS=(1,0,0) file='swirl3-r.dat'
  additional variables in file: T K L FU at ID=RGN1

**SWIRler PROFile** RADIal mdot=50.0 kg/s center=(0.5,0.5,0.5) AXIS=(1,0,0)
- FUEL mdotf=5 kg/s file='swirl3-r.dat'
  additional variables in file: T K L FU at ID=RGN1 **ALWAYs** detailed DIAGnostics on.

The contents of file ‘swirl3-r.dat’:

Swirler mapping file for radial swirler:

<table>
<thead>
<tr>
<th>X</th>
<th>U</th>
<th>Ur</th>
<th>Ut</th>
<th>T</th>
<th>K</th>
<th>L</th>
<th>FU</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-0.5</td>
<td>-0.0</td>
<td>0.0</td>
<td>300</td>
<td>0.005</td>
<td>0.1</td>
<td>0.01</td>
</tr>
<tr>
<td>0.1</td>
<td>-0.4</td>
<td>-0.1</td>
<td>0.1</td>
<td>350</td>
<td>0.004</td>
<td>0.15</td>
<td>0.02</td>
</tr>
<tr>
<td>0.2</td>
<td>-0.3</td>
<td>-0.2</td>
<td>0.2</td>
<td>400</td>
<td>0.003</td>
<td>0.2</td>
<td>0.03</td>
</tr>
<tr>
<td>0.3</td>
<td>-0.2</td>
<td>-0.3</td>
<td>0.3</td>
<td>450</td>
<td>0.002</td>
<td>0.25</td>
<td>0.04</td>
</tr>
<tr>
<td>0.4</td>
<td>-0.1</td>
<td>-0.4</td>
<td>0.4</td>
<td>500</td>
<td>0.001</td>
<td>0.3</td>
<td>0.05</td>
</tr>
<tr>
<td>0.5</td>
<td>0</td>
<td>-0.5</td>
<td>0.5</td>
<td>550</td>
<td>0.0001</td>
<td>0.35</td>
<td>0.06</td>
</tr>
<tr>
<td>0.6</td>
<td>0.1</td>
<td>-0.4</td>
<td>0.4</td>
<td>600</td>
<td>0.001</td>
<td>0.4</td>
<td>0.05</td>
</tr>
<tr>
<td>0.7</td>
<td>0.2</td>
<td>-0.3</td>
<td>0.3</td>
<td>650</td>
<td>0.002</td>
<td>0.45</td>
<td>0.04</td>
</tr>
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<td>0.3</td>
<td>-0.2</td>
<td>0.2</td>
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<td>0.003</td>
<td>0.5</td>
<td>0.03</td>
</tr>
<tr>
<td>0.9</td>
<td>0.4</td>
<td>-0.1</td>
<td>0.1</td>
<td>750</td>
<td>0.004</td>
<td>0.55</td>
<td>0.02</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5</td>
<td>-0.0</td>
<td>0.0</td>
<td>800</td>
<td>0.005</td>
<td>0.6</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Keyword Commands

COMMAND SYMMETRY

PURPOSE To identify an external boundary of the computational domain as a symmetry plane or axis.

SYNTAX SYMM {dir} [subrgn] [OFF]

dir The orientation index for the symmetry boundary. See Section 3.5 for available choices. There is no default value; a value must be specified.

subrgn The subregion to be identified as a symmetry boundary. If no subregion is specified, the outermost "dir" oriented boundary of the entire computational domain is selected.

OFF Previously specified symmetry boundary for the identified subregion is deactivated. A new specification for this subregion may follow.

COMMENTS

A symmetry boundary, by definition, is assumed to be a boundary where the normal fluxes for all dependent variables are zero; that is no amount of the property in question leaves or enters the symmetry boundary.

EXAMPLES

SYMMetry at Y- boundary
SYMMetry at Y- for ID=B_SYMMETRY
SYMMetry OFF for Y- and ID=B_SYMMETRY
COMMAND   THERMAL

PURPOSE   To specify thermal properties of the porous matrix, or of the planar or linear features. This command is effective only for the PORFLOW™ Software Tool.

SYNTAX   THER [Cp, KTs, αL, αT] [subrgn]

Cp   Specific heat of the dry solid, Cps (≥ 0), with typical units as [J/(kg °K)]. The default value is 1000 if GAS or DENSITY GAS command is given otherwise it is 1.

KTs   Thermal conductivity of the dry solid, KTs (≥ 0), with typical units as [J/(m-s °K)]. The default value is 0.

αL   Longitudinal dispersivity, αL (≥ 0) with typical units as [m]. The default value is 0.

αT   Transverse dispersivity, αT (≥ 0) with typical units as [m]. The default value is 0.

subrgn   The subregion for which the input is specified. See Section 3.4 for more details. If no subregion is specified, then entire computational domain is selected.

APPLICABILITY   This command is available only for the PORFLOW™ Software Tool.

COMMENTS   More complex functional relations for specific heat can be specified by the SPECIFIC HEAT command, those for the thermal conductivity by the CONDUCTIVITY command and for the dispersivity by the DISPERSIVITY command. Those commands provide greater flexibility and their use is recommended over this command.

EXAMPLES   

THERmal properties cs = 26, kt = 45
THERmal props cs = 26, ks = 45, alfal = 0, alfat = 0.
THERmal properties ce = 26, ke = 45, alphal = 10, alfat = 2
Keyword Commands

**COMMAND**  TIDE

**PURPOSE**  To specify the height of the tide at an open boundary as a function of time and space. This command is effective only for the TIDAL™ Software Tool.

**MODE 1:**  Tide as a Cosine or Sine Function

**SYNTAX**  TIDE [dir] {COSI|SINE} {N} \{τ₁, a₁, Φ₁\} \{τₙ, aₙ, Φₙ\}

- **dir**  One of the character strings: EAST, WEST, NORTH, or SOUTH. It denotes the boundary of the domain of interest where the water elevation is specified as a function of time and space. If no direction is specified, then the tidal boundary is assumed to be at the west.

- **COSI**  The tide is a cosine function given by:

  \[ \eta = \sum_{n=1}^{N} \eta_n^n \cos (f^n t + \phi^n), \]

- **SINE**  The tide is a sine function given by:

  \[ \eta = \sum_{n=1}^{N} \eta_n^n \sin (f^n t + \phi^n), \]

- **N**  Number of sets of harmonic tidal components that follow. The default value is 0.

- **τ₁**  The time period of the 1<sup>st</sup> component of the tide. The default value is 0.

- **a₁**  The amplitude of the 1<sup>st</sup> component of the tide. The default value is 0.

- **Φ₁**  The phase of the 1<sup>st</sup> component of the tide. The default value is 0.

- **τₙ, aₙ, Φₙ**  Triplets of period, amplitude, phase lag for the 2<sup>nd</sup> through N<sup>th</sup> component of the tide.

**APPLICABILITY**  This command is available only for the TIDAL™ Software Tool.

**EXAMPLES**

- **TIDE** is COSIne function, 1 set: period=24 hrs, amplitude=30 cm, phase=12 hrs
- **TIDE** SOUTH is the sum of SINE functions, 2 sets: (24, 30, 0) (676, 10, 0)
MODE 2: Tide specified as a table of Time and Height

SYNTAX

TIDE [dir] {N\_sets} \{t\_1, \eta\_1\} \{t\_n, \eta\_n\}

\text{dir} \quad \text{One of the character strings: \textit{EAST, WEST, NORT}, or \textit{SOUTH}. It denotes the boundary of the domain of interest where the water elevation is specified as a function of time and space. If no direction is specified, then the tidal boundary is assumed to be at the west.}

N\_sets \quad \text{Number of sets of tide values which follow. The default value is 0.}

t\_1 \quad \text{The time at which the first tide height is specified. The default value is 0.}

\eta\_1 \quad \text{The tide height at time } t\_1. \text{ The default value is 0.}

t\_n, \ldots, \eta\_n \quad \text{Pairs of time and tide height for one complete tidal cycle}

APPLICABILITY

This command is available only for the \textit{TIDAL™} Software Tool.

EXAMPLES

TIDE WEST: (time, height) table, 5 sets: (0, 10) (3, 15) (9, 20) (12, 25) (24, 10)
MODE 3: Tide as a Linear Function of Distance and Time

SYNTAX

```
TIDE {LINE} {dir} {N_sets} {t_{11}, \eta_{11}, \eta_{12}} \{\xi_{\text{start}}, \xi_{\text{end}}\}
```

LINE

The tidal boundary condition at the specified boundary is taken to be a linear function of both time and distance along the boundary.

`dir`

One of the character strings: `EAST`, `WEST`, `NORTH`, or `SOUTH`. It denotes the boundary of the domain of interest where the water elevation is specified as a function of time and space. If no direction is specified, then the tidal boundary is assumed to be at the west.

`N_sets`

Number of sets of tide values which follow. There is no default value; a value must be specified.

`t_{11}`

The time at which the first tide height is specified.

`\eta_{11}`

The value of the tide at the first location (`Nn+1` below) on the specified boundary.

`\eta_{12}`

The value of the tide at the second location (`Nn+2` below) on the specified boundary.

`t_n, \eta_{n1}, \eta_{n2}`

Triplets of time, and tide at the first and second locations in the manner of `t_1, \eta_{11}, \eta_{12}`.

`\xi_{\text{start}}, \xi_{\text{end}}`

Grid coordinates of the starting and ending locations on the boundary for linear interpolation of the tide.

APPLICABILITY

This command is available only for the `TIDAL™` Software Tool.

EXAMPLES

```
TIDE NORth LINEar 3 sets: (0,1,0) (5.E4,5,10) (1.E5,0,1) at X: 0, 1000
```
MODE 4:  Tide Height Determined by a Connected Reservoir

SYNTAX  TIDE  {RESE} [dir] {Q_R}

RESE  The tidal boundary condition for tide height, \( \eta \), as a function of time, \( t \), at the specified boundary is given by:

\[
\frac{\partial \eta}{\partial t} = + \frac{Q}{Q_R},
\]

Here \( Q \) is the actual computed flow rate at the boundary and \( Q_R \) is the specified capacity factor.

dir  One of the character strings: EAST, WEST, NORTH, or SOUTH. It denotes the boundary of the domain of interest where the water elevation is specified as a function of time and space. If no direction is specified, then the tidal boundary is assumed to be at the west.

Q_R  The reservoir capacity factor. The value must be greater than or equal to zero. The default value is 0.

EXAMPLES

TIDE EAST boundary: REServoir, capacity factor = 1.0E10
Keyword Commands

COMMAND  TIME

PURPOSE  To set the initial simulation time for a problem.

