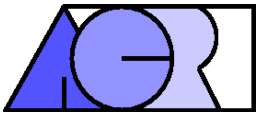
ACRi Software Tools

ANSWER™ ◆ PORFLOW™ ◆ TIDAL™

KEYWORD COMMANDS

VERSION 6.3

Rev: 3



USA ● ACRi ● 1931 Stradella Road, Bel Air, CA 90077, USA ● +1-310-471-3023 ● www.ACRiCFD.com
India ● ACRi InfoTech ● Bangalore (india) ● +91-80-2668 8585 ● Dharamsala ● +91 1892 221675
France ● ACRi SAS ● Sophia Antipolis, France ● 33-492 96 75 00 ● www.ACRi.fr

COPYRIGHT NOTICE

June 27, 2010

IMPORTANT -- PLEASE READ CAREFULLY BEFORE USING THIS SOFTWARE

SOFTWARE LICENSE AGREEMENT

Please read this license agreement before using this SOFTWARE. This agreement is a legal contract between you (the CUSTOMER) and Analytic & Computational Research, Inc. (ACRi) governing the use of this SOFTWARE. Your first use of this SOFTWARE indicates your acceptance of the terms of this agreement. *Please note that in some instances, the software license is on an annual basis and you must pay an annual fee for continued use of the* SOFTWARE*. If an annual fee is applicable, this will be conveyed to you at the time of purchase and be indicated on your invoice or in a License Agreement.* If you do not wish to comply with the terms of this agreement, return the SOFTWARE within 30 days and your money will be refunded. If you have any questions concerning this agreement, please contact ACRi, attn. Software Sales, 1931 Stradella road, Bel Air, CA 90077 or call (+1) (310) 471-3023 or send us email at sales@acriCFD.com.

1. CUSTOMER may use the SOFTWARE on a single-user computer or a single terminal or workstation of a multi-user computer or network. Each installation, terminal or workstation must be separately licensed by ACRi.
2. CUSTOMER may not sublicense, assign, rent, lease or transfer the software or license to another party without the explicit written consent of ACRi. The software is licensed to the CUSTOMER as the END USER. CUSTOMER may not use the SOFTWARE for the purposes of another party or use the SOFTWARE for performing simulations for, or consulting with, another party that result in derived income for the CUSTOMER without obtaining explicit written consent of ACRi and without paying a royalty of 15% on such income.
3. CUSTOMER may not incorporate, or allow another party to incorporate the SOFTWARE, in whole or in part, in any other software.
4. CUSTOMER's license to use the SOFTWARE becomes effective only after the CUSTOMER has paid all amounts which are agreed to by the CUSTOMER and the CUSTOMER has received written notification from ACRi that the LICENSE is now active.
5. This AGREEMENT is effective until terminated.
6. This AGREEMENT is subject to immediate termination if CUSTOMER violates any of its provisions.
7. In the event of termination of this AGREEMENT, CUSTOMER shall discontinue all further use of the SOFTWARE and return all copies of the SOFTWARE and documentation supplied by ACRi.
8. Upon termination, customer shall provide written notice that all use of the SOFTWARE has ended.
9. ACRi warrants that the diskettes or electronic files containing the SOFTWARE and accompanying documentation are free of defects in materials and workmanship for a period of 30 days from the date of purchase. In the event of notification of any physical defects in diskettes or documentation, ACRi will replace the defective diskettes and documentation.
10. ACRi disclaims all other warranties, expressed or implied, including but not limited to implied warranties of fitness or usefulness for a particular purpose, either with respect to defects in the diskettes, and documentation, or with respect to any defects of coding and logic in the SOFTWARE, even if such defects are known to ACRi or have been brought to ACRi's attention.
11. ACRi will not be liable to CUSTOMER, or any other party, for consequential loss or damages arising from the use, operation, or modification of the SOFTWARE by CUSTOMER. ACRi will not be responsible for any loss, damage, or claim resulting from reliance by CUSTOMER or any other party on results obtained by use of the SOFTWARE.

If any provision of this AGREEMENT shall be unlawful, void, or for any reason unenforceable, then that provision shall be deemed severable from this AGREEMENT and shall not affect the validity and enforceability of the remaining provisions of this AGREEMENT.

WARRANTY

No warranty expressed or implied, is provided that this document is complete or accurate in all respects. The information contained in this document, and the software that it describes, are subject to change without notice.

NOTICE

The ACRi Software Tools contain multiple options which are described in this document. Which of these options is actually present in your installation of the Software Tool may depend upon the type of contract under which the software was acquired. If you have any questions about the presence or absence of a particular option, please contact ACRi.

PREFACE

During the past 30 years, ACRi Software Tools **ANSWER™, PORFLOW™, TIDAL™** and **CFDStudio™**, have evolved from simple mathematical models for flow and heat transfer into comprehensive **C**omputational **F**luid **D**ynamics **Software Tools for analysis of a wide range of engineering and environmental applications** for a wide range of problems. These tools provide for coupled transport of fluid, heat and multiple chemical species in complex geometry. These are able to simulate the transient or steady state behavior of compressible or incompressible fluids in diverse host media and multiple phases with chemical reactions, combustion and other complex physical processes.

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:

Analytic & Computational Research, Inc. (ACRi).
1931 Stradella Road, Bel Air, California, 90077
Email: techsupport@ACRiCFD.com Phone: +1 310-471-3023
Web: www.ACRiCFD.com & www.acri.fr

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.

CONTENTS

LIST OF TABLES

LIST OF FIGURES

NOTATION

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
a	A constant or exponent	various	various	Various
a_R	Absorptivity coefficient	L^{-1}	1/m	1/ft
b	A constant or exponent	various	various	various
c	A constant or exponent	various	various	various
c	Speed of sound	$L\ t^{-1}$	m/s	ft/s
C_D	Drag coefficient	-----	-----	-----
C_P	Specific heat	$L^2\ t^{-2}\ T^{-1}$	J/(kg K)	BTU/(lbm°F)
E	Black body radiation energy	$M\ t^{-3}$	W/m^2	BTU/ft^2
f	A frequency	t^{-1}	1/s	1/s
F	General transport variable	various	various	various
g	Gravitational acceleration	$L\ t^{-2}$	m/s^2	ft/s^2
h	Enthalpy	$L^2\ t^{-2}$	m^2/s^2	ft^2/s^2
h^o	Enthalpy of formation of a species	$L^2\ t^{-2}$	m^2/s^2	ft^2/s^2
h_s	Stagnation enthalpy	$L^2\ t^{-2}$	m^2/s^2	ft^2/s^2
H_R	Heat of reaction	$L^2\ t^{-2}$	m^2/s^2	ft^2/s^2
I	Radiation intensity	$M\ t^{-3}$	W/m^2	BTU/ft^2
k	Kinetic energy of turbulence	$L^2\ t^{-2}$	m^2/s^2	ft^2/s^2
m	Rate of injection of fluid per unit volume	$M\ L^{-3}\ t^{-1}$	$kg/(m^3 s)$	$lbm/(ft^3 s)$
m	Mass fraction of a species	-----	-----	-----
M	Molecular weight	$M\ mol^{-1}$	kg/mol	lbm/mol
N	Coordinate normal to a boundary	L	m	ft
N_{sn}	Density of soot nuclei	L^{-3}	$1/m^3$	$1/ft^3$
N_{ss}	Concentration of soot particles	$M\ L^{-3}$	kg/m^3	lbm/ft^3
P	Thermodynamic pressure	$M\ L^{-1}\ t^{-2}$	N/m^2	lbf/ft^2
P_R	Reference value of Thermodynamic pressure	$M\ L^{-1}\ t^{-2}$	N/m^2	lbf/ft^2
P_k	Rate of production of turbulent energy	$M\ L^{-1}\ t^{-3}$	W/m^3	$BTU/(ft^3 s)$
r	Radius of curvature	L	m	ft
R	Radiation flux	$M\ t^{-3}$	W/m^2	BTU/ft^2

... Notation continued

NOTATION - Continued

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
R	Gas constant	$L^2 t^{-2} T^{-1}$	J/(kg K)	BTU/(lbm °F)
Re	Reynolds number	-----	-----	-----
R_U	Universal gas constant	$L^2 t^{-2} T^{-1}$	J/(kg-mol K)	BTU/(lbm-mol R)
s	Reaction or decay rate of a property	$M L^{-3} t^{-1}$	$kg/(m^3 s)$	$lbm/(ft^3 s)$
s_R	Scattering coefficient	L^{-1}	1/m	1/ft
S	Source of a fluid property	various	various	various
t	Time	t	s	s
T	Thermodynamic Temperature	T	K	R
T_a	Convert temperature to absolute units	T	K	R
T_c	Critical temperature of the fluid	T	K	R
uu	Autocorrelation of U	$L^2 t^{-2}$	m^2/s^2	ft^2/s^2
U	Fluid velocity in x-direction	$L t^{-1}$	m/s	ft/s
vv	Autocorrelation of V	$L^2 t^{-2}$	m^2/s^2	ft^2/s^2
V	Fluid velocity in y-direction	$L t^{-1}$	m/s	ft/s
V_i	Velocity in i^{th} direction	$L t^{-1}$	m/s	ft/s
ww	Autocorrelation of W	$L^2 t^{-2}$	m^2/s^2	ft^2/s^2
W	Fluid velocity in z-direction	$L t^{-1}$	m/s	ft/s
x	x-coordinate	L	m	ft
y	y-coordinate	L	m	ft
z	z-coordinate	L	m	ft

GREEK SYMBOLS

Symbol	MEANING	UNITS		
		GENERIC	SI	FPS
α	A coefficient	various	various	various
β	A coefficient	various	various	various
γ	Ratio of specific heats	-----	-----	-----
Γ	Diffusion coefficient	$M\ L^{-1}\ t^{-1}$	kg/(m s)	lbm/(ft s)
ε	Rate of dissipation of turbulence energy	$L^2\ t^{-3}$	J/(kg s)	BTU/(lbm s)
ε	A small quantity	-----	-----	-----
θ	Angular coordinate	radian	radian	radian
κ	Von Karman Constant	-----	-----	-----
λ	Decay rate constant	t^{-1}	1/s	1/s
μ	Fluid viscosity	$M\ L^{-1}\ t^{-1}$	kg/(m s)	lbm/(ft s)
ρ	Fluid density	$M\ L^{-3}$	kg/m^3	lbm/ft^3
σ	Prandtl or Schmidt number	-----	-----	-----
σ	Stefan-Boltzman constant	$M\ t^{-3}\ T^{-4}$	$J/(m^2\ s\ K^4)$	$Btu/(ft^2\ s\ R^4)$
τ	Shear stress	$M\ L^{-1}\ t^{-2}$	N/m^2	lbf/ft^2
φ	Density-related variable	$M\ L^{-3}$	kg/m^3	lbm/ft^3
φ_E	Equivalence ratio	-----	-----	-----
χ	Fuel fraction in fine or ambient scale of flow	-----	-----	-----

SUBSCRIPTS

SYMBOL	PERTAINING TO
e	Effective value of a fluid property
Φ	Fluid property F
i	The i^{th} coordinate direction or i^{th} phase
inj	Injected fluid
j	The j^{th} coordinate direction or j^{th} phase
k	The k^{th} coordinate direction or k^{th} phase
t	Turbulent state of fluid
t	The time coordinate
w	The wall
x	The x direction
y	The y or r direction
z	The z or θ direction

SUPERSCRIPTS

SYMBOL	PERTAINING TO
Φ	Pertaining to property Φ
j	Pertaining to the j^{th} coordinate direction or j^{th} phase
t	Pertaining to the time coordinate
*	Approximate or reference value of a variable
'	Variation in the value of a variable
n	Pertaining to the n^{th} fluid or the n^{th} chemical species
k	Pertaining to the k^{th} time step

CHAPTER **1**

ACRi FREEFORM™ COMMAND LANGUAGE

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

Number	Character	Description	ASCII Sequence #
1	' '	Space or Blank	32
2	(	Left parenthesis	40
3	)	Right parenthesis	41
4	,	Comma	44
5	:	Colon	58
6	;	Semicolon	59
7	=	Equal sign	61
8	|	Vertical Line	124
9	Tab	Horizontal Tab Character	9

.