SYNTAX   TIME  {N1}

N1        The starting time ($\geq 0$) for simulations. The default value is 0.

EXAMPLES

TIME = 50 years at start of simulations
COMMAND TITLE

PURPOSE To specify the problem title.

SYNTAX TITL followed by character information

COMMENTS The specification must be restricted to one 80 character record. Title specification is included in all output files generated by the ACRi Software.

EXAMPLES

TITLe ILLUSTRATIVE PROBLEM - DEFAULT SET UP - 07/01/93: ACRi/akr
COMMAND: TORTUOSITY

PURPOSE: To define tortuosity factor for the flow path in the porous material matrix. This command is effective only for the PORFLOW™ Software Tool.

SYNTAX: TORT [V₁, V₂, V₃] [subrgn]

V₁, V₂, V₃: The x, y and z direction components, respectively, of the tortuosity factor τᵢⱼ as shown in the equation below that are used to compute the effective diffusivity. Only components in the principal directions are used. The default value is 1.

\[ \Gamma^T_{ij} = (1 - \theta_T) k_S + \theta_T s \frac{\kappa_i}{\kappa} \] + \theta_E S \cdot \rho D_{ij} \]

\[ \Gamma^\phi_{ij} = \theta_D \tau_{ij} S \cdot \rho \cdot D^\phi_M + \theta_E S \cdot \rho \cdot D_{ij} \]

\[ D_{ij} = \alpha_T \delta_{ij} v + (\alpha_L \cdot \alpha_T v_i v_j \) \]

Where the superscript “n” denotes the nth fluid phase and:

- \( \Gamma^T_{ij}, \Gamma^\phi_{ij} \) are the diffusion coefficients for thermal and species equations,
- \( \theta_E, \theta_T, \theta_D \) are the effective, total and diffusional porosities of the material,
- \( k_S, k_i \) are the solid and fluid thermal conductivities,
- \( D_M \) is the molecular diffusivity of the species,
- \( D_{ij} \) is the dispersion tensor,
- \( v_i, v \) are the components of particle velocity and the modulus of velocity,
- \( S \) is the saturation of the fluid phase,
- \( \alpha_L, \alpha_T \) are the longitudinal and transverse dispersion coefficients,
- \( \rho \) is the density of fluid,
- \( \tau_{ij} \) is the tortuosity or constrictivity tensor.

APPLICABILITY, EXAMPLES

This command is currently available only for the PORFLOW™ Software Tool.

TORTUOSITY factors: 0.7, 0.6, 0.9
COMMAND: TRACK

PURPOSE: To compute particle tracks and their corresponding elapsed time in the flow field.

MODE 1: Particle Locations and Tracking Options

SYNTAX: TRAC [fname] [TABL] [STOP] [option] {N1, ..Nn} [Vstop, η0, Nfrq]

fname: The name of the file to which the output is directed. See Section 3.3 for additional information. If no name is specified then the output is directed to a file with the same name as the Standard Output file but with the extension removed and replaced by “_TRACK.TMP”. For example, if the Standard Output file is “PROBLEM.OUT”, then the file is named “PROBLEM_TRACK.TMP”. At any time only one track file can be open. If a new file name is given, then the previous file is closed and output is directed to the new file. A summary of output is also printed to the standard output device at the end of simulations.

TABL: The particle track data are printed in a tabular form at the end of simulations.

STOP: The particle stopping criterion is explicitly specified as one of the options listed in the table below. If no stopping criterion is specified then the particle is tracked to the end of simulations or till it reaches or crosses a boundary element.

option: The stopping option for the particle; the modifier STOP must be present for one of these options to be effective.

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>Particle tracking stops if its x-coordinate exceeds the Nn+1\textsuperscript{th} numerical value.</td>
</tr>
<tr>
<td>Y or R</td>
<td>Particle tracking stops if its y-coordinate exceeds the Nn+1\textsuperscript{th} numerical value.</td>
</tr>
<tr>
<td>Z or THETA</td>
<td>Particle tracking stops if its z-coordinate exceeds the Nn+1\textsuperscript{th} numerical value.</td>
</tr>
<tr>
<td>DIST</td>
<td>Particle tracking stops when its distance from the point of release exceeds the Nn+1\textsuperscript{th} numerical value. This is default option if STOP modifier is specified.</td>
</tr>
<tr>
<td>TIME</td>
<td>Particle tracking stops when the time exceeds the Nn+1\textsuperscript{th} numerical value.</td>
</tr>
<tr>
<td>ELAP</td>
<td>Particle tracking stops when the elapsed time from its moment of release exceeds the Nn+1\textsuperscript{th} numerical value.</td>
</tr>
<tr>
<td>FREE</td>
<td>Particle tracking stops if it reaches a free surface or zone of saturation.</td>
</tr>
</tbody>
</table>

N1, .., Nn: The coordinates of the starting location of the particle. Two values are required for the 2D and 3 for 3D input modes.

Vstop: The numerical value pertaining to the stopping criterion as described under options listed in the table above. There is no default value. A dummy numerical value must be specified if any numerical input follows for the time or frequency input below.

η0: In the transient solution mode, the starting time for the particle; the default value is 0. In the steady state solution mode, the time interval for the particle computations; the default value is 1.

Nfrq: The frequency index for providing the output in the particle track file. The output is obtained every Nn+3 (≥1) steps. For example, a specification of 10 result in output at the 10th, 20th, 30th, etc. step. If no input is specified, the frequency is assumed to be 1.
EXAMPLES

TRACks for particle start at: (35.0, 5.27)
TRACks for particle start at: (1.22, 10.0, 19.3) print TABLEs also
TRACK particle at: (1.22, 10.0) print TABLEs and save on file "TRACK.SAV"
TRACK particle at: (1.22, 10.0, 19.3) STOP at X=100. Starting time = 20 years
TRACK at: (1.2, 10.0) stop_distance 150 m; delta_t 0.1 yrs (steady state mode)
TRACks at: (35.0, 5.27) STOP TIME 200. Start at 0 yrs; output every 20 steps
TRACks for particle start at: (1.22, 10.0, 19.3) STOP at FREE surface.
TRACks at: (35.0, 5.27) STOP ELAPsed TIME 100. on file "PARTICLE.TRK"
MODE 2: Particle Tracking Factors

SYNTAX  
TRAC \{FACT\} [subrgn] [MULT | DIVI] \{V_{factor}\}

FACT  The particle velocity in the specified region is multiplied or divided by a specified factor.

subrgn  The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

MULT  Particle velocity in the selected region is multiplied by \(V_{factor}\). This is the default option.

DIVI  Particle velocity in the selected region is divided by \(V_{factor}\).

\(V_{factor}\)  The numerical value of the factor to modify the particle velocity. There is no default value.

EXAMPLES

TRACking FACTor for the particle is 0.5!! to account for retardation
TRACking FACTor: is 0.5 in the currently SELECTed subregion
TRACking FACTor is 2.5 in the subregion with ID=FAST
TRACking FACTor: DIVide particle velocity by 2.0!! To account for retardation
Keyword Commands

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>TRANSFER</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To specify the transfer of mass flux and fluid properties from one subregion to another.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>Direct Transfer of Computed Flux</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>TRANSFER [FLUX] [LOCA] [subrgn]</td>
</tr>
</tbody>
</table>

**FLUX**

The flux of mass is transferred from one surface to another. This type of transfer can only be defined by a LOCATE command with MATCHed pair option. The purpose of this command is to simulate embedded objects in the flow field such as pipes, pumps, propellers and swirlers which are not explicitly resolved by the computational grid. The gross effect of such embedded objects is to transfer fluid flux and properties (with or without modification) from one location to another. For effective use of this option the object should be declared as a blocked region (BLOCK command) or the values of all the variables within the object should be fixed with the FIX command.

The flux computed at the 1st surface ("donor") of a matched pair of surfaces is transferred to the 2nd surface ("receptor"). Both surfaces must be internal to computational domain; external surfaces are not allowed. There must be a one-to-one correspondence in the number of segments between the two surfaces.

The mass flux is computed at each segment of the donor surface from velocity components at the element located just upstream of the surface. This is then assumed to be the mass flux at the corresponding receptor surface. Any mass flux computed internally at the receptor surface is ignored. The momentum loss at the donor surface is equal to mass flux multiplied by the velocity components. At the receptor surface, by default, the flow enters normal to the surface. However, this can be changed by the LOCAL modifier below.

The loss (sink) of a conserved variable at the donor surfaces is computed as mass flux multiplied by the value of the variable at the element just upstream of the surface. An equal amount (source) is then injected at the element just downstream of the receptor surface.

**LOCA**

By default the flow at the receptor surface is assumed to enter with a velocity vector that is normal to the surface. If the LOCAL modifier is present, then it is assumed that the velocity components of the flow entering the receptor are equal to the locally prevailing values. Thus there is no net effect of the entering flow on the local momentum.

**subrgn**

The subregion for flux transfer. The subregion must have been previously defined by a LOCATE MATCH command. A subregion must be defined; there is no default value.

**EXAMPLES**

TRANSFER FLUXes from 1st surface (entrance) of subregion ID=Q_TRANSFER to the 2nd surface (exit)
TRANSFER FLUXes from 1st surface of SELECTed subregion to the 2nd with LOCAL momentum
MODE 2: Transfer of Computed Amount as Flux or Source

SYNTAX

```
TRANSFER {FLUX|SOUR} {func(ξ)} {N₁, N₂, .., Nₙ} [fname] [LOCA] [subrgn] [TOTA] [VOLU | AREA] [INTE]
```

**FLUX**

Same as Mode 1 except that the user specifies the mass flux rate at the matched surfaces. Fluid is extracted from elements just upstream of the 1st of a matched pair of surfaces and transferred to the corresponding elements just downstream of the 2nd surface. This is the default mode.

**SOUR**

Similar to **FLUX** modifier except that the mass is transferred as a source rather than as flux.

**func**

One of the modifiers listed in Table 4.2.1 that denotes the functional form of the source. If no function is specified, the value is assumed to be constant.

**ξ**

One of the independent variables listed in Table 4.2.2 if no independent variable is specified, the variable is assumed to be time.

**N₁,..,Nₙ**

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

**fname**

The name of the file containing the numerical values N₂ through Nₙ. This option is available only for selected functions. See Section 3.3 for additional information.

**LOCA**

See Mode 1 Specification.

**subrgn**

The sub region for flux or source transfer. If the **SOURCE** modifier without **AREA** is present, then the sub region must have been previously defined by a **LOCATE MATCH** or a **LOCATE CORRELATED** command. Otherwise the sub region must have been previously defined by a **LOCATE MATCH** command. A subregion must be defined; there is no default value.

**TOTA**

By default, the amount of source specified, or computed from **func** (ξ), is applied to each element of the **subrgn**. If this modifier is present then the amount is assumed to be the total quantity over whole of the **subrgn**. In this case, the source is distributed equally to all the elements of the **subrgn** unless the **VOLUme** or **AREA** modifiers are present.

**VOLU**

If the **TOTAL** modifier is absent, the source for each element is computed as: Q=qδV. Here q is computed from **func** (ξ) and N₁,..., Nₙ and, δV is the volume of the element. If the **TOTAL** modifier is present, the amount for each element is equal to: Q=qδV/V, where V is the volume of the total **subrgn**.

**AREA**

If **TOTAL** modifier is absent, the source for each element is computed as: Q=qδA, if **TOTAL** modifier is present, the source is computed as: Q=qδA/A. Here δA is the area of the element boundary and A is the total area of at the 1st (inlet) surface.

**INTE**

By default wall function treatment at the walls of the object is deactivated and the diffusive flux at the wall is set to zero. If the **INTERNAL** modifier is present then the wall treatment is retained and the wall diffusive flux is included in the computations.
EXAMPLES

Generic examples for this command are given in Section 4.4. The keyword `TRANSFER` must replace the keyword and the dependent variable (Φ) used in these examples. Some additional examples that illustrate the use of the attributes specific to this command are given below.

`TRANSfer FLUX = 0.0256` 1st surface (entrance) of subregion ID=Q_TRANSFER to the 2nd surface (exit)
`TRANSfer SOURce TOTAL amount of 0.0256 for SELECTed subregion`
`TRANSfer SOURce = 0.0256 per unit VOLUME for SELECTed region; treat as INTERNAL source`
`TRANSfer FLUX = 0.0256 per unit AREA for SELECTed region`
`TRANSfer SOURce TOTAL amount of 0.0256 and per unit VOLUME for SELECTed region`
`TRANSfer SOURce is TABLE per unit AREA: 3 sets (TIME, value) (0, 0.01), (100, 0.10), (200, -0.20)`
`TRANSfer FLUX is TABLE per unit AREA: 3 sets (TIME, value) from file ‘TRANSFER.FIL’`
MODE 3: Transfer Based Upon Drag Coefficient and Pressure Difference

SYNTAX

TRANSFER {DRAG} [FLUX|SOUR] [LOCA] [subrgn] [VOLU|AREA] [REVE] [INTE] {C_D} [D, β]

DRAG

The amount of mass transferred from one location to another is computed from a pressure gradient based drag law. It is assumed that flow occurs as a result of pressure difference across the object defined by the two surfaces. The fluid is extracted from elements just upstream of the 1st of a matched pair of surfaces and transferred to the corresponding elements just downstream of the 2nd surface. In all other respects command mode is identical to Mode 1. The flow rate is computed as:

\[ q = \rho \delta A \left( \frac{1}{2 C_D} \frac{P_{in} - P_{out}}{\rho} \left( \frac{\rho D}{\mu} \right)^\beta \right) \]

In the equation above:

- \( \rho \) is the fluid density
- \( \delta A \) is area of a segment (each element boundary) of the 1st surface through which the flow is extracted,
- \( C_D \) is the drag coefficient,
- \( P_{in} \) is the average pressure across the inlet surface (determined by taking an area-based average of the pressure at each segment of the surface) of the sub region,
- \( P_{out} \) is the average pressure across the outlet surface of the sub region,
- \( D \) is the hydraulic diameter that defines an appropriate Reynolds number,
- \( \mu \) is the dynamic viscosity, and
- \( \beta \) is an exponent that represents the dependence of the drag on Reynolds number (For laminar flow \( \beta \) is unity; for turbulent flow \( \beta \) is a weak function of Reynolds number. At high Reynolds number, for smooth pipes, the empirical value of \( C_D \) is 0.0791 and that of \( \beta \) is 0.25. Often for fully turbulent flow, the effect of Reynolds number on \( \beta \) is ignored and its value taken as zero).

FLUX See Mode 2 Specification.

SOUR See Mode 2 Specification.

LOCA See Mode 1 Specification.

subrgn The sub region for mass transfer which must have been previously defined by a LOCATE MATCH command. There is no default value.

VOLU See Mode 2 Specification.

AREA See Mode 2 Specification.

INTE See Mode 2 Specification.

REVE By default flow can only occur from 1st surface to the 2nd surface irrespective of the pressure gradient. If \( P_2 \) exceeds \( P_1 \) the source is set to zero. If this modifier is present then reverse flow is allowed if the pressure gradient is from the 2nd to the 1st surface.

\( C_D \) The drag coefficient, \( C_D \). There is no default value for this input.

\( D \) The hydraulic diameter, \( D \), that defines the Reynolds number. This value is required only if the exponent \( \beta \) is specified. There is no default value for this input.

\( \beta \) The exponent \( \beta \) for the drag coefficient. The default value is zero.
This mode of the **TRANSFER** command is automatically selected if the **DRAG** modifier is present and there are no more than 3 numerical values on the command.

**EXAMPLES**

```
TRANsfer DRAG C_drag = 0.10 for subregion ID=Q_TRANSFER
TRANsfer as FLUX DRAG C-drug = 0.5 Length scale = 0.2 beta=0.25 ID=Q_TRANSFER
TRANsfer DRAG as SOURCE:  CD = 0.10 Hydraulic Dia = 0.2 beta =0.25 by VOLUME ID=Q_TRANSFER
TRANsfer DRAG as FLUX:  CD = 0.10 Hydraulic Dia = 0.2 beta =0.25 by AREA ID=Q_TRANSFER
TRANsfer DRAG SOURCE:  CD=0.10 Hyd_Dia=0.2 beta =0.25 allow REVERse flow ID=Q_TRANSFER
```
MODE 4: Transfer due to Pressure Difference across Sub-Grid Scale Holes

SYNTAX

TRANSFER {DRAG} {FLUX | SOUR} [LOCA] [subrgn] [VOLU | AREA] [REVE] [INTE] {CD, D, N, L} \{β\}

DRAG

The amount of mass transferred from one location to another is computed from a pressure gradient based drag law. This simulates flow through small holes that are not explicitly resolved by the grid. It is assumed that flow occurs as a result of pressure difference across the holes. The fluid is extracted from elements just upstream of the 1st of a matched pair of surfaces and transferred to the corresponding elements just downstream of the 2nd surface. The flow rate is computed as:

\[
q = \rho N \frac{\pi D^2}{4} \left[ \frac{1}{2 CD} \frac{P_{in} - P_{out}}{\rho} \left( \frac{\rho D}{\mu} \right)^{\beta} \frac{D}{L} \right]^{1 - \beta},
\]

In the equation above:

- \(\rho\) is the fluid density
- \(N\) is the number of holes,
- \(D\) is the diameter of holes,
- \(CD\) is the drag coefficient,
- \(P_{in}\) is the average pressure across the inlet surface (determined by taking an area-based average of the pressure at each segment of the surface) of the sub region,
- \(P_{out}\) is the average pressure across the outlet surface of the sub region,
- \(D\) is the hydraulic diameter that defines an appropriate Reynolds number,
- \(\mu\) is the dynamic viscosity,
- \(L\) is the length of each hole, and
- \(\beta\) is an exponent that represents the dependence of the drag on Reynolds number (For laminar flow \(\beta\) is unity; for turbulent flow \(\beta\) is a weak function of Reynolds number. At high Reynolds number, for smooth pipes, the empirical value of \(CD\) is 0.0791 and that of \(\beta\) is 0.25. Often for fully turbulent flow, the effect of Reynolds number on \(\beta\) is ignored and its value taken as zero).

FLUX

See Mode 2 Specification.

SOUR

See Mode 2 Specification.

LOCA

See Mode 1 Specification.

subrgn

See Mode 3 Specification.

VOLU

See Mode 2 Specification.

AREA

See Mode 2 Specification.

INTE

See Mode 2 Specification.

REVE

See Mode 3 Specification.

\(CD\)

The drag coefficient, \(CD\), for the holes. There is no default value for this input.

\(D\)

The diameter, \(D\), of the holes through which mass is transferred in response to a pressure gradient. There is no default value for this input.

\(N\)

Total number of holes, \(N\). There is no default value for this input.

\(L\)

Average length of the holes, \(L\). There is no default value for this input.

\(\beta\)

The exponent \(\beta\) for the drag coefficient. The default value is zero.
COMMENTS

This mode of the TRANSFER command is automatically selected if the DRAG modifier is present and there are at least 4 numerical values on the command.

EXAMPLES

\texttt{TRAN}sf\texttt{f}e\texttt{r} \texttt{C}_{\text{drag}}= 0.10 \text{ dia}= 0.001, \text{ number}=200, \text{ Length}= 0.005, \text{ for subregion ID}=Q\_\text{TRANSFER}
\texttt{TRAN}sf\texttt{f}e\texttt{r} \texttt{C}_{\text{drag}}= 0.10 \text{ dia}= 0.001, \text{ number}=200, \text{ L}= 0.005, \text{ beta}=0.25 \text{ ID}=Q\_\text{TRANSFER}
\texttt{TRAN}sf\texttt{f}e\texttt{r} \texttt{C}_{\text{drag}}= 0.10 \text{ dia}= 0.001, \text{ n}=200, \text{ L}= 0.005, \text{ distribution by VOLUMe ID}=Q\_\text{TRANSFER}
\texttt{TRAN}sf\texttt{f}e\texttt{r} \texttt{C}_{\text{drag}}= 0.10 \text{ dia}= 0.001, \text{ n}=200, \text{ L}= 0.005, \text{ distribution by AREA ID}=Q\_\text{TRANSFER}
\texttt{TRAN}sf\texttt{f}e\texttt{r} \texttt{C}_{\text{drag}}= 0.10 \text{ dia}= 0.001, \text{ n}=200, \text{ L}= 0.005, \text{ Allow REVERse flow; ID}=Q\_\text{TRANSFER}
**COMMAND** TRANSPORT

**PURPOSE** To specify the transport properties of the host porous matrix, or of planar or linear features. This command is effective only for the PORFLOW™ Software Tool.