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    !789.123
```

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
!****////// ARRAY = 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.)

CHAPTER 2

INPUT AND OUTPUT OPTIONS

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

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

..... Table 6.1.1 continued

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

NO.	KEYWORD	INPUT FUNCTION

41	**GEOM**ETRY	Specify or modify problem geometry
42	**GAS**	Specify gas constant and parameters
43	**GEOM**ETRY	Specify or modify problem geometry
44	**GRAV**ITY	Specify constants of gravitational acceleration
45	**GRID**	Number of grid nodes in the x, y and z directions
46	**HIST**ORY	Provide time history output at selected nodes
47	**HYDR**AULIC	Hydraulic properties of porous matrix
48	**IF**	To initiate the IF-ELSE-ENDIF construct
49	**INCL**UDE	To include a file at run time in the input data stream
50	**INDE**NT	To allow command input to be indented
51	**INIT**IAL	Initial conditions for state variables
52	**INJE**CTION	Specification for injection of Liquid Films and Sprays
53	**INLE**T	To specify an inflow boundary for the domain of computation
54	**INTE**GRATION	Index for selection of integration profile
55	**LAMI**NAR	Specify laminar flow
56	**LAND**	Define Land Boundary
57	**LATE**NT	Specify latent heat of fluid
58	**LIMI**T	Set upper and lower limits for dependent variables
59	**LOCA**TE	Specify location of sub-regions or boundaries
60	**MATE**RIAL	Specify material types and properties
61	**MATR**IX	Specify Options for solution of matrix of equations
62	**META**	Specify a meta command file to generate multiple simulations
63	**MOVE**	Specify moving surface within flow domain
64	**MULT**IPHASE	Specify multi-phase or multi-fluid hydraulic characteristics
65	**NOZZ**LE	Specify liquid fuel nozzle injection parameters
66	**OPEN**	Specify an open boundary through which fluid may enter or leave
67	**OPTI**ON	Modify built-in default options
68	**OUTL**ET	Specify an outflow boundary for the domain of computation
69	**OUTP**UT	Frequency and extent of tabular output
70	**OXID**IZER	Oxygen to nitrogen ratio in the oxidizer stream
71	**PAUS**E	Cause a temporary pause in processing
72	**PAUS**E	Cause a temporary pause in processing
73	**PERM**EABILITY	Specify permeability of the porous medium
74	**PHAS**E	Specify phase change mode and constants
75	**PORO**SITY	Specify material porosity for porous matrix
76	**PRAN**DTL	Specify Prandtl numbers
77	**PREC**IPITATE	Specify precipitation reaction from fluid to solid phase
78	**PRIN**T	Print flow rate, sources and statistical measures of variables
79	**PROB**LEM	Specify general nature and type of problem
80	**PROP**ERTY	Option for mode of property specification

..... Table 6.1.1 continued

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

NO.	KEYWORD	INPUT FUNCTION
81	**QUIT**	Terminate solution process
82	**RADI**ATION	Activate thermal radiation calculation

83	**REAC**TION	Specify reaction rate constants
84	**READ**	Read initial conditions from archive file
85	**REFE**RENCE	Reference values for key variables
86	**REGE**NERATION	Specify regeneration rate for chemical decay chain
87	**RELA**X	Relaxation factors for governing variables
88	**RENA**ME	Allows renaming of output variables listed in Table 6.8.1
89	**RETA**RDATION	Specify retardation coefficient for a transport variable
90	**SAVE**	Frequency of output to archive file
91	**SCAL**E	Internal scaling of specified input
92	**SCHM**IDT	Specify Schmidt numbers
93	**SCRE**EN	Echo some of the diagnostic output to screen
94	**SELE**CT	Specify location of sub-regions or boundaries
95	**SET**	Set value of a variable as a function of space and time
96	**SOLI**D	Specify conjugate heat transfer and properties
97	**SOLV**E	Start of solution of equations
98	**SOOT**	Activate soot computations and specify constants
99	**SOUR**CE	Specify source, injection or withdrawal terms
100	**SPEC**IFIC HEAT	Select specific heat options and constants for the fluid
101	**STAC**K	To specify stack transformation operations
102	**STAT**ISTICS	Obtain output of statistical parameters of variables
103	**STOR**AGE	Specify storage coefficient for a governing transport equation
104	**SWIR**L	To specify characteristics of swirl imposed on flow
105	**SYMM**ETRY	To identify an external boundary as a symmetry plane or axis
106	**THER**MAL	Thermal properties of solid or porous matrix
107	**TIDE**	Specify history of tide at a boundary
108	**TIME**	Set initial time for simulations
109	**TITL**E	Problem title specification
110	**TORT**UOSITY	Specificy tortuosity of the porous matrix
111	**TRAC**K	Compute Particle tracks and corresponding elapsed time in flow field
112	**TRAN**SFER	Transfer mass and property variables within the computational domain
113	**TRAN**SPORT	Transport properties of porous matrix
114	**TURB**ULENT	Select turbulent model and specify constants
115	**USER**	User identification for input and output files
116	**VELO**CITY	Select method of computation of Darcy velocity
117	**VISC**OSITY	Select fluid viscosity options
118	**WALL**	Specify internal walls within domain of interest
119	**WRIT**E	Generate output of variables
120	**ZONE**	Specify host media zones

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 2.2.1: FUNCTIONAL UNITS OF ACRi™ SOFTWARE TOOLS COMMANDS

ORDER	FUNCTION	RELATED KEYWORD COMMAND
1	Identification	**BANNER**, **TITLE**, **USER**
2	Grid specification	**ADAPTIVE**, **CONNECTIVITY**, **COORDINATE**, **GEOMETRY**, **GRID**, **SCALE**
3	Problem definition	**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**
4	Initial and boundary conditions	**ADIABATIC**, **BOUNDARY**, **FIX**, **FLOW**, **FRICTION**, **INITIAL**, **INLET**, **OPEN**, **OUTLET**, **PERIODIC**, **READ**, **SET**, **SWIRL**, **SYMMETRY**, **TIDE**,**TIME**
5	Fluid and Host Matrix Properties and constants	**CONDUCTION**, **DENSITY**, **DIFFUSION**, **DISTRIBUTION**, **FLUID**, **FUEL**, **HYDRAULIC**, **GAS**, **LATENT**, **MULTIPHASE**, **OXIDIZER**, **PERMEABILITY**, **POROSITY**, **PRANDTL**, **PROPERTY**, **REFERENCE**, **RETARDATION**, **SCHMIDT**, **SPECIFIC**, **STORAGE**, **THERMAL**, **TORTUOSITY**, **TRANSPORT**, **VISCOSITY**
6	Nature of Flow	**COMPRESSIBLE**, **LAMINAR**, **RADIATION**, **REACTION**, **SOLID**, **SOOT**, **TURBULENT**
7	Source and sink specifications	**ARRHENIUS**, **CORIOLIS**, **EBU**, **DECAY**, **PRECIPITATE**, **REACTION**, **REGENERATION**, **SOURCE**
8	Solution options	**DISABLE**, **INTEGRATION**, **LIMIT**, **MATRIX**, **RELAX**
9	Output control	**CLOSE**, **CORRELATION**, **DEBUG**, **DIAGNOSTIC**, **FLUX**, **HISTORY**, **PRINT**, **OUTPUT**, **SAVE**, **SCREEN**, **STACK**, **STATISTICS**, **TRACK**, **VELOCITY**, **WRITE**
10	Operational control	**ALLOCATE**, **CONVERGENCE**, **DEFINE**, **ELSE**, **END**, **ENDIF**, **FILE**, **IF**, **INDENT**, **META**, **PAUSE**, **QUIT**, **SOLVE**

[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 2.4.1: I/O FILE UNITS AND THEIR DEFAULT ASSIGNMENT

UNIT #	DEFAULT FILE NAME	FUNCTION OF THE FILE
15	Console	Read user input commands from standard input device.
16	xxx.out	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
81	ACRINIT.ACR	ACRi Initialization file
82	ACRIMSG.ACR	ACRi file for diagnostic and error messages, and formats
Auto	zzz_LCNS.ACR	ACRi user License file. The string zzz is replaced by a set of characters that is unique to each user.
Auto	xxx_DEBUG.TMP	User specific diagnostic and debug output (**DEBU**G).
Auto	xxx_GRID_QUALITY.TMP	Grid quality information (**DEBU**G **GEOM**ETRY **FILE**).
Auto	acr_MTRXxxx.TMP	Solution Matrix Coefficients (**DEBU**G **MATR**IX). The string xxx is replaced by an identifier for the variable for which the output is generated
Auto	xxx_FLUX.TMP***	Write data for fluxes crossing a sub-region boundary (**FLUX**).
Auto	xxx_DIAGNOSTIC.TMP***	Internally generated file with step-by-step diagnostics of convergence history for each variable for which a transport equation is solved (**DIAG**NOSTIC).
Auto	xxx_HISTORY.TMP	Time-history data file (**HIST**ORY).
Auto	xxx_HISTORY_XYZ.TMP	Time-history at specified locations (**HIST**ORY **COOR**DINATE).
Auto	xxx_SOURCE.TMP	Time-history of source of variables (**HIST**ORY **SOUR**CE.
Auto	xxx_STORAGE.TMP	Time-history of storage of variables (**HIST**ORY **STOR**AGE).
Auto	acr_REDBLACK.TMP	Red/Black matrix split information (**MATR**IX **REDB**LACK).
Auto	acr_NOZZLE.TMP	Nozzle spray trajectory information (**NOZZ**LE **TRAJ**ECTORY).
Auto	xxx_PRINT_FORCE.TMP	Time-history of forces or moments on a surface (**PRIN**T **FORC**E).
11	xxx.SAV***	Write data file for restart, archiving and post-processing (**SAVE**).
Auto	xxx_RESTART.TMP***	ACRi restart file (**SAVE REST**ART, **READ REST**ART,).
12	xxx_TABLE.SAV***	Write archive data file in tabular form (**SAVE TABL**E).
Auto	xxx_STATS.TMP	Statistics information pertaining to variables (**STAT**ISTICS).
Auto	xxx_TRACK.TMP***	Particle Track information for the flow field (**TRAC**K).
Auto	acr_XYZ_CRNR.TMP	Corner coordinates for each element (**WRIT**E **CORN**ERS).
Auto	xxx_VRTX_MAP.TMP	Vertex Mapping information automatically generated if needed.

***** 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 **DEBU**G, **DIAG**NOSTIC, **FLUX**, and **OUTP**UT commands. The **DEBU**G command provides a printout of numerical error parameters, which are useful in evaluating the accuracy of numerical solution. The **DIAG**NOSTIC 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 **OUTP**UT 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 2.7.1: DEPENDENT VARIABLES OF ACRi™ SOFTWARE TOOLS

ACRi™ Software	Software Symbol	Mathematical Symbol	Description of the Variable
ANSWER™ TIDAL™	U	U	Velocity component in x-direction
ANSWER™ TIDAL™	V	V	Velocity component in y or r-direction
ANSWER™	W	W	Velocity component in z or θ-direction
ANSWER™	PP	φ	Density and Pressure correction variable
ALL	HT	h or h_s	Enthalpy or Stagnation enthalpy (See Note below)
ALL	T	T	Temperature
ANSWER™	K	K	Kinetic energy of turbulence
ANSWER™	E	ε	Dissipation of turbulence energy (See Note below)
ANSWER™	FF	m_C	Mass fraction of total carbon
ANSWER™	FH	m_H	Mass fraction of total hydrogen
ANSWER™	FO	m_O	Mass fraction of total oxygen
ANSWER™	FU	m_{CnHm}	Mass fraction of fuel species
ANSWER™	CH	m_{CnHm-2}	Mass fraction of H_2-stripped fuel
ANSWER™	CO	m_{CO}	Mass fraction of carbon monoxide
ANSWER™	H2	m_{H2}	Mass fraction of hydrogen
ANSWER™	RA	$(R_x+R_y+R_z)/3$	Net incoming thermal radiation flux.
ANSWER™	SN	S_N	Concentration of soot nuclei
ANSWER™	S1	S_1	Concentration of small soot particles
ANSWER™	S2	S_2	Concentration of large soot particles
PORFLOW™	P	P^1	Pressure head for 1st (primary) fluid phase
PORFLOW™	P2	P^2	Pressure head for 2nd fluid phase
PORFLOW™	P3	P^3	Pressure head for 3rd fluid phase
TIDAL™	ETA	η	Fluid elevation above datum
PORFLOW™ & TIDAL™	C, C2,C3, C4	C^k	Mass concentration of 1st through 4th species in fluid
ALL	User defined	none	Variables defined by the user with the ALLOCATE command or one of the above variables renamed by the user with the RENAME command.

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. Table 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 (**CONN**ECTIVITY 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 **OUTP**UT, **SAVE** and **WRIT**E 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 **OUTP**UT 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 **WRIT**E 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 flied, the vorticity, stresses, strains, and some special variables. Please see the **OUTP**UT 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 **OUTP**UT and **SAVE** commands for a detailed description of this output.

TABLE 2.8.1: STANDARD VARIABLES OF ANSWER™ SOFTWARE TOOL

Software Symbol	Mathematical Symbol	Description of the Variable
U	U	Velocity component in x-direction
V	V	Velocity component in y or r-direction
W	W	Velocity component in z or θ-direction
P	P	Fluid pressure
HT	h or h_s	Enthalpy or Stagnation enthalpy
T	T	Fluid Temperature
K	k	Kinetic energy of turbulence
E	ε	Dissipation of turbulence energy
L	ℓ	Length scale of turbulence
FF	m_C	Mass fraction of total carbon
FH	m_H	Mass fraction of total hydrogen
FO	m_O	Mass fraction of total oxygen
FU	m_{CnHm}	Mass fraction of fuel species
CH	m_{CnHm-2}	Mass fraction of H_2-stripped fuel
CO	m_{CO}	Mass fraction of carbon monoxide
H2	m_{H2}	Mass fraction of hydrogen
O2	m_{O2}	Mass fraction of oxygen
H2O	m_{H2O}	Mass fraction of water
CO2	m_{CO2}	Mass fraction of carbon dioxide
NO	M_{NO}	Mass fraction of Nitrogen Oxides
NO2	M_{NO2}	Mass fraction of Nitrogen Di-oxides
FG	G	The property g for the fuel fluctuation equation
FM	f_m	The mean-mixture fraction for for the fuel fluctuation equation
PV	f_v	The mixture variance for the fuel fluctuation equation
SN	S_N	Concentration of soot nuclei
LF		Liquid mass fraction from the nozzle injections
AD		Average droplet diameter for nozzle injections
S1	S_1	Concentration of small soot particles
S2	S_2	Concentration of large soot particles
RA	$(R_x+R_y+R_z)/3$	Net incoming thermal radiation flux.
RGAS	R	The specific gas constant for the gaseous mixture
MU	μ	Effective viscosity of fluid
RHO	ρ	Mass density of fluid
POR	Θ_E	Effective porosity of a grid element
PHYD		Hydraulic head of the fluid
EBYK	ε/k	Turbulence time constant
CP	C_p	Specific Heat of fluid mixture
SPEED	V	Modulus of Velocity = $Sqrt(u^2+v^2+w^2)$
EDYN	$0.5\ V^2$	Dynamic energy of fluid
PDYN	$0.5\ \rho\ V^2$	Dynamic pressure of fluid
PTOTAL	$P+0.5\ V^2$	Total pressure of fluid
MACH	c/a	Mach Number for the fluid = V/sqrt[(γ-1)CpT]
VOL	δV	Volume of the Element
X, Y, Z	x, y, z	X, Y and Z Coordinates of the Node Location
User-Specific	---	User-specific variables defined in the **acrNAMES.ACR** file
Dynamically Allocated	---	Dynamically allocated variables with **ALLO**CATE or **RENA**ME commands

TABLE 2.8.2: STANDARD VARIABLES OF PORFLOW™ SOFTWARE TOOL

Software Symbol	Mathematical Symbol	Description of the Variable
U	U	Velocity component in x-direction
V	V	Velocity component in y or r-direction
W	W	Velocity component in z or θ-direction
P	P	Fluid pressure
HT	h or h_s	Enthalpy or Stagnation enthalpy
T	T	Fluid Temperature
POR	Θ_E	Effective porosity of a grid element
PORT	Θ_T	Total porosity of a grid element
PORD	Θ_D	Diffusional porosity of a grid element
PHYD		Hydraulic head of the fluid
CP	C_p	Specific Heat of fluid mixture
SPEED	V	Modulus of Velocity = Sqrt(u^2+v^2+w^2)
EDYN	0.5 V^2	Dynamic energy of fluid
PDYN	0.5 ρ V^2	Dynamic pressure of fluid
PTOTAL	P+0.5 V^2	Total pressure of fluid
MACH	c/a	Mach Number for the fluid = V/sqrt[(γ-1)CpT]
C, C2,C3, C4	C^k	Mass concentration of 1st through 4th species in fluid
S, S2, S3	S^1, S^2, S^3	Saturation fraction for the 1st, 2nd and 3rd fluid phase
RHO, RHO2,	R^1, R^2	Normalized Density of the 1st and 2nd fluid phase
RHOG	R^3	Normalized Density of the 3rd (gas) fluid phase
RHOS	ρ_s	Mass density of solid matrix
H, H2, H3	H^1, H^2, H^3	Total hydraulic head for the 1st, 2nd and 3rd fluid phase
MOIS	Φ_E	Effective moisture in the first fluid phase
MU	μ/μ^*	Viscosity ratio for the primary Fluid
QX, QY, QZ		X, Y and Z components of element-average Darcy Velocity
VOL	δV	Volume of the Element
X, Y, Z	x, y, z	X, Y and Z Coordinates of the Node Location
User defined	---	User-defined variables with **ALLO**CATE or **RENA**ME commands

TABLE 2.8.3: STANDARD VARIABLES OF TIDAL™ SOFTWARE TOOL

Software Symbol	Mathematical Symbol	Description of the Variable
U	U	Velocity component in x-direction
V	V	Velocity component in y or r-direction
W	W	Velocity component in z or θ-direction
HT	h or h_s	Enthalpy or Stagnation enthalpy
T	T	Fluid Temperature
RHO	ρ	Mass density of fluid
CP	C_p	Specific Heat of fluid mixture
SPEED	V	Modulus of Velocity = Sqrt($u^2+v^2+w^2$)
EDYN	$0.5\ V^2$	Dynamic energy of fluid
PDYN	$0.5\ \rho\ V^2$	Dynamic pressure of fluid
PTOTAL	$P+0.5\ V^2$	Total pressure of fluid
C, C2,C3, C4	C^k	Mass concentration of 1^{st} through 4^{th} species in fluid
ETA	η	Fluid elevation above datum
H	H	Total fluid depth = h +η
DEPT	h	Bathymetric depth below datum
PA	P_a	Atmospheric pressure
WIND	w	Wind speed
ANGL	Θ	Angle that the wind vector makes with the positive direction of x
VOL	δV	Volume of the Element
X, Y, Z	x, y, z	X, Y and Z Coordinates of the Node Location
User defined	---	User-defined variables with **ALLO**CATE or **RENA**ME commands

TABLE 2.8.4: SUPPLEMENTARY VARIABLES OF ACRi™ SOFTWARE TOOLS

Software Symbol	Variable Basis	Variable Type	Description of the Variable
XC, YC, ZC	Vertex	Real	x, y and z coordinates for element vertices
VOLF	Face	Real	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.
VOLR	Face	Real	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.
AFX, AFY, AFZ	Face	Real	The x, y and z components of the area vector for an element face.
FC	Face	Real	Convective mass flux across an element interface.
FD	Face	Real	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)
NCRN	Vertex	Integer	Element to vertex connectivity
NBRS	List	Integer	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.
NFACE	List	Integer	Element to surface number connectivity. For each element, the list contains the surface numbers that comprise the element boundary.
LINK	List	Integer	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.
MTYP	Node	Integer	Material Type index

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 BLOC**K, **SAVE TABLE** and **SAVE REST**ART 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 BLOC**K command provides flexibility in the selection of variables, the output frequency and the nature of data records (formatted or unformatted). In the **SAVE BLOC**K 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 TABL**E 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 REST**ART mode is strictly meant for restart of a given problem and is generated only in **UNFO**RMATTED 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 **REST**ART modifier. This file is in an unformatted format and is machine specific. This file can only be read with the **READ** command with a **REST**ART 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

```
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.
 /
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
```

(This page left intentionally blank)

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^{th} 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.

V_{frq} 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 "**FORM**ATTED" mode. Some commands also allow an "**UNFO**RMATTED" 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 **LOCA**TE or **SELE**CT command (in this document "**LOCA**TE" is used to identify both these commands). Multiple modes of **LOCA**TE command are available to accommodate a diversity of input and output requirements. Each **LOCA**TE 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 **LOCA**TE command for a subregion may also be specified without a unique identifier, then this subregion may be identified on a subsequent command by specifying **LOCA**TE or **SELE**CT as a modifier till the occurrence of the .next **LOCA**TE 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 3.4.1: VALID SUBREGION IDENTIFICATION MODIFIERS

subrgn	Interpretation
SELE	The input applies to the most recently defined subregion of the **LOCA**TE or **SELE**CT command. Same as **LOCA**TE modifier.
LOCA	The input applies to the most recently defined subregion of the **LOCA**TE or **SELE**CT command. Same as **SELE**CT modifier.
ID=idsub	The input applies to the subregion that was assigned the identity 'idsub' in a previous **LOCA**TE or **SELE**CT command.

*The **LOCA**TE 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 **LOCA**TE command specifies only a boundary, then only the nodes falling at the boundary are included in the subregion.

However, if a **LOCA**TE 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 **FIEL**D modifier is present on a **LOCA**TE 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 **FIEL**D 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 **FIEL**D modifier is ignored if the **LOCA**TE 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

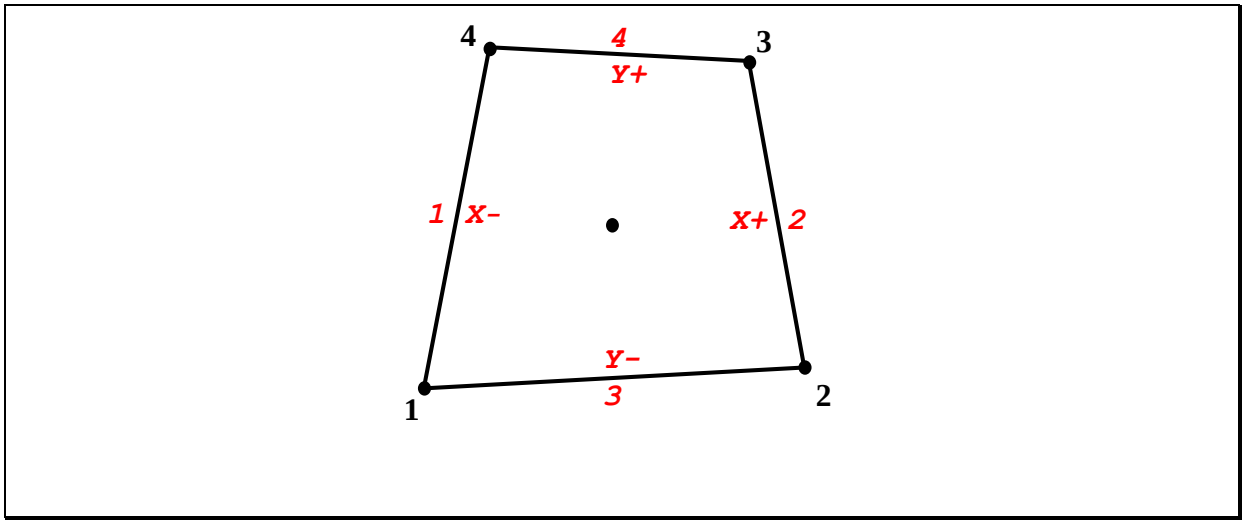
Some of the commands refer to input for the boundaries of the problem. These boundaries may be the external boundaries, which enclose the domain of computation, or these may be internal boundaries that are located within the domain of computation. For these commands the boundary orientation is identified either explicitly on the command by a direction modifier or it is specified as an integral part of the sub-domain specification by the **LOCA**TE command with a **PAIR**ED 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 **LOCA**TE 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 3.5.1 BOUNDARY IDENTIFICATION INDEX

Orientation	Interpretation
X-	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.
X+	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 3.5.1
Y-	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 3.5.1
Y+	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 3.5.1
Z-	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.
Z+	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 3.5.1.

Vertex and Face Number Nomenclature for a Quadrilateral Element



Vertex and Face number Nomenclature for a Hexahedral Element

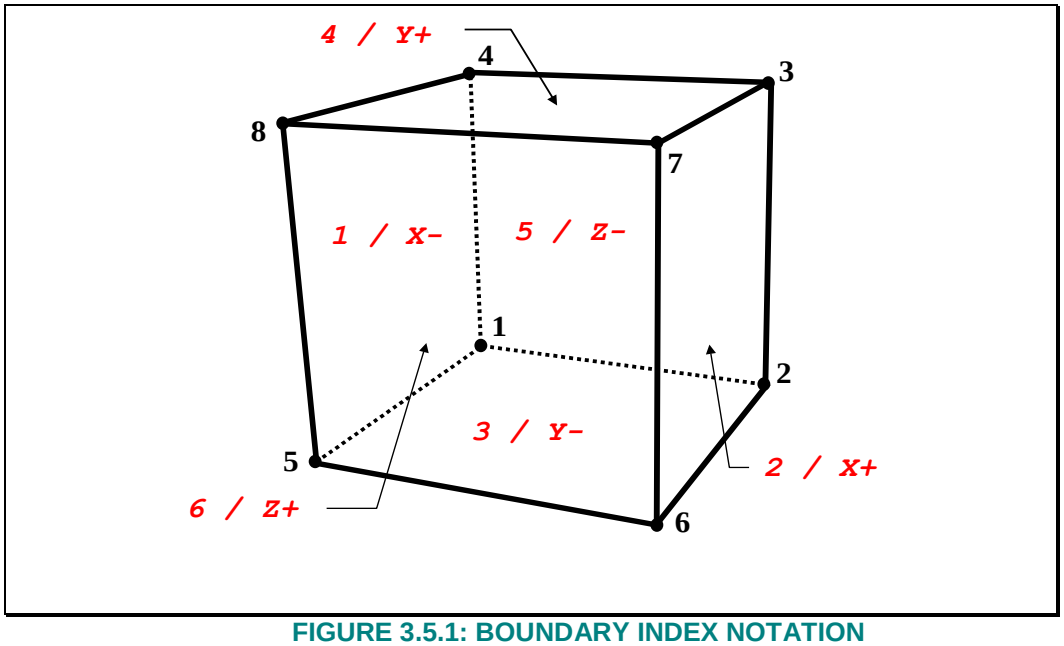


FIGURE 3.5.1: BOUNDARY INDEX NOTATION

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 3.6.1: VALID MODIFIERS FOR PHASE DESIGNATION

User Specification of phase	Interpretation For The Corresponding Command
FIRSt	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.
SECOND	The input is for the second phase of the fluid.
THIRd	The input is for the third phase of the fluid. This modifier is available only for the **PORFLOW™** Software Tool.
GAS	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 **FIRS**t modified for a single-phase gas, the **SECO**ND modifier for a liquid-gas, and the **THIR**d modifier for a liquid-liquid-gas simulation.
VAPO	Same as **GAS** Modifier

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.

(This section left intentionally blank)

CHAPTER 4

FUNCTIONAL INPUT FOR FREEFROM 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:

$$\Phi = \Phi(\xi) \tag{4.1.1}$$

here Φ 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 Φ 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 Φ is specified as an arbitrary function of ξ. The desired value is obtained as a step-wise or piece-wise linear, quadratic or cubic approximation over the values of Φ in the neighborhood of the given value of ξ. This can be expressed as:

$$\text{Given : } \Phi(\xi) = \Phi_n(\xi_n);\ \ 1<n<N$$

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

Where α=β=γ=0 for step wise, α=1; β=γ=0 for linear, α=1; β=1/2; γ=0 for quadratic and α=1; β=1/2; γ=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 ξ used in the above interpolation relation is computed as:

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

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

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

$$\Phi(\xi_N + \delta\xi) = \Phi_N + \left(\frac{\partial\Phi}{\partial\xi}\delta\xi\right)_N;\ \ \xi > \xi_N \tag{4.1.4}$$

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:

$$\Phi_n = A_n;\ \ 1<n\le N, \tag{4.1.5}$$

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:

$$\Phi_n(t) = A_n;\ \ 1<n\le N, \tag{4.1.6}$$

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:

$$\Phi_n^t = \Phi_n^m + \alpha \frac{t - t^m}{t^{m+1} - t^m} (\Phi_n^{m+1} - \Phi_n^m); \quad t^m \le t < t^{m+1}. \tag{4.1.7}$$

Where the coefficient α 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 π. 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. For set of N values, all the three distributions are all given by::

$$\Phi_n = x_n; \quad 1 < n \le N, \tag{4.1.8}$$

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 uniform random number sequence is defined by a mean value (μ) and a range (R). For a sub-domain with a total of N nodes, the PNR, denoted by x_n, are then generated by the algorithm and assigned in order of the occurrence of the nodes in the sub-domain according to: The probability density function (pdf) and the cumulative distribution function (cdf) for this distribution are:

$$\text{pdf}(x) = \frac{1}{R}, \quad \mu - \frac{R}{2} \le x \le \mu + \frac{R}{2}; \quad 0 \text{ for all other } x \tag{4.1.9}$$

$$\text{cdf}(x) = \frac{x - R/2}{R}, \quad \mu - \frac{R}{2} \le x \le \mu + \frac{R}{2}; \quad 0 \text{ if } x < \mu - \frac{R}{2}; \quad 1 \text{ if } x > \mu + \frac{R}{2} \tag{4.1.10}$$

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

$$E(x) = \mu; \quad m(x) = \mu; \quad \text{Var}(x) = \frac{R^2}{12} \tag{4.1.11}$$

The Normal or Gaussian probability density function (pdf) is defined by a mean,μ, and a standard deviation, σ. 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:

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

$$\text{cdf}(x) = \frac{1}{2} + \frac{1}{2} \text{erf} \frac{x - \mu}{\sqrt{2\sigma^2}}, \tag{4.1.13}$$

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

$$E(x) = \mu; \quad m(x) = \mu; \quad \text{Var}(x) = \sigma^2 \tag{4.1.14}$$

:

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:

$$\text{pdf(x)} \quad = \quad \frac{1}{x\sqrt{2\pi\sigma^2}} \exp\left[- \frac{\{\ln(x) - \mu\}^2}{2\sigma^2} \right], \tag{4.1.15}$$

$$\text{cdf(x)} = \frac{1}{2} + \frac{1}{2} \text{erf} \frac{\ln(x) - \mu}{\sigma\sqrt{2}}, \tag{4.1.16}$$

The mean, E(x), the median, m(x), and the variance of the Log-Normal distribution are given by:

$$E(x) \; = \; e^{\mu + \sigma^2/2}; \quad m \; = \; e^{\mu}; \quad \text{Var(x)} = \left(e^{\sigma^2} - 1 \right) e^{2\mu + \sigma^2} \tag{4.1.17}$$

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

4.1.5 The Constant Function

$$\Phi = A \tag{4.1.18}$$

4.1.6 Replacement Function

$$\Phi = \xi \tag{4.1.19}$$

4.1.7 Multivariate Polynomial Functions

$$\Phi = A_0 + \sum_{n=1}^{N} A_n \, \xi_n, \quad 1 \le N \le 7 \tag{4.1.20}$$

$$\Phi = A_0 + \sum_{n=1}^{N} \left(A_n \, \xi_n + B_n \, \xi_n^2 \right), \quad 1 \le N \le 7 \tag{4.1.21}$$

$$\Phi = A_0 + \sum_{n=1}^{N} \left(A_n \, \xi_n + B_n \, \xi_n^2 + C_n \, \xi_n^3 \right), \quad 1 \le N \le 7 \tag{4.1.22}$$

4.1.8 The Higher Order Polynomial Functions

$$\Phi = A + B \, \xi + C \, \xi^2 + D \, \xi^3 + E \, \xi^4 \tag{4.1.23}$$

$$\Phi = A + B \, \xi + C \, \xi^2 + D \, \xi^3 + E \, \xi^4 + F \, \xi^5, \tag{4.1.24}$$

$$\Phi = A + B \, \xi + C \, \xi^2 + D \, \xi^3 + E \, \xi^4 + F \, \xi^5 + G \, \xi^6, \tag{4.1.25}$$

$$\Phi = A + B \, \xi + C \, \xi^2 + D \, \xi^3 + E \, \xi^4 + F \, \xi^5 + G \, \xi^6 + H \, \xi^7, \tag{4.1.26}$$

4.1.9 The Power Functions

$$\Phi = A \, (\, \xi + B \,)^C + D, \tag{4.1.27}$$

$$\Phi = A \, \left| \xi + B \right|^C + D, \tag{4.1.28}$$

4.1.10 The Exponential Functions

$$\Phi = A \exp(\, B \, \xi + C \,) + D, \tag{4.1.29}$$

$$\Phi = \sum_{n=1}^{N} A_n \exp(B_n \, \xi + C_n) + D, \tag{4.1.30}$$

4.1.11 The Logarithmic Functions

$$\Phi = A \ln(\, B \, \xi + C \,) + D, \tag{4.1.31}$$

$$\Phi = \sum_{n=1}^{N} A_n \ln(B_n \xi + C_n) + D, \quad (4.1.32)$$

4.1.12 The Trigonometric Functions

$$\Phi = A \sin(B \xi + C) + D, \quad (4.1.33)$$

$$\Phi = \sum_{n=1}^{N} A_n \sin[2\pi \frac{\xi + C_n}{B_n}] + D \quad (4.1.34)$$

$$\Phi = A \cos(B \xi + C) + D, \quad (4.1.35)$$

$$\Phi = \sum_{n=1}^{N} A_n \cos[2\pi \frac{\xi + C_n}{B_n}] + D \quad (4.1.36)$$

$$\Phi = A \tan(B \xi + C) + D, \quad (4.1.37)$$

$$\Phi = \sum_{n=1}^{N} A_n \tan[2\pi \frac{\xi + C_n}{B_n}] + D \quad (4.1.38)$$

$$\Phi = A \arcsin(B \xi + C) + D, \quad (4.1.39)$$

$$\Phi = \sum_{n=1}^{N} A_n \arcsin[2\pi \frac{\xi + C_n}{B_n}] + D \quad (4.1.40)$$

$$\Phi = A \arccos(B \xi + C) + D, \quad (4.1.41)$$

$$\Phi = \sum_{n=1}^{N} A_n \arccos[2\pi \frac{\xi + C_n}{B_n}] + D \quad (4.1.42)$$

$$\Phi = A \arctan(B \xi + C) + D, \quad (4.1.43$$

$$\Phi = \sum_{n=1}^{N} A_n \arctan[2\pi \frac{\xi + C_n}{B_n}] + D \quad (4.1.44)$$

4.1.13 Rational Functions

$$\Phi = \frac{A + B\xi}{C + D\xi}, \quad (4.1.45)$$

$$\Phi = \frac{(A + B\xi)^E}{(C + D\xi)^F}, \quad (4.1.46)$$

4.1.14 Power of Ten Function

$$\Phi = A\, 10^{\frac{B}{\xi + C}} + D \quad (4.1.47)$$

4.1.15 Inverse Exponential Function

$$\Phi = A \exp(\frac{B}{\xi + C}) + D, \quad (4.1.48)$$

4.1.16 Gate Function