**MODE 1:** Diffusivity and Dispersivity for a Species

**SYNTAX**\[
\text{TRAN} \{ \Phi \} \{ \alpha \} [D_M, \alpha_L, \alpha_T] [\text{SECO}|\text{SOLI}] [\text{WET}] [\text{subrgn}]
\]

\( \Phi \) A symbol to denote the dependent variable for which the transport properties are specified. The valid symbols are those pertaining to transport equations of Table 2.7.1. By default, the specification is assumed to be for the 1st transport equation or chemical species.

\( \alpha \) The partition coefficient, \( k_d (\geq 0) \), that relates the species concentration in the solid to that in the fluid phase. However, if a PROPERTY command with the same symbol and EFFECTIVE modifier was previously specified, the input value is interpreted as the retardation factor, \( R_D (> 0) \). The equations below explain the interpretation of this input. The default value for \( k_d \) is 0 and that for \( R_D \) is 1. Please see the STORAGE command (COMMENTS Section) for a full discussion of the interpretation of \( k_d \) and \( R_D \).

\( D_M \) Molecular diffusivity, \( D_M (\geq 0) \) for the species. The default value is 0.

\( \alpha_L \) The coefficient of longitudinal dispersivity: \( \alpha_L (\geq 0) \). The default value is 0.

\( \alpha_T \) The coefficient of transverse dispersivity: \( \alpha_T (\geq 0) \). The default value is 0.

\( \text{SECO} \) By default the species transport occurs in the 1st phase of the fluid. If \( \text{SECO} \) is present, then the species transport is in the 2nd fluid phase. This means that the convective fluxes, saturation and fluid properties for the 2nd phase are used to solve the governing equations. The pressure equation for the 2nd phase must be solved for this modifier to be effective.

\( \text{SOLI} \) By default the transport of mass species occurs in a fluid phase. If this modifier is present then the transport is in the solid phase of the porous matrix and the governing transport equation is:

\[
\frac{\partial}{\partial t} \left[ (1 - \theta_E) \rho_S C_k^k \right] = \frac{\partial}{\partial x_j} \left( \rho_S \Gamma_{ij} \frac{\partial C_k}{\partial x_j} \right) + S_c^k (1 - \theta_E) \rho_S \gamma^k
\]

\( \text{WET} \) The modifier is effective only if the SOLID modifier is also present on the command. By default, the accumulation term for the solid phase transport assumes that the total amount of solid is available for transport of the species. If this modifier is present, then only the wetted part of the solid participates in transport. That is the accumulation term of the above equation and is further multiplied by the saturation, \( S \), of the first fluid phase.

\( \text{subrgn} \) The subregion for which the input is specified. See Section 3.4 for more details. If no subregion is specified, then entire computational domain is selected.

**APPLICABILITY**

This command is available only for the PORFLOW™ Software Tool.

**COMMENTS**

More complex functional relations for \( \alpha \) can be specified by the DISTRIBUTION command, those for the diffusivity by the CONDUCTIVITY command and for the dispersivity by the DISPERSIVITY command. Those commands provide greater flexibility and their use is recommended over this command.

**COMMENTS**

This command is a compact input mode to specify constant values for the transport properties for mass species. If these properties vary as functions of other variables, then the individual components of the input can be specified (or overwritten) by the STORAGE, CONDUCTION and DISPERSION commands.
TRANsport properties: kd=1, Dm=5.24, alpha L=10, alpha T=1
TRANsport properties for C2: kd=1, Dm=5.24, alpha L=10, alpha T=1
TRANsport for C2 Rd=21, dm=0, alpha_L=10, alpha_T=1
TRANsport for C2 in SOLid phase kd=0, dm=1.E-5
TRANsport for C2 only in WET part of SOLid phase.
MODE 2:  Exponential Diffusivity Relation for a Species

SYNTAX  TRAN [Φ] {EXPO} {α} [DM, β, γ] [SECO|SOLI] [WET] [subrgn]

Φ  A symbol to denote the dependent variable for which the transport properties are specified. The valid symbols are those pertaining to transport equations of Table 2.7.1. By default, the specification is assumed to be for the 1st transport equation or chemical species.

EXPO  The diffusion coefficient for the species, Γ, is computed from the exponential relation:

\[ Γ = D_M \beta \exp(γS Θ_D) \]

where S is the phase saturation and Θ_D is the diffusional porosity. Other symbols are described below.

α  See mode 1 of command.

DM  Molecular diffusivity D_M (≥ 0) for the chemical species. The default value is 0.

β  The coefficient β (≥ 0) of the diffusional relation given above. The default value is 0.

γ  The coefficient γ (≥ 0) of the diffusional relation given above. The default value is 0.

SECO  See mode 1 of command.

SOLI  See mode 1 of command.

WET  See mode 1 of command.

subrgn  See mode 1 of command.

APPLICABILITY  This command is available only for the PORFLOW™ Software Tool.

EXAMPLES  TRANsport EXPOnential form: kd=1.1E-3, dm=1.2, a1=10, a2 = 5
Keyword Commands

COMMAND TURBULENCE

PURPOSE To select the appropriate turbulence model and specify the empirical constants. This command is available only for the ANSWER™ Software Tool.

MODE 1: Selection of Two Equation Turbulence Model

SYNTAX TURB {model} [LOWR] [COMP]

model The turbulence model to be used. By default the standard k-ε model is used.

<table>
<thead>
<tr>
<th>model</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHIE</td>
<td>Chien (1982) low Reynolds number model is used.</td>
</tr>
<tr>
<td>CUBI</td>
<td>Cubic k-ε model of Shih et al. (1997) is employed.</td>
</tr>
<tr>
<td>LRR</td>
<td>Launder, Reece and Rodi (1975) Reynolds stress model is used.</td>
</tr>
<tr>
<td>LS</td>
<td>Launder-Sharma (1974) low Reynolds number model is used.</td>
</tr>
<tr>
<td>MENT</td>
<td>Menter (1996) two layer blended k-ε/ k-ω model is employed.</td>
</tr>
<tr>
<td>QUAD</td>
<td>Quadratic k-ε model of Shih et al. (1997) is employed.</td>
</tr>
<tr>
<td>RNG</td>
<td>RNG enhancements to the k-ε model are employed.</td>
</tr>
<tr>
<td>RSM</td>
<td>Reynolds stress model of Craft et al. (1996) &amp; Iocovides et al. (1996) is used</td>
</tr>
<tr>
<td>SSA</td>
<td>So and Sarkar (1997) low Reynolds number model is used.</td>
</tr>
<tr>
<td>SST</td>
<td>Menter (1996) low Reynolds number shear-stress transport model is used.</td>
</tr>
<tr>
<td>WILC</td>
<td>Wilcox (1993) k-ω model is employed.</td>
</tr>
<tr>
<td>YSM</td>
<td>Yang and Shih (1993) low Reynolds number model is used.</td>
</tr>
</tbody>
</table>

LOWR This modifier is effective in the absence of any explicit selection of a low Reynolds number model. For the standard k-ε model, the Launder and Sharma (1974) low Reynolds number option is used. For the QUADratic and CUBIC models, the Yang and Shih (1993) low Reynolds option is used.

SECO This modifier is effective only in the presence of the CUBIC modifier. In this case, a second option of the Yang & Shih (1993) low Reynolds number enhancement is selected.

COMP By default, for incompressible flow, the contribution of the divergence term to the kinetic energy production is ignored. This term is typically negligible for subsonic flows. If this modifier is present, then this contribution is included.

COMMENTS

Turbulence modeling still remains more of an art than science. The standard k-ε model is widely used and has a measure of acceptability. However, it is known to have many shortcomings. In particular, its use for flows with high swirl, high streamline curvature or strong pressure gradients may not prove satisfactory. Many of the other models should be considered experimental at this stage. Some of these perform well for certain class of flows. Caution should be exercised in evaluating the results obtained from all turbulence models. ACRi makes some of the models available only by special arrangement.

EXAMPLES

TURBulence model standard k-ε
TURBulence model k-ε with LOWReynolds number extensions
TURBulence model k-ε with CHIen low Reynolds number extensions
TURBulence model LRR version of rsm
TURBulence model RSM of launder & Craft
MODE 2: Selection of LES Turbulence Model

SYNTAX:

\[
\text{TURB} \ \{ \text{LES} \} \ \{ \text{SMAG} | \text{DEDU} | \text{DYNA} \} \ [C_s]
\]

SMAG

Smagorinsky (1963) Large Eddy Simulation Model is used. This is the default option.

DEDU

The 2nd order Deductive LES of Lee and Meecham (1996) is used.

DYNA

The deductive dynamic LES model of Lee, Kim & Runchal (2003) is used. In the default mode of the dynamic model, the constant (Cs) that is used to compute the turbulent eddy viscosity for this model is a function of space and time that is automatically computed. The specified value of the \( C_s \) is ignored. However, if the modifier SMAGorinsky is simultaneously present, then specified value of the \( C_s \) constant is added to the value computed by the model.

\( C_s \)

The Smagorinsky constant \( C_s \) (>0). The default value is 0.05.

COMMENTS

Turbulence modeling still remains more of an art than science. The LES models are widely used and have a measure of acceptability. However, these models are known to have many shortcomings. In particular, the use of such models for flows where wall effects may dominate the flow may not prove satisfactory. These models should be considered experimental at this stage though they may perform well for certain class of flows. Caution should be exercised in evaluating the results obtained from all turbulence models. ACRI makes some of the models available only by special arrangement.

EXAMPLES

- TURBulence model is LES
- TURBulence model is DYNAMIC LES
- TURBulence model is DYNAMIC LES with default value of SMAGorinsky constant
- TURBulence model is DYNAMIC LES with SMAGorinsky constant \( C_s=0.04 \)
MODE 3: Empirical Constants for Turbulent Flows

SYNTAX  

TURB \{ \kappa, E, C_\mu, C_{\varepsilon 1}, C_{\varepsilon 2} \}

\kappa  
The constant \( \kappa \ (>0) \) of the log law of wall. The default value is 0.4187.

E,  
The constant \( E (>0) \) of the log law of wall. The default value is 9.793.

C_\mu  
The constant \( C_\mu (>0) \) of the \( k-\varepsilon \) model. The default value is 0.09.

C_{\varepsilon 1}  
The constant \( C_{\varepsilon 1} (>0) \) of the \( k-\varepsilon \) model. The default value is 1.44.

C_{\varepsilon 2}  
The constant \( C_{\varepsilon 2} (>0) \) of the \( k-\varepsilon \) model. The default value is 1.92.

COMMENTS  

The default values are for the ‘standard’ \( k-\varepsilon \) model of turbulence. Some of the other models have their own built-in default values. This mode of the command may be invoked in a single mixed command with the Mode 1 of the command.