$$\Phi = \beta A B \sqrt{|\xi - C|} \; ; \quad \beta = 1 \quad \text{if} \quad \xi > C \quad \text{otherwise} \quad \beta = 1; \quad (4.1.49)$$

4.1.17 Sutherland Function

$$\Phi = A \frac{B + C}{\xi + C} \left(\xi / B \right)^{3/2} \tag{4.1.50}$$

4.1.18 Multivariate Linear Sum

$$\Phi = \sum_{n=1}^{N} \xi_n \tag{4.1.51}$$

$$\Phi = \sum_{n=1}^{N} A_n \, \xi_n + A_{N+1} \tag{4.1.52}$$

4.1.19 Multivariate Square Sum

$$\Phi = \sum_{n=1}^{N} \xi_n^2 \tag{4.1.53}$$

$$\Phi = \sum_{n=1}^{N} A_n \, \xi_n^2 + A_{N+1} \tag{4.1.54}$$

4.1.20 Multivariate Square Root of Sum of Squares

$$\Phi = \sqrt{\sum_{n=1}^{N} \xi_n^2} \tag{4.1.55}$$

$$\Phi = \sqrt{\sum_{n=1}^{N} A_n \, \xi_n^2 + A_{N+1}} \tag{4.1.56}$$

4.2 COMMAND INPUT OF FUNCTIONAL FORM

The functional form of input can be used with a number of commands. Currently these include the **ABSO**RPTIVITY, **BORE**HOLE, **BOUN**DARY, **COND**UCTION, **DENS**ITY, **DIFF**USION, **DIST**RIBUTION, **FLOW**, **FRAC**TURE, **GAS**, **RADI**ATION, **RETA**RDATION, **SET, SOUR**CE, **SPEC**IFIC heat, **STOR**AGE, **SWIR**L, **TRAN**SFER, and **VISCO**SITY 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 ξ, respectively. Valid input options for **func** and their corresponding interpretations are given in Tables 4.2.1. Valid input options for independent variable ξ 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, ξ at the same location. However, if the modifier "STAC" is present on a command then the function is evaluated with the value of ξ at the most recent location specified by the STAC**K **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 4.2.1: VALID INPUT FUNCTIONAL FORMS

Function	Option	Dependent Variable Computed From
TABL		Equation 4.1.2 with STEP, LINE, QUAD or CUBI modifiers
TABL	PERI	Equations 4.1.2 and 4.1.3 with STEP, LINE, QUAD or CUBI modifiers
TABL	EXTR	Equations 4.1.2 and 4.1.4 with STEP or LINE or QUAD modifiers
NODE		Equation 4.1.5
NODE	TIME	Equation 4.1.7 with STEP (α=0) or LINE (α=1) modifier
RANDOM	UNIF	Equation 4.1.9
RANDOM	GAUS	Equation 4.1.12
RANDOM	LOG	Equation 4.1.15
CONS		Equation 4.1.18
EQUAL		Equation 4.1.19
LINE		Equation 4.1.20
CUBI		Equation 4.1.21
QUAD		Equation 4.1.22
POLY		Equation 4.1.20 through Equation 4.1.26
POWE		Equation 4.1.27
POWE	MODU	Equation 4.1.28
EXP or EXPO		Equation 4.1.29
EXP or EXPO	SERIes	Equation 4.1.30
LN or LOG		Equation 4.1.31
LN or LOG	SERIes	Equation 4.1.32
SIN or SINE		Equation 4.1.33
SIN or SINE	SERIes	Equation 4.1.34
COS or COSI		Equation 4.1.35
COS or COSI	SERIes	Equation 4.1.36
TAN or TANG		Equation 4.1.37
TAN or TANG	SERIes	Equation 4.1.38
ASIN		Equation 4.1.39
ASIN	SERIes	Equation 4.1.40
ACOS		Equation 4.1.41
ACOS	SERIes	Equation 4.1.42
ATAN		Equation 4.1.43
ATAN	SERIes	Equation 4.1.44
RATI		Equation 4.1.45
RATI		Equation 4.1.46
POWER	TEN	Equation 4.1.47
EXP or EXPO	INVE	Equation 4.1.48
GATE		Equation 4.1.49
SUTHERLAND		Equation 4.1.50
SUM		Equation 4.1.51 or Equation 5.1.52
SQUA		Equation 4.1.53 or Equation 5.1.54
ROOT		Equation 4.1.55 or Equation 5.1.56
USER	GLOBal	User-defined function called only once for the computational domain.

TABLE 4.2.2: VALID INDEPENDENT VARIABLES

User Specification ξ	Denotes Independent Variable
TIME	t
X	Coordinate x
Y or R	Coordinate y (or r for radial geometry)
Z or THETa	Coordinate z (or θ for radial geometry)
Any of the symbols in Table 2.8.1-3	The corresponding variable listed in Table 2.8.1 -3

TABLE 4.2.3: NUMERICAL INPUT FOR THE TABLE SPECIFICATION

Numerical Value	Interpretation
N1	The number of sets of input in the table that are specified by Equation 4.1.2.
N2, ... , Nn	The pairs of values, ξ_n and θ_n (in that order), for Equation 4.1.2. A total of 2*N1 values (N1 sets) must be specified.

TABLE 4.2.4: NUMERICAL INPUT FOR SIMPLE ANALYTIC FUNCTIONS

Numerical Value	Interpretation
N1, ... , Nn	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.

TABLE 4.2.5: NUMERICAL INPUT FOR THE SERIES FUNCTIONS

Numerical Values	Interpretation
N1	The number of sets of input in the series specified by Equations given above nwuth the “SERIES” modifier.
N2, ... , Nn-1	The triplet of values of A_n, B_n and C_n (in that order), for the series functions. A total of 3*N1 values (N1 sets) must be specified.
Nn	The datum A_0 for the function.

TABLE 4.2.6: NUMERICAL INPUT FOR USER SPECIFIED FUNCTIONS

Numerical Value	Interpretation
N1	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.
N2, ... , Nn	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.

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 **DENS**ITY, **SET**, **VISC**OSITY and a number of other commands. The availability for a particular command is indicated by the presence of the "**operation**" on the command.

TABLE 4.3.1: ADDITIONAL OPERATIONS ON FUNCTIONS

operation	Operation Performed
REPLACE	The computed value replaces the existing value for that variable. This is the default option.
ADD	The computed value is added to the existing value for that variable.
SUBTRACT	The computed value is subtracted from the existing value for that variable.
MULTIPLY	The computed value multiplies the existing value for that variable.
DIVIDE	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.
ABS or **ABSO**	The absolute value of the computed function is taken. This modifier may be present along with one of the **REPL**ACE, **ADD, SUBT**RACT, **MULT**IPLY or **DIVI**DE modifiers
POSITIVE	The negative values for the computed function are set of zero This modifier may be present along with one of the **REPL**ACE, **ADD, SUBT**RACT, **MULT**IPLY or **DIVI**DE modifiers
NEGATIVE	The positive values for the computed function are set of zero. This modifier may be present along with one of the **REPL**ACE, **ADD, SUBT**RACT, **MULT**IPLY or **DIVI**DE modifiers

In case of multiple specification of **REPL**ACE, **ADD, SUBT**RACT, **MULT**IPLY and **DIVI**DE modifiers, the first specification takes precedence over others. Similarly in case of multiple specification of **ABS** or **ABSO**, **POSI**TIVE and **NEGA**TIVE, the first specification takes precedence over others

4.4 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 **SOUR**CE command would specify the source for that variable and, the **BOUN**DARY 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

Illustrative Commands
//// Constant boundary temperature of 30. BOUNDARY value at X+ is CONSTANT T = 30.
//// Source for temperature is a constant value for active subregion SOURce for T: = 100 W/m^3 in currently SELEcted subregion
//// Field values of T set as a power law of pressure in previously identified subregion SET T as POWEr law: [1.020 * (P + 0.] ^ 0.50 + 100] in subregion ID=ZON1
//// Boundary temperature is a sinusoidal function of time BOUNdary value at Y+: function: T = 10. * SIN (0.003 * TIME +0.5) +10.
//// Field values of temperature set as a polynomial function of coordinate X SET T: POLYnomial in X: (10, 0.5, 0, -0.1, 0.)
//// Boundary temperature is a linear function of y coordinate BOUNdary value at X+ boundary LINEar function: T = 30. -0.015 * Y
//// Temperature is a cosine function of time SET T as 100 * COSIne (0.00274 * TIME)
//// Temperature is an exponentially decaying function of time SET T as 100 * EXP (-0.001 * TIME) +100.
//// Source for temperature is a linear function of Pressure SOURce LINEar function (T = 0. -0.10 * P)
//// Source for temperature is a cosine function of time SOURce T COSIne function of TIME: 100, 0.00274, 0., +10.5
//// Thermal conductivity for temperature is a linear function of temperature itself CONDuctivity for T LINEar function: 0. -0.10 * T

TABLE 4.4.2: EXAMPLES OF ANALYTIC FUNCTION SERIES

Illustrative Commands
//// Boundary P is a function of T (temperature) BOUNdary value for P at Y- boundary: COSIne SERIes in T: 3 sets (0, 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.
//// Field values for temperature set as sinusoidal function of Y coordinate SET T as SINE SERIes in Y: 3 sets: (0, 5, 1), (100, 10, 1), (200, 20, 3)
//// Source for temperature is a 3 term cosine series in velocity U SOURce T as COSIne SERIes in U: 3 sets (0, 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.
//// Boundary flux for T is a 3 part sinusoidal function of temperature BOUNdary T at Y- boundary FLUX type: SINE SERIes in T: 3 sets (0., 5, 1), (100, 10, 1), (200, 20, 3) datum= 0., h=1.E-4
//// Source for temperature is a function of temperature (itself) SOURce T SINE SERIes in T: 3 sets: (0, 5, 1), (100, 10, 1), (200, 20, 3)
//// Source for T as an exponential function of time SOURce T: EXPOnential SERIes in TIME; with 3 terms (0.1, 1.0) (0.05, 0.1) (0.001, 01), base value = 0.
//// Field value of U velocity is set as a function of Temperature SET value for U as COSIne SERIes in T: 3 sets (0., 5, 1), (100, 10, 1), (200, 20, 3) datum = 10.
//// Pressure set as a 24 part cosine series; coefficients are contained in file named 'COSVALS' SET P as COSIne SERIes of T: 24 sets from file 'COSVALS'

TABLE 4.4.3: EXAMPLES OF TABULAR FUNCTIONS

Illustrative Commands
//// The value of P at the boundary is a tabular function of time BOUNdary P value at Y- boundary: TABLe of values: 3 sets (TIME, value) (0., 0.01), (100, 0.10), (200, -0.20)
//// The flux of P at the boundary is a tabular function of time BOUNdary P at X-: FLUX is a TABLe in TIME: 3 sets (0., 5), (100, 15), (200, 3.5), h=0.001
//// The field values of temperature are set as a tabular function of time SET T as TABLe of values: 3 sets: (0., 0.01), (100, 0.10), (200, -0.20)
//// As above except that step-wise, rather than the linear, interpolation is used SET T is STEP wise TABLe: 3 sets: (0., 0.01), (100, 0.10), (200, -0.20)
//// As above except that the values will be repeated after 200 time units SET T is PERIodic TABLe with STEP wise interpolation: 3 sets: (0., 0.01), (100, 0.10), (200, -0.20)
//// Table with linear interpolation but time input set to result in steep step-like interpolation SET T for as TABLe of values: with 6 sets: (TIME, value) (0., 0.0) (1.0000, 0.0) (1.0001, 1.0) (2., 1.0) (2.0001, 0.5) (3.0000, 0.2)
//// Table with linear interpolation but input from a file SET T for domain as function of TIME: 20 sets from file 'TIMEVALS'

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} [V_1,..V_m] [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 **STRU**CTURED mode if the **subrgn** was defined with a **LOCA**TE 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 **UNST**UCTURED 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 **LOCA**TE 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 **LOCA**TE command. It should be noted that if the **LOCA**TE 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 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 **LOCA**TE command which can be examined by including a file name on the **LOCA**TE command.

fname The name of the file for numerical values unless the values are directly specified by **V_1….V_m** below. See Section 3.3 for additional information.

V_1….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. Note that the modifiers **FIEL** 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 **NODE**S for **SELE**CTED region from **'ACTIVAL'** in **STRU**CTURED mode
SET T in **ID=RGN1** region from file **'RGN1VAL'** only for the **FIEL**D 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:

SET **{Φ} {TIME} [LINE|STEP] {NODE|STRU|UNST} fname} [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.

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.

LINE The time step interpolation is linear; this is the default option.

STEP The time step interpolation is step function (Equation 4.1.4).

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.

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

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 **SELE**CTED region in **STRU**CTURED mode
SET T at **NODE**S function of **TIME ID=RGN1** file= **'RGN1VAL'** only for the **FIEL**D nodes.

4.7 USER-DEFINED INPUT OPTIONS

Some commands permit input of user-defined functions or options. These options are permitted for all the all 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.

(This section left intentionally blank)

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.

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 **LOCA**TE or **SELE**CT 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 **ACTI**VE 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 LOCA**TE **or SELE**CT **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 **ACTI**VE 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**

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 **BOUN**DARY 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 **BOUN**DARY**, INIT**IAL**, READ or SET** commands. The **ADIA**BATIC 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 **BOUN**DARY command. For the species transport variables, the **ADIA**BATIC **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 **ANSWER™** 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

$$S_{mj,k} = C_A S_o \exp(-C_E / T)\rho^{(a+b+c)} m_j^a m_k^b m_l^c$$

N2 The Arrhenius activation energy constant, C_E (≥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

Symbol	N1	N2	N3	N4	N5
FU	2.0893×10^{22}	2.48×10^{4}	0.50	1.07	0.40
CH	5.0117×10^{19}	2.50×10^{4}	0.90	1.18	-0.37
CO	3.9811×10^{19}	2.00×10^{4}	1.00	0.25	0.50
H2	3.3113×10^{18}	2.05×10^{4}	0.85	1.42	-0.56

EXAMPLES

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

* The Rate Expression equation
where

$S_{mj,k}$ 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

COMMAND **BANNER**

PURPOSE 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.

SYNTAX **BANN**

EXAMPLES

BANNER page output at this stage

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_{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.

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 of 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_{ROUGH} and C_{ROUGH} constants(below).

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_{ROUG} 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_{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.

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**, **INIT**IAL 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_{ROUG} 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=ξ] [ALL | NONE] [[RATE=λ] | [MULT=β] [PLAN] [I | J | K=N_{IJK}] [AVER=N_{avg} | 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:

$$\frac{dr}{dt} = \alpha_1 \gamma^4 - \alpha_2 \gamma^3 + \alpha_3 \gamma^2 - \alpha_4 \gamma + \alpha 5 - \frac{\alpha_6}{\gamma}$$

Where γ 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:

$$\left[\frac{dr}{dt}\right]_{\theta \geq 0} = \left[\frac{dr}{dt}\right]_{\theta=0} [\mathrm{Cos}\theta]^{1/2}$$

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

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

Units	α_1	α_2	α_3	α_4	α_5	α_6
Ft/hr	45.654996	232.2931	469.5247	470.37554	232.73686	45.203241
m/sx10^3	3.8654563	19.667482	39.753091	39.825129	19.705054	3.8272077

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.

$\psi = \rho/\rho^*$	1.0	1.05	1.10	1.15	1.20
dr/dt (m/s) x10^6	3.783	2.409	1.368	0.5371	0.01146
dr/dt (m/day)	0.327	0.208	0.118	0.046	0.001

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 dislodges and becomes part of 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.

RATE If this modifier is present, then the built-in correlation is bypassed and the rate of surface dissolution or melting is assumed to be equal to **λ**.

λ 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 **β**.

β The multiplicative factor for the dissolution or melting rate if the modifier **MULT** is present.

PLAN The computation of dissolution rate (dr/dt) requires the location of specific gravity, **ψ**. By default, **ψ** is computed at the fluid element next to the wall between the fluid and the solid (salt). If this modifier is present, **ψ** 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.

AVER The specific gravity is computed from an average of values prevailing at a number of elements opposite the wall element or with reference to the plane specified by N_{IJK} and the depth of averaging specified by N_{avg}.

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 transact 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 * N23D where N is number of elements in the blocks and N23D 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 if 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.

ROUG See Mode 1 of command.

Z_{ROUGH} See Mode 1 of command.

TYPE See Mode 1 of command.

C_{ROUG} 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_{STOR}] [ROUG=Z_{rough}] [TYPE=C_{rough}] [DELA=N_{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_{ROUG} 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 mast 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

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

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

BLOCKage	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 sub-domain are selected to be part of the borehole.

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

$$\text{Area} = (\pi/4)\,(D_{outer}^{2} - D_{inner}^{2})$$

EXAMPLES

BOREHOLE for ID=BOREHOLE_1 dia = 0.2
BOREHOLE ID= BOREHOLE_2 Y: D=0.2, Inner d=0.1 DETAIL

MODE 2: **Specification of a Borehole with Diameter as a Functional Form**

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

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.

ξ 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 Se Mode 1.

dir Se Mode 1..

ALL Se Mode 1..

NONE Se 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] {V_B} [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.

option	INTERPRETATION
VALU	Value of the variable at the boundary node is specified as: $\Phi=\Phi_0$ where Φ_0 Is the specified numerical value. This is the default option.
FLUX	**q**, the flux of the variable at the boundary node is specified according to the equation: $q=-\Gamma\frac{\partial\Phi}{\partial N}$ where Γ 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.
GRAD	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.
MIXE	The flux of the variable at the boundary is specified according to the equation: $q=-\Gamma\frac{\partial\Phi}{\partial N}=\pm h(\Phi-\Phi_O)$ where h is a transfer coefficient, and Φ_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.
FLOW	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.
EXTR	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.

subopt The nature of the **MIXE**D boundary condition.

subopt	INTERPRETATION
FLUX	Mixed boundary condition is specified in terms of the flux of the variable. This is the default option.
GRAD	Mixed boundary condition is specified in terms of the gradient of the variable (the **MIXE**D condition with $\Gamma = 1$).

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.

V_B The value of the variable Φ_0 if **VALU**E or **MIXE**D modifier is present, the flux, **q**, if the **FLUX** modifier is present, and the outward normal gradient $\partial\Phi/\partial N$ if the **GRAD** modifier is present. If no modifier is specified, then the **VALU**E modifier is assumed to be present by default. There is no default value.

h The transfer coefficient **h** for the **MIXE**D 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 **BOUN**DARY 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 (**ID=idsub**; see Section 3.4 and **LOCA**TE command) may be replaced by a new specification provided the previously specified boundary condition is explicitly disabled by the **BOUN**DARY **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 **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

BOUNdary for P: at X- boundary, value = 0
BOUNdary GRADient at X+ boundary for all variables is = 0.
BOUNdary for T: orientation index X+ value = 10.
BOUNdary for T at X+: value = 10 at ID=UPPEr subregion
BOUNdary for T at Y- boundary: FLUX = 10 at the selected segment
BOUNdary for P at Y- boundary: GRAD = -2.5 at the selected segment
BOUNdary for T at Y+ boundary: MIXEd type: equilibrium value=5 h=0.5
BOUNdary T: Y+; MIXEd FLUX: v=1, h=0.1 for segment with ID=MIDDle
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 [Φ] [func[ξ]] {N_1, N_2, .., N_n | fname} [option] [subopt] [dir] [subrgn] [h]**

Φ 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 **VALU**E, **FLUX**, **GRAD** and **MIXE**D modifiers. 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_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, **Φ**. In the **GRAD**IENT mode, the input units are those of **Φ** 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 (**BOUN**DARY) 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
```