EXAMPLES  

TURBulence kappa=0.4, E=9.
TURBulence kappa=0.4, E=9., CMU=0.09, Ce1 = 1.4, Ce2 = 2.0
TURBulence model RSM kappa=0.4, E=9., CMU=0.09     !! Differential Reynolds stresses Model
COMMAND UPTAKE

PURPOSE To specify uptake and precipitation reactions of dissolved species. This command is effective only for the PORFLOW™ Software Tool.

COMMENTS

This command is identical to the PRECIPITATION command.

EXAMPLES

See PRECIPITATION command
COMMAND  USER

PURPOSE  To specify the user identification for the problem.

SYNTAX  USER  followed by character information

COMMENTS

The specification must be restricted to one 80 character record. User identification is included in all output files generated by the ACRi Software Tool.

EXAMPLES

USER  ACRi - AKR demonstration
COMMAND VELOCITY

PURPOSE To specify the direct computation of Darcy velocity from pressure field. This command is effective only for the PORFLOW™ Software Tool.

SYNTAX VELO {PRES}

PRES By default the representative Darcy velocity at a grid node is computed by dividing the arithmetic average of the flux by the average directed area of the faces. For example, for the hexahedral element shown in Figure 3.2.1, the U, V and W velocity components are computed as the averages of flux at each of the faces divided by the total face area and multiplied by the directed area in the x, y and z direction, respectively. If PRESSURE modifier is present, then the velocity components are directly computed from the hydraulic conductive and the local pressure gradient.

COMMENTS

The PORFLOW™ Software Tool directly computes the fluxes from the continuity equation at cell boundaries (see Figure 3.2.1). The fluxes are computed with the hydraulic conductivity computed at the cell faces. The cell-face value of hydraulic conductivity is different from the value at the node depending on the method of averaging (see the PROPERTY command). This command computes the Darcy velocity from the hydraulic conductivity and the local pressure gradient at the nodal point located within the cell. Thus strictly speaking, the Darcy velocity computed by this command represents the local cell velocity. On the other hand, the fluxes, and the implied velocity, at the cell face are more representative of the numerical solution which satisfies the governing equation.

EXAMPLES

VELOcity directly from PRESSURE gradient
Keyword Commands

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>VISCOSITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>PURPOSE</td>
<td>To specify the viscosity and to select associated options.</td>
</tr>
<tr>
<td>MODE 1:</td>
<td>Generic Functional Form for Viscosity</td>
</tr>
<tr>
<td>SYNTAX</td>
<td>VISC {func[$]} {N1, N2, .., Nn {fname} {EFFE {operation} {ALWA} {phase} {subrgn}}</td>
</tr>
</tbody>
</table>

**func**

One of the modifiers listed in Table 4.2.1 that denotes the functional form of the input. For this input, the function specifies the value of the viscosity for the corresponding phase. If no function is specified then the value is assumed to be constant.

**ξ**

One of the independent variables listed in Table 4.2.2. If no independent variable is specified, the variable is assumed to be time.

**N1,...,Nn**

The numerical constants and coefficients for the selected function. See Section 4.4 for more details. There are no default values for this input.

**fname**

The name of the file containing the numerical values N through Nn. This option is available only for selected functions. See Section 3.3 for additional information.

**EFFE**

By default for turbulent flow in ANSWER™ Software Tool, the specification is assumed to be for the molecular dynamic viscosity. The turbulent eddy viscosity is added to the molecular viscosity. If this modifier is present, then the specified value becomes the total viscosity for the fluid. For PORFLOW™ Software Tool this modifier is assumed to be present by default.

**operation**

Available modifiers are REPLACE, ADD, SUBTRACT, MULTIPLY, DIVIDE, ABS, ABSOLUTE, POSITIVE and NEGATIVE. See Section 4.3 for further details.

**ALWA**

By default, for PORFLOW™ Software Tool the VISCOSITY command is implemented immediately and only once – as soon as the command is encountered. If this modifier is present then the command is executed immediately as well as repeatedly at the beginning of each time step (or iterative step in steady state mode) of the solution procedure. For ANSWER™ Software Tool this modifier is assumed to be present by default.

**phase**

The phase for which the input is specified. See Section 3.6 for available options. By default the input pertains to the 1st phase of the fluid. This modifier is currently available only for the ANSWER™ and PORFLOW™ Software Tools.

**subrgn**

The subregion for which the input is specified. See Section 3.4. If no subregion is specified, the entire computational domain is selected.

**COMMENTS**

The effective viscosity for the fluid (combined molecular and turbulent components) may also be set by the SET Command with MU modifier. In this case the modifier ALWAYS must be specified if the viscosity is to be set as the specified function throughout the solution process. Otherwise the values will be set only at the time of specification and may be subsequently overwritten by other computations. The VISCOSITY command is recommended as the preferred mode of input.

The effective viscosity may also be set by the CONDUCTIVITY command with U, V or W modifiers. This option allows the specification of anisotropic viscosity; that is the coefficient of viscosity can be specified as a vector so that the components in the 3 principal directions are different from each other. In this mode, the viscosity vector for each velocity component can be independently specified for each velocity component.

The VISCOSITY, SET and CONDUCTIVITY commands may be specified in combination. In this case, the CONDUCTIVITY commands will take precedence over all other commands.

**COMMENTS**

If a constant value is specified for whole of the field, then it is used as reference value. The reference value is used in ANSWER™ to compute reference Reynolds number for the flow and to account for the effect of wall in turbulent flow through wall functions.

In PORFLOW™ the reference value is used to compute the effect of varying viscosity on the hydraulic conductivity of the matrix. The effective hydraulic conductivity, Keff, is computed as:

\[
K_{\text{eff}} = \frac{\text{reference value}}{\text{viscosity}}
\]
\[ K_{ij} = K_{ij}^* \frac{\mu^*}{\mu} \]

Where \( K_{ij}^* \) is the reference value of hydraulic conductivity specified through the CONDUCTIVITY or HYDRAulic commandS, and \( \mu \) and \( \mu^* \) are, respectively, the local and reference values of viscosity.

**EXAMPLES**

VISCosity for primary fluid: \( \mu^* = 1.002E^{-3} \) (water at 20 deg C)
VISCosity UNIFORM SECONDary phase: \( \mu^* = 8E^{-2} \) (Engine oil at 20 deg C)
VISCosity for primary fluid: \( \mu^* = 1.002E^{-3} \) for region ID=LOWER_Domain
VISCosity REFERENCE value = 0.544E^{-3}

Generic examples for this command are given in Section 4.4. The command keyword (VISC) must replace the keyword used in these examples.
Keyword Commands

MODE 2:       Pre-Defined Viscosity Functions

SYNTAX        VISC  {SUTH | POWE | EXPO} [phase] [μ₀] [α] [β] [T_a]

CONS          The fluid viscosity is constant. This is the default option.

SUTH          Sutherland equation for viscosity of gases is used:

\[ \mu = \mu_0 \left( \frac{T + \beta}{T + \beta} \right)^{3/2} \]

For this relation, T must be in absolute units. If no numerical values are specified; then the
default values are \( \mu_0 = 1.827 \times 10^{-5} \), \( \alpha = 291 \), \( \beta = 120 \) that provide the viscosity of gaseous air in
units of \([N.s/m^2]\).

POWE          The special version of empirical Seeton fit (C.J. Seeton, UIUC, 2006) for viscosity of liquids is
used:

\[ \mu = \mu_0 \left( \frac{\alpha}{T + T_a - \beta} \right) \]

The default values are \( \mu_0 = 2.414 \times 10^{-5} \), \( \alpha = 247.8 \), \( \beta = 140 \) that provide the viscosity of water in
units of \([N.s/m^2]\) with an accuracy of 2.5% in the temperature range from 0 to 370 °C.

EXPO          Exponential variation in fluid viscosity according to the equation:

\[ \mu = \mu_0 \exp \left( \frac{\alpha}{T + T_a} \right) \]

If no numerical values are specified; then the default values are \( \mu_0 = 7.20912 \times 10^{-6} \), \( \alpha = 1436 \).
These provide the viscosity of water in units of \([N.s/m^2]\).

EFFE          See Mode 1 of Command.
ADD           See Mode 1 of Command.
phase        See Mode 2 of Command.
μ₀           The 1st viscosity constant. See above for default values.
α           The 2nd viscosity constant. See above for default values.
β           The 3rd viscosity constant. See above for default values.
T_a          The absolute temperature base. If no value is specified, the default value is 273.15 except if
the compressible mode of ANSWER™ Software Tool is invoked. In that case, the
temperature must be in absolute units and the default value is 0.

COMMENTS

If these viscosity relations are invoked and no other VISCOSITY command is given to set the reference value
(see Mode 1 of command), then the reference value is set to 8.90439E-4 for the POWER and EXPONENTIAL
options and equal to the value of \( \mu_0 \) for the SUTHERLAND option.
EXAMPLES

VISCosity EXPOnential option
VISCosity from SUTHERLAND equation
VISCosity EXPOnential option: \( \mu^* = 0.544E^{-3}, \ b = 1450 \) K for FIELD values
Keyword Commands

<table>
<thead>
<tr>
<th>COMMAND</th>
<th>WALL</th>
</tr>
</thead>
</table>

**PURPOSE**
To specify wall boundary or boundary conditions for a problem. This command is effective only for the ANSWER™ Software Tool.

**MODE 1:**
Specify Walls at Undefined Outer Boundaries

**SYNTAX**
WALL [ORTH][MOVI][ROUG=Z_{rough}][TYPE=C_{rough}]

**ORTH**
By default it is assumed that walls may not be orthogonal to the grid coordinates. Therefore the computation of wall functions and turbulence energy production term requires extensive arithmetic operations. If this modifier is present, then a simpler set of formulae are used on the assumption that the walls are aligned with coordinate directions.

**MOVI**
By default all walls and solid blocks are assumed to be stationary. Irrespective of the user input, the initial values of velocity components and, energy, length scale and dissipation of turbulence are all set to zero at all walls and obstacles. This modifier disables this feature so that all non-zero initial values for these variables are retained as such. Independent of this modifier, external moving walls may be specified by the BOUNDARY command.

**ROUG**
This mode of the command is operational only for the ANSWER™ software. If this modifier is present, then the wall of the block is assumed to be hydro-dynamically rough for turbulent flow. The height and type of roughness is specified by the Z_{ROUGH} and C_{ROUGH} constants.

**Z_{ROUGH}**
The average roughness height for the wall. It should be noted that the roughness should be small compared to the grid size in the vicinity of the wall. Further the roughness theory is only valid for the range of Y+ values that put it in fully turbulent region of the log-law of the wall.