MODE 3: **Total Pressure Boundary Condition**

SYNTAX **BOUN {TOTA} {P} [func[ξ]] {N_1, N_2, .., N_n | fname} [N_{n+1},.. N_{n+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:

$P_{Total} = P + \frac{1}{2}\rho(u^2 + v^2 + w^2)$, Where $\mathbf{P_{Total}}$, 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.

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 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.

N_{n+1},.. N_{n+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.

APPLICABILTY

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 (**BOUN**DARY) 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 TOTAL P at X+ boundary = 2.E.5
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., -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

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

SYNTAX **BOUN {Φ} {DISC|GATE } {dir} [subrgn] {C_D} [P|PRES=P_B] [AREA=A_B] [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, ρ 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.

Φ One of the symbols U, V or W to denote the velocity component to be set by the command.

dir See Mode 1 specification.

subrgn See Mode 1 specification.

C_D The discharge coefficient for the boundary

P|PRESS 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 boundary segment; 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.

APPLICABILTY

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, AREA=0.02

MODE 5: **Gate boundary conditions for Tide Height**

SYNTAX **BOUN {ETA} {GATE} {IN|OUT} [func[ξ] {N_1, N_2, .., N_n|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.

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 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.

dir See Mode 1 specification.

subrgn See Mode 1 specification.

APPLICABILTY

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 (**BOUN**DARY) 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 **LOCA**TE or **SELE**CT 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

BOUNDARY for T at Y+ boundary for ID=UPPER turned OFF

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.

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

$$S_{BF} = \theta^2 (1+C_F Re_K)\frac{\mu}{K} V_j$$

$$Re_K = \frac{\rho\theta |V|\sqrt{K}}{\mu}$$

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],
ρ	is the mass density of the fluid, [M/L^3]
θ	is the porosity of medium,[0]
V_j	is the j^{th} component of fluid (particle) velocity [L/t]
μ	is fluid viscosity [M/(Lt]
p	is the fluid thermodynamic pressure [M/(L 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],
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::

$$V_{dj} = -\frac{K_H}{1+C_F Re_K}\left(\frac{\partial P}{\partial x_j}+\frac{\rho g_j}{\rho^* g}\right)$$

$$K_H = \frac{\rho^* g}{\mu} K; \qquad P = \frac{p - p^*}{\rho^* g}$$

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 PERM**EABILITY **command.** For the **PORFLOW™** Software Tool, the hydraulic conductivity specified through the **HYDR**AULIC or **COND**UCTIB+VITY 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

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]} {N_1, N_2, .., N_n | 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 **MULT**IPHASE 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.

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 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.

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 (**MULT**IPHASE 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 n^{th} phase fluid, the capillary pressure, Ψ^n is computed from:

$$\Psi^n = P^n - P^{n+1}$$

If the **CAPI**LLARY command is present, then the computed value is further modified as per the specification on the command. The n^{th} phase saturation, S^n, is then computed from the specified soil-characteristic by the **MULT**IPHASE command. Though specifics of the $S^n(\Psi^n)$ depend on the command, in general, the following conditions prevail for most characteristics.

$$\Psi^1 < 0 \rightarrow S^1 < 1; \quad \Psi^1 \geq 0 \rightarrow S^1 = 1$$

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

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 TABL**E) 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

CLOSe SAVE file
CLOSe archive TABLe output file now
CLOSe file by name 'MYOLDFILE'

COMMAND COMPRESSIBLE

PURPOSE To select compressible flow option. This command is effective only for the **ANSWER™** Software Tool.

MODE 1: Mild Compressibility Option

SYNTAX COMP {MILD} [ATMO] [N1]

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 $\partial\rho/\partial p$ 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.

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

In this equation the constant α has the units of 1/p.

ATMO The constant α 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 α 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 α is assumed to be a local variable and is computed as:

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

Where γ is the specific heat ratio, ρ 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, $\mathbf{h_s}$, rather than enthalpy, $\mathbf{h_T}$ That is, the mean and turbulence kinetic energy of fluid is added to the enthalpy as defined by the below equation

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

$$h_T = \sum_j \mathbf{m_j}\, \mathbf{h_j}\ ; \quad \sum_j \mathbf{m_j} = 1\ ,$$

$$\mathbf{h_j} = \mathbf{h_j^o} + \int_T C_{Pj}\, dT\ ,$$

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

where

h_j is the enthalpy, and mj, the mass fraction, of the j^{th} chemical species,
h_j^o is the heat of formation of the j^{th} species,
Cp_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.

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

MODE 2: **Full Compressibility Option**

SYNTAX **COMP [DENS|SIMP|SYMM|DIRE|COUP] [ISEN|ISOT] [ISOP] [INVI] [FIXE] [RHOU] [N_1]**

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, h_s, is assumed to be conserved and the temperature is computed from:

$$T = (h_s - 0.5\,V^2)\,/\,C_p$$

where V is the flow speed and C_p 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.

N_1 The constant C (>0) of the pressure perturbation equation as given below. The default value is 1.4.

$$P' = \rho' C R T$$

Where C is equal to unity for an isothermal process, and is equal to, γ, 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

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} {Γ_{xx}, Γ_{yy}, [Γ_{zz}]} [SATU|TOTA] [option] [subrgn]

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

Γ_{xx}, Γ_{yy}, Γ_{zz} 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.

option	INTERPRETATION
REPL	The computed value replaces the existing value. This is the default option.
ADD	The computed value is added to the existing value.
SUBT	The computed value is subtracted from the existing value.
MULT	The computed value multiplies the existing value.
DIVI	The computed value divides the existing value. A value of 1.E-30 is added to the divisor if it is zero.

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] {N_1, N_2, .., N_n | 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.

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 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.

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 **COND {P} {RELA} {func[ξ]} {N_1, N_2, .., N_n | fname} [option] } [GRAD] [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.

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.

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 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 conducvity 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]} {N_1, N_2, .., N_n|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 ^{o}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.

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 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.

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 **DISP**ERSION 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-sold 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 ^{o}K)].

T Same as above.

SECO The thermal conductivity of the 2nd fluid phase is specified.

Γ The constant and uniform value of the thermal conductivity for the 2nd 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 2nd phase fluid. If a 3rd fluid phase is present then the thermal conductivity for the 3rd phase is assumed to be zero; user can not specify a value for the 3rd phase.

EXAMPLES

CONDUCTIVITY for **T SECO**ND phase value =**1.E-5**

MODE 6: **Thermal Conductivity of the Solid Component of a Fluid-Solid Matrix**

SYNTAX **COND {HT|T} {SOLI} {func[ξ]} {N_1, N_2, .., N_n|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 ^{o}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.

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 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.

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-sold 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]} {N_1, N_2, .., N_n|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.

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 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.

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 **DISP**ERSION 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. m^2/s). The kinetic units are converted to mass units by multiplication with reference density (see **REFE**rence command).

MASS By default **PORFLOW™** input for mass species is assumed to be in kinetic units (e.g. m^2/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 **REFE**rence command).

option Option selected for the operation to be performed.

option	INTERPRETATION
REPL	The computed value replaces the existing value. This is the default option.
ADD	The computed value is added to the existing value.
SUBT	The computed value is subtracted from the existing value.
MULT	The computed value multiplies the existing value.
DIVI	The computed value divides the existing value. A value of 1.E-30 is added to the divisor if it is zero.

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 **DISP**ERSIVITY and **TORT**UOSITY 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.

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

SYNTAX **COND {Φ} {NODE|STRU|UNST|fname} [V_1,..V_m] [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 **STRU**CTURED mode if the **subrgn** was defined with a **LOCA**TE command in terms of grid indices or in the **UNST**UCTURED 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 **LOCA**TE command which can be examined by including a file name on the **LOCA**TE command.

fname The name of the file for numerical values unless the values are directly specified by **V_1….V_m** below. See Section 3.3 for additional information.

V_1….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.

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

CONDuctiivity by NODE for P variable for ID=SUBRGN1 ! 3 nodes in this region – **PORFLOW™**
1.5, 11.5, 10.
CONDuctiivity for P NODE in STRUctured mode from File “KHYD.FIL”
CONDuctiivity for P STRUctured mode from File “KHYD.FIL” for Field NODES only
CONDuctiivity 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]} {N_1, N_2, .., N_n|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 **CONT**ACT 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.

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 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.

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

$$q_{\Phi} = \frac{A_f\,(\Phi_1 - \Phi_2)}{\frac{ds_1}{\Gamma_1} + \frac{ds_2}{\Gamma_2} + \frac{1}{h}}$$

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:

$$q_{\Phi} = q_{\Phi_{internal}} + h\,A_f\,(\Phi_1 - \Phi_2)$$

TOTA The diffusive flux at the surface is computed as:

$$q_{\Phi} = h\,A_f\,(\Phi_1 - \Phi_2)$$

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, α_φ, β_φ]**

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, μ_j, and the diffusion coefficient, Γ_j, in the selected direction are computed from:

$$\mu_j = \frac{\mu}{[1+\beta\, Ri]^{\alpha}} \quad ; \qquad \Gamma_j = \frac{\Gamma}{[1+\beta_\varphi\, Ri]^{\alpha_\varphi}}$$

Where subscript "j" denotes the direction specified by the **dir** modifier, μ and Γ are, respectively, the scalar values of the viscosity and diffusion coefficients (specified by user or computed from built-in formulae), and α, β, α_φ and β_φ empirical constants. The Richardson number, Ri, is defined as:

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

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

$$-\frac{\mu_e}{\rho^2}\frac{\partial \rho}{\partial x_i}\frac{\partial P}{\partial x_i}$$

If this command with a **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 **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 **UNLI**MITED 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 **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.

α, β, α_φ, β_φ 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 **ANSWER™** Software Tool

EXAMPLES

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

MODE 11 **Treatment of Skew Diffusion Terms**

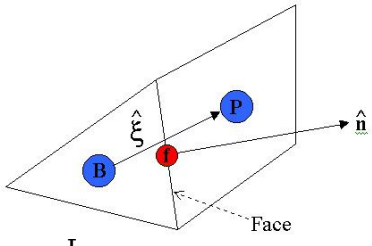
SYNTAX **COND {SKEW|SECO} [POSI] [Φ]**

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:

$$Q_D = -\Gamma_{ij}^f \frac{\partial \Phi}{\partial x_j} n_i A_f \quad ,$$



where summation convention is implied, and Γ_{ij}^f 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:

$$\frac{Q_D}{\Phi_B - \Phi_P} > 0; \quad \Phi_B - \Phi_P \neq 0$$

$$Q_D = 0; \qquad \Phi_B - \Phi_P = 0$$

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 Φ_B and Φ_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 Γ_{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):

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

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

where α_L and α_T are, respectively, the longitudinal and transverse dispersivities for the porous matrix, δ_{ij} is the Kronecker delta function, v_i is the fluid particle velocity vector, $\underline{\mathbf{V}}$ is its magnitude, V_i is the Darcy velocity vector and θ_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 **BOUN**DARY 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

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 **(**ξ_n**,**η **)** 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 **(**ξ_n**,** η**,** ζ**)** 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 **(**ξ_n**,**η**,**ζ**)** direction for each element is defined by the order in which the vertices appear on this record. The local ξ_n axis is oriented from vertex 1 to vertex 2, the η axis from vertex 1 to vertex 4, and the ζ 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.

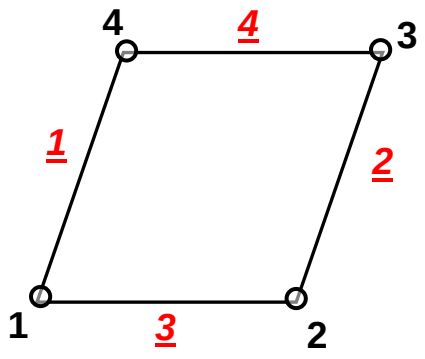
COMMENTS

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

CONNectivity information on file "VERT2ELM.CNC"
CONNectivity of VERTices to elements on file "VERT2ELM.CNC"



Quadrilateral

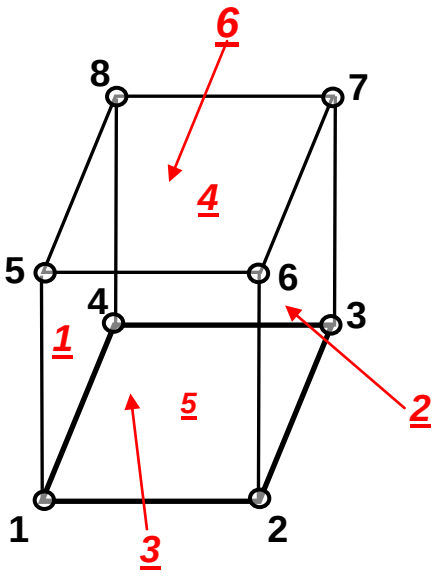
Assume that the vertex connectivity record for this element reads as follows:

Cell #	Cell Type	# of Corners,	Vertex List:
?	2	4	1, 2, 3, 4

Side Number	Vertex Numbers
1	1, 4
2	2, 3
3	1, 2
4	3, 4

The right hand rule implies that: $(\vec{r}_{12} \times \vec{r}_{13}) \bullet \vec{k} > 0$, 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:

Cell #,	Cell Type,	# of Corners,	Vertex List:
?	6	8	1, 2, 3, 4, 5, 6, 7, 8

Side Number	Vertex Numbers
1	1, 4, 8, 5
2	3, 2, 6, 7
3	2, 1, 5, 6
4	4, 3, 7, 8
5	1, 2, 3, 4
6	5, 8, 7, 6

The right hand rule implies that: $(\vec{r}_{12} \times \vec{r}_{14}) \bullet \vec{r}_{15} > 0$, where $\vec{r}_{12}$ 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.