**TYPE**
This mode of the command is operational only for the ANSWER™ software. This modifier specifies the nature of the roughness. Roughness can be of many types including those of sand-grain, ribbed, finned and random. A factor in the corresponding roughness relations (C_{ROUGH}) accounts for these differences. This modifier is effective only if the modifier ROUG is also present.

**C_{ROUGH}**
The factor that accounts for roughness type. The default value is 0.5 which is generally considered to be suitable for sand-grain type of roughness. The recommended values generally lie between 0.5 and 1.0.

**COMMENTS**
If this command is present then all the outer boundaries of the domain of computation that are not explicitly defined through the INLET, OPEN, OUTLET, PERIODIC and SYMMETRY commands are defined to be walls. At a wall, the turbulence variables are forced to conform to certain preset conditions, the velocities and temperatures are fixed and gradients of the species are set to zero. The defaults for wall temperature and species can be changed by explicit user commands (ADIABATIC and WALL). The wall is assumed to coincide with the element boundary.

**EXAMPLES**

WALL by default at external boundaries
WALL by default at undefined external boundaries; ORTHogonal
WALL by default at undefined external boundaries; ORTHogonal and MOVing
WALL by default at external boundaries ROUGHness height=0.001; TYPE=0.6
MODE 2: Specify Boundary Conditions at Walls

SYNTAX WALL {Φ} [FIX|ADIA|GRAD|EXTR]

Φ One or more symbols that denote the dependent variables for which the wall boundary conditions are specified. Valid symbols are listed in Table 2.7.1. There is no default value; a symbol must be specified

FIX The wall values of the specified variables are fixed. The actual value may be fixed by the BOUNDARY, INITIAL, READ or SET commands

ADIA The gradient of the specified variables at the wall is set to zero.

GRAD Same as ADIABATIC; the gradient of the specified variables at the wall is set to zero.

EXTR The specified variables at the wall are computed from linear extrapolation of the values from the nearest in-field locations.

COMMENTS This command allows the user to set the boundary conditions at the walls globally. Multiple commands may be used to accommodate different requirements for different variables. The wall boundary conditions can also be set by BOUNDARY and ADIABATIC commands. By default, at a wall, the turbulence variables are forced to conform to certain preset conditions, the velocities and temperatures are fixed and gradients of the species are set to zero

EXAMPLES

WALL present at the SELECTed region; determine orientation from subregion
WALL for SELECTed region with orientation of X-
WALL for SELECTed region with orientation of Z+
MODE 3: Specify Individual Wall Location and Boundary Conditions

SYNTAX

```
WALL {dir} [subrgn] [FIX|ADIA] [ROUG=Zrough] [TYPE=Crough]
```

dir The orientation index for the wall. See Section 3.5 for available choices. There is no default value; a value must be specified.

subrgn The subregion to be identified as a wall. See Section 3.4. If no subregion is specified, the outermost dir oriented boundary of the entire computational domain is selected.

FIX The wall is assumed to be at fixed temperature. For the external wall, the temperature may be specified by BOUNDARY, INITIAL, READ or SET commands. For an internal wall, temperature is assumed to be the average of the fluid temperature prevailing at the two nearest elements that straddle the wall. This specification takes precedence over any global boundary specification by WALL (Mode 1) or BOUNDARY command.

ADIA The gradient of the specified temperature at the wall is set to zero.

ROUG See Mode 1 of command.

ZROUGH See Mode 1 of command.

TYPE See Mode 1 of command.

CRough See Mode 1 of command.

COMMENTS

This command may be used either for external walls or infinitesimally thin internal walls. Any thick walls should be specified by the BLOckage command. For an external wall the values of the variables at the boundary can be set by the BOUNDARY, INITIAL, READ or SET commands. For an internal wall, normal gradients of all variables except velocity and temperature are set to zero. It is assumed that all internal walls are stationary; hence all velocity components are set to zero. The temperature boundary condition may be specified as indicated above.

EXAMPLES

```
WALL with orientation of X-
WALL at Y+
WALL for SELEcted region with orientation of Z+
WALL with orientation of Y+ at ID=OUTEr boundary
WALL with orientation of Y+ at ID=OUTEr boundary with ADIA boundary
```
MODE 4: Open a Segment of a Previously Specified Wall

SYNTAX

WALL {OPEN} {dir} [subrgn]

OPEN
All previously specified walls are searched and if the boundary segments identified by the dir and subrgn on the command match any previous wall segments, then the wall segment is removed. This essentially replaces a wall segment by an opening which may be subsequently used for specification of, say, an inlet or outlet.

dir
The orientation index for the boundary. See Section 3.5 for available choices. There is no default value; a value must be specified.

subrgn
The subregion to be removed from an existing wall. See Section 3.4. If no subregion is specified, the outermost dir oriented boundary of the entire computational domain is selected.

COMMENTS
This command is intended to provide a compact method of opening a hole or slot in a previously specified wall. It should be noted, that at the time of specification, only the previously specified walls are searched to remove wall segments. The same segments may be subsequently re-specified by, say, a WALL command.

EXAMPLES
WALL OPEN any previously specified walls at Y+ of the SELECTed region
WALL OPEN any previous wall for Y+ of ID=HOLEINWALL
MODE 5: Drill a Hole in a Previously Specified Wall

SYNTAX

```
WALL {HOOLE} {dir} {subrgn} {d\text{hole}} [N_{11}, \ldots, N_{nn}] [IJK | ELEM] [N_{vec1}, \ldots, N_{vecm}] [\varepsilon]
```

**HOLE**

Wall segments falling within the range specified by the input are removed from the wall previously specified by the same dir and subrgn modifiers. The hole is circular or elliptic based on the specification of the direction normals for the plane.

**dir**
The orientation index for an existing wall. See Section 3.5 for available choices. There is no default value; a value must be specified.

**subrgn**
The subregion designation of an existing wall. See Section 3.4. If no subregion is specified, the outermost dir oriented boundary of the entire computational domain is selected.

**d\text{hole}**
The diameter of the hole to be “drilled” in the specified wall.

**N_{11}, \ldots, N_{nn}**
In the absence of the IJK or ELEM modifier, these specify the (x, y) or the (x, y, z) coordinates of the center of the circular hole. In the presence of IJK or ELEM modifier these are interpreted as given below.

**IJK**
The numerical input $[N_{11}, \ldots, N_{nn}]$ specifies the grid indices (I, J) or (I, J, K) of the element. The center of the hole is assumed to coincide with the center (node) of the element. 2 values must be specified for 2D and 3 for 3D geometry. This option can be used only for structured grids. Only the internal elements can be specified.

**ELEM**
The numerical input $[N_{11}, \ldots, N_{nn}]$ specifies the element which is at the center of the hole. Only 1 value must be specified. This option can be used for structured or unstructured grids. Only the internal elements can be specified.

**N_{vec1}, \ldots, N_{vecm}**
The components of a vector normal to the plane in which the center of the hole is located. The values may be in arbitrary units and are internally converted to unit normals. Up to 3 values may be specified. At least one value must be specified. An elliptic hole can be drilled by appropriate choice of the normal vector.

**\varepsilon**
The tolerance in the direction normal to the plane of the hole. The logic employed computes the normal and tangential distance of the existing wall element centers (nodes) from the center of hole in the specified plane. If the tangential distance is ≤ to the radius of the hole, then the wall segment is removed provided its normal distance from the plane is less than the tolerance. By default the tolerance is set to $10^{-30}$ so that all elements in the projected plane of the hole are captured. This input is used to specify a different tolerance to capture only wall segments within a certain distance from the plane. If specified, the intervening values for all 3 components of the unit normal (even if zero) must be specified.

**COMMENTS**

This command is intended to provide a compact method of opening a hole or slot in a previously specified wall. **It should be noted, that only the specified wall is searched to remove wall segments.** The removed segments may be subsequently re-specified by, say, a WALL command.

**EXAMPLES**

```
WALL HOLE dia = 0.018 at (0.012, 0.3) normal (1, 0) in X+ wall of ID=WALLHOLE
WALL HOLE dia = 0.018 at (0.012, 0.3) normal (1, 2) in X+ ID=WALL to=0.1
WALL HOLE dia = 0.018 at (0.012, 0.3, 0.1) normal (0, 1, 0) in Y+ wall of ID=HOLEINWALL
WALL HOLE dia = 0.01 at IJK (10, 15, 5) normal (0, 1, 0) in Y+ wall of ID=WALL
WALL HOLE dia = 0.01 at ELEMent 989 normal (0, 1, 0) in Y+ wall of ID=WALL
```
COMMAND  WRITE

PURPOSE  To generate output of selected variables on demand.

MODE 1:  Write Selected Variables to Standard Output File or User-Specified File

SYNTAX  WRIT {Φ} [SCALE|STAC|UNIT|ELEM] [N[α][β][fname][subrgn]]

Φ  One or more of the symbols that represent the variables for which output is desired. The valid symbols are listed in Tables 2.8.1-3 and 2.8.4. There is no default value.

SCAL  All output variables, Φ’s, are scaled with α, β according to the relation:

Φ_{out} = α \Phi_{computed} + β

STAC  The output variable is scaled by coefficients a and b specified on a previous STACK WRITE command according to:

Φ_{out} = a \Phi_{computed} + b

In this mode each variable can be scaled by its own a, b as specified by previous STACK WRITE commands. See also comments below for further clarification.

UNIT  If this modifier is specified then the each output variable is scaled to the range of zero to unity according to the relation:

Φ_{out} = Φ_{min} + (Φ_{computed} – Φ_{min}) / (Φ_{max} – Φ_{min})

Here Φ_{min} and Φ_{max} are, respectively, the minimum and maximum computed values of the Φ variable in the whole of the computational domain.

ELEM  If this modifier is specified then the each output variable is in reference to the value of that variable at the element number specified by the input N; that is:

Φ_{out} = \Phi_{computed} – Φ_{N}

Here Φ_{N} is the value of Φ at element number denoted by N

N  The element number for the reference element location if ELEM modifier is present. This input must be omitted if the ELEM modifier is not present.

α  The scaling factor for the variables if the SCAL modifier is specified. This input must be omitted if the SCAL modifier is not present.

β  The additive factor for the variables if the SCAL modifier is specified. This input must be omitted if the SCAL modifier is not present.

fname  The name of the file to which the output is directed. See Section 3.3 for additional information. If no file name is specified, then the variables are written to the Standard Output file

subrgn  The subregion for computations. If no subregion is specified, the entire domain is selected.

COMMENTS  This command provides an alternative mode of output in comparison with the OUTPUT command. The output is obtained in the form of a list. Where possible the list is organized by element or node number. Output is provided as soon as the command is encountered.

The SCAL, STAC, UNIT and ELEM modifiers are effective only for real variables. These are ignored for integer variables. The STAC modifier is also ignored if no previous STACK WRITE command was specified.

EXAMPLES  

WRITe V and T  WRITe V and T to ‘file.VT’  WRITe U, V, P and T in SELElected subregion to ‘FLOW.FIL’  WRITe U, V, P and T in region ID=SUBSET1 to ‘FLOW.FIL’  WRITe U, V, P and T after scaling with STAC for region ID=SUBSET1 to ‘FLOW.FIL’  WRITe V, T, NFACE, NBRS, MTYP and FC to ‘output.mix’
**MODE 2:** Write Boundary Specific Variable Values and Statistics.

**SYNTAX**

\[
\text{WRIT } \{\Phi\} \{\text{option}\} \{\text{walltype}\} \{\text{SUMM}\} \{\text{SCALE}\} | \{\text{STAC}\} | \{\text{UNIT}\} | \{\text{ELEM}\} \{N\{\alpha\}\{\beta\}\}
\]

\[
\{\text{dir}\} \{\text{fname}\}
\]

**Φ**

One or more of the symbols that represent the variables for which output is desired. The valid symbols are those listed in Table 2.8.1-3 and Table 2.8.4. **There is no default value.**

**option**

The boundary type for which output is required. **Only one option may be selected for each command.**

<table>
<thead>
<tr>
<th>option</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>INLE</td>
<td>Only the boundaries specified by the INLET command are selected.</td>
</tr>
<tr>
<td>OUTL</td>
<td>Only the boundaries specified by the OUTLET command are selected.</td>
</tr>
<tr>
<td>OPEN</td>
<td>Only the boundaries specified by the OPEN command are selected.</td>
</tr>
<tr>
<td>IO</td>
<td>All boundaries specified by INLET, OUTLET or OPEN commands are selected.</td>
</tr>
<tr>
<td>BOUN</td>
<td>All external boundaries of the specified (or default) subregion are selected.</td>
</tr>
<tr>
<td>SYMM</td>
<td>Only the boundaries specified by the SYMMETRY command are selected.</td>
</tr>
<tr>
<td>WALL</td>
<td>Only the walls are selected.</td>
</tr>
</tbody>
</table>

**walltype**

The type of wall to be selected for output if the WALL modifier is present.

<table>
<thead>
<tr>
<th>walltype</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALL</td>
<td>All walls are selected. <strong>This is the default option.</strong></td>
</tr>
<tr>
<td>EXTE</td>
<td>Only the exterior walls of the computational domain are selected.</td>
</tr>
<tr>
<td>INTE</td>
<td>Only the walls located in the interior of the computational domain are selected.</td>
</tr>
<tr>
<td>BLOC</td>
<td>Only the walls of the blocks (BLOCK command) are selected.</td>
</tr>
</tbody>
</table>

**SUMM**

By default, the output generated by this command includes the detailed information for each element of the boundary as well as an overall summary for the boundary as a whole. If this modifier is present, then only the summary information is generated; the element by element details are suppressed.

See Mode 1 Specification.

See Mode 1 Specification.

See Mode 1 Specification.

See Mode 1 Specification.

See Mode 1 Specification.

See Mode 1 Specification.

The subregion for computations. If no subregion is specified, the entire domain is selected.

The orientation index for the boundary. See Section 3.5 for available choices. If no input is given, then the output is obtained for all boundaries of the selected type.

The file name for output. By default the output is printed only to the standard output device. If a file name is specified, then the output is printed to the named file.
EXAMPLES

WRITe T and RHO for all INLET boundaries
WRITe T and RHO only for INLET boundaries; scale output with STACK coefficients
WRITe T and RHO only for INLET boundaries in X- direction to file ‘INLETX.FIL’
WRITe T and RHO only for INLET boundaries defined by ID=INLET in X- direction.
WRITe SUMMARY for U, T and RHO for INLET boundaries defined by ID=INLET in X- direction.
WRITe U, V, P, T and RHO for all OUTlet boundaries in X+ direction to ‘OUTLET.VAL’ file
WRITe T and RHO only for WALLs to the file ‘WALLS.PR’B
WRITe T and RHO only for EXTERior WALLs to the file ‘WALL_EXT.PR’B
WRITe T and RHO only for axis of SYMMetry in Y- direction.
WRITe T for all external BOUNdaries.
MODE 3:  Write a Profile of Values at Selected Locations

SYNTAX  WRIT  {Φ} [INTE] [method] [STAC] [subrgn] [fname]

Φ  One or more of the symbols that represent the variables for which output is desired. Up to 9 symbols may be specified on one command. The valid symbols are those listed in Table 2.8.1-3 and Table 2.8.4. There is no default value.

INTE  The variable values at the selected locations are computed by linear or inverse distance squared interpolation from the computed values at the nearest neighboring nodes.

method  The method of interpolation for computing values at the specified (x, y, z) locations. Only one method may be selected for each command.

<table>
<thead>
<tr>
<th>method</th>
<th>INTERPRETATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>LINE</td>
<td>The values are computed by inverse linear distance interpolation from the computed values at nearest neighbors. This is the default option.</td>
</tr>
<tr>
<td>SQUA</td>
<td>The values are computed by inverse distance squared interpolation from the computed values at nearest neighbors.</td>
</tr>
<tr>
<td>AVER</td>
<td>The values are computed by arithmetic average of computed values at nearest neighbors.</td>
</tr>
<tr>
<td>NEAR</td>
<td>The value is set equal to that at the nearest neighbor.</td>
</tr>
<tr>
<td>X</td>
<td>Same as LINE except that the distance is set equal to the separation in the x-coordinate.</td>
</tr>
<tr>
<td>Y</td>
<td>Same as LINE except that distance is set equal to the separation in the y-coordinate.</td>
</tr>
<tr>
<td>Z</td>
<td>Same as LINE except that the distance is equal to the separation in the z-coordinate.</td>
</tr>
</tbody>
</table>

STAC  The output variable is scaled by coefficients a and b specified on a previous STACK WRITE command according to:

Φ_{out} = a Φ_{computed} + b

The STAC modifier is effective only for real variables. It is ignored if no previous STACK WRITE command was specified.

subrgn  The sub region for output. The sub region must have been previously specified by a LOCATE LIST COORDINATE command. Any other sub region specification will lead to an error condition. There is no default value.

fname  The file name for output. By default the output is printed only to the standard output device. If a file name is specified, then the output is printed to the named file.

EXAMPLES

WRITe U, V, P and T by INTEerpolation for ID=L_PROFILE
WRITe U, V, P and T by SQUAred INTEerpolation for ID=L_PROFILE
WRITe U, V, P and T by INTEerpolation for ID=L_PROFILE
WRITe U by AVERAGE INTEerpolation for ID=L_PROFILE on file: ‘PROFILE.U’
WRITe U, V, P and T by X direction INTEerpolation for ID=L_PROFILE on file: ‘PROFILEX.VAR’
MODE 4: Write Selected Variables to User-Specified File in Block Mode

SYNTAX

```
WRIT {Φ} {BLOC} [HEAD] [FIEL] {fname}
```

Φ
One or more of the symbols that represent the variables for which output is desired. The valid symbols are those listed in Table 2.8.1-3, and the node or element-based variables listed in Table 2.8.4. There is no default value.

BLOC
The variables are written in the block format. One record is written for each variable. If the grid is structured then the variable is written in the manner of the FORTRAN DO loop (over the grid indices I, J, K). If the grid is unstructured, then the record for the variable is sequential over element numbers starting with the 1<sup>st</sup> element.

HEAD
By default only the numeric values for the selected variable(s) are written to the file without any header information. If the HEADER modifier is present, then a two line header in the standard ACRi SAVE file format appears before each set of variable values.

FIEL
Only the inner field nodes or elements are written to the output file. The boundary nodes are omitted. This modifier is active only if the BLOCK modifier is simultaneously present. By default both the field and the boundary elements are written to the record.

fname
The name of the file to which the output is directed. See Section 3.3 for additional information. There is no default file name; a file name must be specified.

EXAMPLES

```
WRITe T in BLOCK format to file named ‘value.T’
WRITe U, V and W in BLOCK format to file ‘value.UVW’
WRITe U, V, W, T, C, FU in BLOCK format to file named ‘mixed.val’
WRITe FIELd values of U and X in BLOCK format ‘UandX.val’
WRITe in BLOCK format values of X Y Z and MYTP to ‘geometry.val’
```
MODE 5: Write Vertex Coordinates to User-Specified File

SYNTAX

WRIT {VERT} {fname}

VERT

A file containing the (x, y, z) coordinates of the vertices is generated. The file contains header information followed by a table of vertex numbers and the corresponding grid coordinates. The vertex data in the file is generated by the FORTRAN STATEMENTS:

DO N = 1, Total_Vertices
   WRITE (IFILE,*) N, (XV (K), K=1, N23D)
ENDDO

Here IFILE is an internally assigned file unit number, XV are the coordinates of the vertices and, N23D is 2 for 2D and 3 for 3D geometry.

fname

The name of the file to which the output is directed. See Section 3.3 for additional information. There is no default file name; a file name must be specified.

EXAMPLES

WRITe VERTices on file=’VERTICES.XYZ’
MODE 6: Write Element Connectivity to User-Specified File

SYNTAX: WRIT {CONN} {fname}

CONN
A file containing the element to vertex connectivity is generated. The command must be given before the first SOLVE command otherwise an empty file will be generated. The file contains header information followed by a table of element numbers and the corresponding vertices that define the element. The connectivity data in the file is generated by the FORTRAN STATEMENTS:

DO M = 1, Total_Elements
   MVLO = NVRTXLO (M)
   MVHI = NVRTXHI (M)
   WRITE (IFILE,*) M, (NVRTX (K), K=MVLO, MVHI)
ENDDO

Here IFILE is an internally assigned file unit number and NVRTXLO and NVRTXHI are the starting and ending locations of the vertices for the m<sup>th</sup> element.

fname
The name of the file to which the output is directed. See Section 3.3 for additional information. There is no default file name; a file name must be specified.

EXAMPLES

WRITe CONNectivity on file="VERTICES.CNC"
MODE 7: Write Element Vertex Coordinates to User-Specified File

SYNTAX  
WRIT {CORN} {fname}

CORN  
A file containing the (x, y, z) coordinates of the vertices for each element is generated. The command must be given before the first SOLVE command otherwise an empty file will be generated. The file contains header information followed by a table of element number, vertex number connected to that element, and the corresponding coordinates for the vertex. The vertex data in the file is generated by the FORTRAN STATEMENTS:

DO M = 1, Total_Elements
   DO N = 1, Vertices_for_this_Element
      WRITE (IFILE,*) M, N, XC (N), YC (N), ZC (N)
   ENDDO
ENDDO

Here IFILE is an internally assigned file unit number, and XC, YC and ZC are, respectively, the (x, y, z) coordinates of the vertex. The vertex numbers for the element are in the same order as those on the CONNECTIVITY command.

fname  
The name of the file to which the output is directed. See Section 3.3 for additional information. There is no default file name; a file name must be specified.

EXAMPLES  
WRITe CORNers of the element vertices on ‘CORNER.XYZ’
Keyword Commands

COMMAND  ZONE

PURPOSE  To specify the material or zone type for the soil or rock formation. This command is effective only for the PORFLOW™ Software Tool. This command has been retained only for backward compatibility. It is no longer necessary to use this command. Its function has been superseded by the LOCATE command.

MODE 1:  Specification of Material Type

SYNTAX  ZONE  \{N_1\} \{N_2, ..., N_n\} [N_{n+1}, N_{n+2}]

MODE 2:  Material Type Data Input from a File

SYNTAX  ZONE  \{fname\}

COMMENTS  This command is retained primarily to provide compatibility for data sets prepared with previous versions of PORFLOW™. Mode 1 and Mode 2 of the MATERIAL, ROCK or SOIL commands, together with LOCATE command, have replaced its function. These latter commands should be used.

EXAMPLES  See Mode 1 of the MATERial command.
REFERENCES


<table>
<thead>
<tr>
<th>Reference</th>
<th>Title</th>
</tr>
</thead>
</table>


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APPENDIX A: FILES PROCESSED DURING EXECUTION

A.0 INTRODUCTION

ACRi Software Tools read a number of files during execution. These help in customizing the installation and managing the progress of the simulation. These are described below.
A.1 ACRNAMES.ACR

ACRi Software Tools define a number of phase space variables by default. These names are contained in the file called ACRINIT.ACR. The user can define and add new phase space variables by the ALLOCATE command. If however a number of variables need to always defined for an installation or for a project then these can be included in a file named “acrNAMES.ACR”. The installation and the working directories are searched for this file at the start of simulations. If this file is present, then these phase space variables are automatically defined. If the file is present in both the installation and the working directory, then the one in the working directory is included. The typical file format is given below.

```
T199 – Technetium 199
I129 - Iodine 129
VRBL1 – 1st Variable to be defined
VRBL0002 – 2nd variable to be defined
```

With these as the contents of the file, 4 new phase space variables will be automatically defined for each simulation by default as if these were included in the ACRINIT.ACR file. Following the variable symbol convention, the symbols for these variables will be constructed from the first “word” of up to 8 characters that appears in the definition before a separator (a space or a “-” in this case). Thus for the above list the symbols will be T199, I129, VRBL1 and VRBL0002.
A.2 ACRDFLT.ACR

If a file named ‘acrDFLT.ACR’ is present in the working directory, then this file is automatically included at the start of simulation. This file is assumed to consist of a number of ACRi FREEFORM™ commands. It is automatically included at the head of the user input command file. As far as the ACRi Software Tool is concerned, this is equivalent to the user having inserted these commands into the input command file.

The purpose of this file is to allow project specific “macro” commands, such as for a given geometry of a reaction system to be automatically included. For example for project control, it may be desirable to have some common project specific files that define some basic components of the simulation and need to be standardized across all users. These can be spun off to a separate “read-only” file that is include for all users of that directory.
A.3 ACRINSRT.ACR

If at time during the simulation, a file named ‘acrINSRT.ACR’ is present in the working directory, then it is automatically inserted in the input command file. ACRi Software searches for this file at the start of each time (or iteration) step of the solution process. As soon as this file is detected, it is inserted in the input command file and the file is deleted. The search continues however, if the file is detected again, it is again included.

This file provides a mechanism for including commands that were omitted for one or reason or another at the launch of the simulation or it can used to modify the input (such as relaxation factors, matrix solvers, boundary conditions or output requirements) during the simulation process.
A.4 ACRSTOP.ACR

If at time during the simulation, a file named ‘acrSTOP.ACR’ is detected in the working directory, then the simulation is automatically terminated. All remaining commands in input command file are executed except the SOLVE command which is ignored. Any output requested is generated and the solution process is terminated.

The contents of this file are not scanned and the action is taken solely on the basis of the name of the file.
A.5 ACRDONE.ACR

A file named ‘acrDONE.ACR’ is generated at the end of the simulations. The purpose of this file is to act as an indicator for other processes that may be running and waiting for the simulation to complete. For example, this file can be used to automatically trigger post-processing of the solution.
APPENDIX B: FILE FORMATS

B.1 INPUT FILE FORMATS

B.1.1 Input file for NODE wise Time-Dependent Function (Section 4.1.3)

A typical file is of the form:

<Optional number of header records>
These must not begin with TIME as the first word in the record>

< A record: such as>
TIME = <value> (TIME must be the first word; command follows FREEFORM input mode)

< One or more records with numerical values which are read according to the FORTRAN Format:
READ(NUNIT,*) (VALUE(N), N=1, NVAL)
Here:
NUNIT is a unit number which is internally assigned
VALUE(N) are the user input values
NVAL is the number of nodes in the ID=<subdomain>. If the number of values specified on the file
exceeds the NVAL; then the extra values are ignored. If the specified number of values is less than
NVAL, then the run is terminated with an error message.

The values for the variable at following times follow the same format. An example of such a file is given below.

FILE TITLE: Temperature at a 12 nodes in sub domain ID=FIX_T as a function of Time.
Temperature is given in absolute Kelvin units.
TIME = 0  (First data set)
300 301 303 298 305 299 301 302 305 304 307 296
Second data set
TIME = 10 (Second data set)
300 299 300 299 300 299 300 299 300 299 300 299
TIME = 25 (Third data set)
300 301 303 298 305 299 301 302 305 304 307 296
TIME = 30 (Second data set)
300 299 300 299 300 299 300 299 300 299 300 299
TIME = 50 (Third data set)
300 299 300 299 300 299 300 299 300 299 300 299
END of File
APPENDIX C: RADM STOCHASTIC TRANSPORT METHODOLOGY

C.1 THEORETICAL DESCRIPTION

C.1.1 Basic Transport Equation

C.1.1 Computational Algorithm

C.2 COMPUTATION OF CONCENTRATION

For each computational element (or cell) the concentration of species is equal to the sum of the mass of particles in the cell divided by the volume of the cell. However in the macro scale simulations, each particle represents a large collection of “molecules” that are distributed around the mean computed position of the particle. The concentration for any element is preferably computed from the intersecting “volume” of the particle with the element. The general relation is:

\[ C_M = \frac{\sum_{n=1}^{n+N} q_n \left( \delta V_n \cap \delta V_M \right)}{\delta V_M} \]  

(C.2.1)

Where

- \( C_M \) is the average concentration of the species in the grid element \( M \),
- \( q_n \) is the mass of the \( n^{th} \) particle
- \( \delta V_n \) is the volume of the \( n^{th} \) particle
- \( \delta V_M \) is the volume of the \( M^{th} \) grid element or cell
- \( N \) is the number of particles in the vicinity of the cell within a given radius of influence, and
- \( \cap \) stands for the intersection of the particle volume with the cell volume.

With \( \alpha^M_n \) is the fractional contribution of the \( n^{th} \) particle to the \( M^{th} \) element, the above formula can be written as:

\[ C_M = \frac{1}{\delta V_M} \sum_{n=1}^{n-N} \alpha^M_n q_n \]

There are many ways to compute the intersecting volume and the radius of influence; some of these are described below.

C.2.1 Species Concentration from Inverse-Distance-Square Algorithm

The distance of the particle, \( d_n \), from the element \( M \) is given as:

\[ d_n^2 = \sum_{i=1}^{i=3} (x_{Mi} - x_{ni})^2 \]

If the particle mass is distributed according to the inverse of the distance squared; then:

\[ \alpha^M_n = \frac{1/d_n^2}{\sum_k 1/d_k^2} \]

Here the subscript \( k \) denotes the immediate neighborhood that consists of the element in which the particle is located and its immediate neighbors. For a hex grid there will be 4 neighbors in 2D and 6 in 3D; therefore the total mass of the particle will be distributed over 5 elements for 2D and 7 for 3D.

C.2.2 Species Concentration from Location of Particle

In this case, the total mass of the particle is assumed to be located in the element of its location: If there are a total of \( k \) particles in the element \( M \), then:

\[ \alpha^M_n = 1 \quad \text{if particle in } M \quad ; \quad \alpha^M_n = 0 \quad \text{otherwise} \]
C.2.3 Species Concentration from Particle density

With the assumption that each particle has a volume based upon its mass and density, the characteristic lengths for the particle ($R_n$), the element ($R_M$) and the distance between the element and the particle ($d_n$) are computed as:

$$R_n = \frac{1}{2}\left(\frac{q_n}{\rho}\right)^{1/3} \quad ; \quad R_M = \frac{1}{2}\delta V_M^{1/3} \quad ; \quad d_n = \sqrt[3]{\frac{1}{\delta M} \sum_{i=1}^{M} (X_{Mi} - X_{ni})^2}$$

Where $X_i$ are the grid coordinates and the subscripts $M$ and $n$ refer to the element and the particle. The particle contribution to this cell is then computed as:

$$\alpha_n^M = \frac{R_M + R_n - d_n}{R_M + R_n} \quad \text{if} \quad d_n < R_M + R_n \quad ; \quad \alpha_n^M = 0 \quad \text{otherwise}$$

C.2.4 Species Concentration from Radius of Influence

The expressions used are:

$$R_M = \frac{1}{2}\delta V_M^{1/3} \quad ; \quad d_n = \sqrt[3]{\frac{1}{\delta M} \sum_{i=1}^{M} (X_{Mi} - X_{ni})^2}$$

$$\alpha_n^M = 1 \quad \text{if} \quad d_n \leq R_M \quad ; \quad \alpha_n^M = \frac{R_M^2}{R_n^2} \quad \text{if} \quad R_M < d_n < \beta R_M \quad ; \quad \alpha_n^M = 0 \quad \text{if} \quad d_n \geq \beta R_M$$