Element Type	# of Vertices	# of Sides	Geometry	Description
1	3	3	2D	Triangle
2	4	4	2D	Quadrilateral
3	4	4	3D	Tetrahedron
4	5	5	3D	Quad-Based Pyramid
5	6	5	3D	Triangle-based Prism
6	8	6	3D	Hexahedron

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)

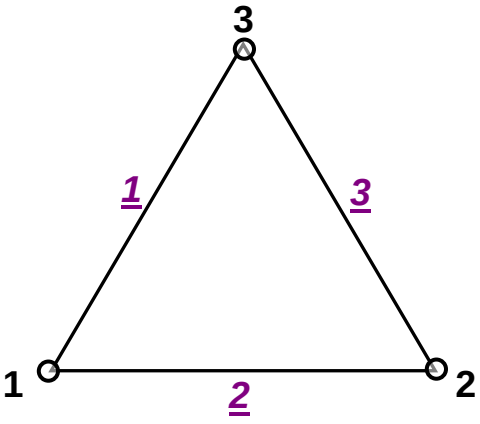
where IFILE is an internally assigned file unit number, M, is the element number, MTYPE is the element type, NVRTX is the number of vertices for the element, and NV are the vertex numbers for the element corners.

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

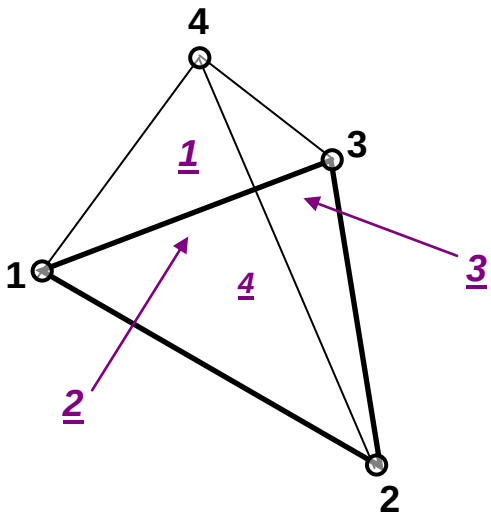
Assume that the vertex connectivity record for this element reads as follows:

Cell #,	Cell Type,	# of Corners,	Vertex List:
?	1	3	1, 2, 3

Side Number	*Vertex Numbers*
1	1, 2
2	2, 3
3	3, 1

The right hand rule implies that: $(\vec{r}_{12} \times \vec{r}_{13}) \bullet \vec{k} > 0$, 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

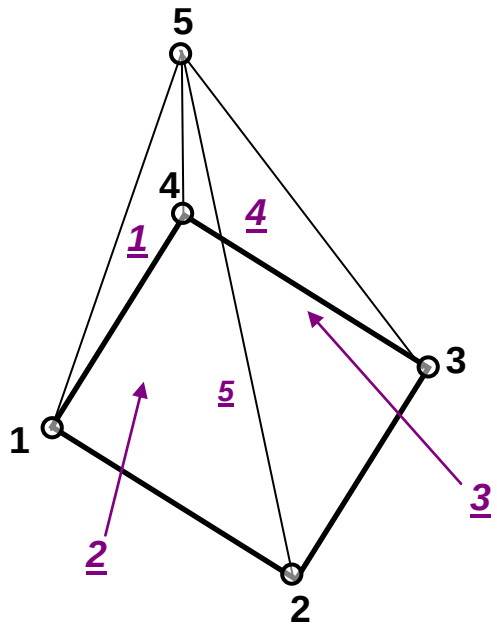
Assume that the vertex connectivity record for this element reads as follows:

Cell #,	Cell Type,	# of Corners,	Vertex List:
?	3	4	1, 2, 3, 4

Side Number	Vertex Numbers
1	1, 3, 4
2	1, 4, 2
3	4, 3, 2
4	1, 2, 3

The right hand rule implies that: $(\vec{r}_{12} \times \vec{r}_{13}) \bullet \vec{r}_{14} > 0$, 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).



Pyramid

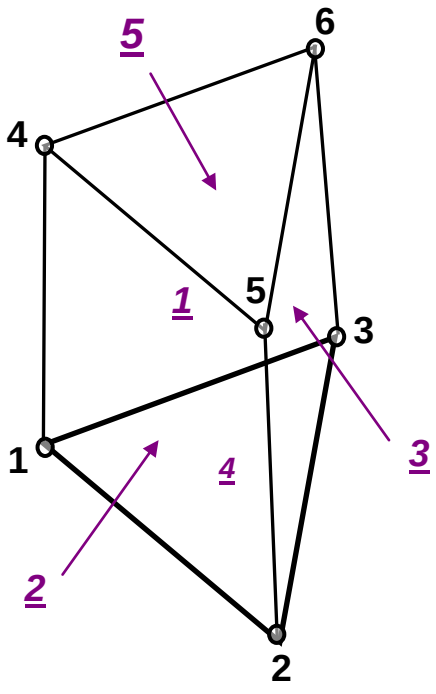
Assume that the vertex connectivity record for this element reads as follows:

Cell #,	Cell Type,	# of Corners,	Vertex List:
?	4	5	1, 2, 3, 4, 5

Side Number	Vertex Numbers
1	1, 4, 5
2	1, 5, 2
3	3, 2, 5
4	4, 3, 5
5	1, 2, 3, 4

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

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



Triangular Prism

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

Cell #,	Cell Type,	# of Corners,	Vertex List:
?	5	6	1, 2, 3, 4, 5, 6

Side Number	Vertex Numbers
1	1, 3, 6, 4
2	2, 1, 4, 5
3	3, 2, 5, 6
4	1, 2, 3
5	4, 6, 5

The right hand rule implies that: $(\vec{r}_{12} \times \vec{r}_{13}) \bullet \vec{r}_{14} > 0$, where $\vec{r}_{12}$ 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.

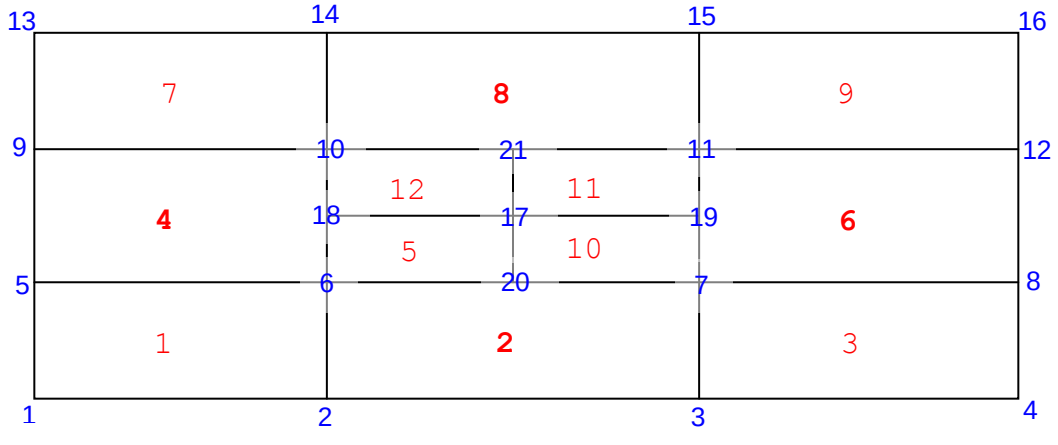
The 1st record in the file consists of a header with two numbers: the number of split elements and the total number of data items in the rest of the file. The header is followed by a number of sets of data equal to the number of split elements. The 1st record of each set consists of the element number 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



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

Element #	Vertex Connectivity			
1	1	2	6	5
2	2	3	7	6
3	3	4	8	7
4	5	6	10	9
5	6	20	17	18
6	7	8	12	11
7	9	10	14	13
8	10	11	15	14
9	11	12	16	15
10	20	7	19	17
11	17	19	11	21
12	18	17	21	10

Then the SPLIt connectivity command is:

CONNectivity 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                                        ! Split Element Number
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                                        ! Split Element Number
0    2    0    0                        ! Face # 2 is split in to 2 segments
5    12                                  ! Element numbers that split face connects to
1    1                                   ! Face # 1 (of Element 5) and Face # 1 (of Element 12)
6                                        ! Split Element Number
2    0    0    0                        ! Face # 1 is split in to 2 segments
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] [ε_{Tol}, N_{ITER}, N_{MIN} X_{ref}]

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 3.6 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:

$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N}\left| A_{ij}\, X_j - B_i \right|$$

$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N}\left| X_j^{new} - X_j^{old} \right|$$

$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N}\left| \frac{X_j^{new} - X_j^{old}}{X_j^{old}} \right| ; \quad \left| X_j^{old} \right| \geq X^{ref}$$

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 specified.

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

$$\varepsilon = \max_i \left| A_{ij}\, X_j - B_i \right|$$

$$\varepsilon = \max_i \left| X_j^{new} - X_j^{old} \right|$$

$$\varepsilon = \max_i \left| \frac{X_j^{new} - X_j^{old}}{X_j^{old}} \right| ; \quad \left| X_j^{old} \right| \geq X^{ref}$$

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.

ε_{Tol} 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 ε falls below this value for the chosen **REFE**RENCE 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 **MATR**IX command.

If no variable (**Φ**) 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 LOCAl 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: LOCAl mode, value = 1.E-4, max iterations 10, min iter= 5; min value 1.E-5
CONV for flow: LOCAl mode, epsilon = 1.E-2, max iterations = 5
CONV LOCAl, 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}, N_{ITER}]**

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.

N_{ITER} 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 **COUP**LED 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 **COUP**LED 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 N_{ITER} 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} [N_{Short}] [N_{Long}] [N_{Start}] [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:

$$\varepsilon_{Long} = \frac{1}{N_{Long}} \sum_{i=1}^{N_{Long}} \varepsilon \qquad \varepsilon_{Long} = \frac{1}{N_{Long}} \sum_{i=1}^{N_{Long}} \varepsilon$$

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

$$\varepsilon > \varepsilon_{Short} > \varepsilon_{Long} \quad \text{and} \quad \varepsilon > \alpha\, \varepsilon_{Short}$$

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

N_{Short} 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.

N_{Long} 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

N_{Start} 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 averring 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 $\varepsilon/\varepsilon_{Tol}$) is printed out as a diagnostic output (see **DIAG**NOSTICS 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 **AVER**AGE over **31** and **151** steps
CONVERGENCE **AVER**AGE over **31** and **151** steps. Start at **50** steps and print **LONG** term average
CONVERGENCE **AVER**AGE 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 (**CONV**ERGENCE **REFE**RENCE 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.

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 **THET**a 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 **DEGR**ee 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 in to 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

COORdinate corners are: (0., 0.) (1., 0.), (0., 1.) and (1., 1.) !! Unit Square
COORdinate: (0,0) (0.707,0.707), (-0.707,0.707) and (0,1.414)! 45 Deg Square
COORdinate: (0,0) (1., 0.), (0., 1.) and (1,1) CYLIndrical system
COORdinates: 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
COORdinates: 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

MODE 5: **Structured or Unstructured Grid: Element Vertex or Grid Node Coordinates**

SYNTAX **COOR {fname} {dir} [CYLI] [DEGR] [BLOC] [NODE] [PLAN] [JIK|JKI|KIJ|KJI|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 x_{ij} must be in the order: x_{11}, x_{21}, x_{31}, ...x_{n1}; x_{12}, x_{22}, x_{32}, ...,x_{n2}; ... and so on. If, say, both x and y coordinates for a 2D grid are simultaneously specified, then the set of values (x_{ij}, y_{ij}) must be in the order: (x_{11}, y_{11}), (x_{21}, y_{21}), (x_{31}, y_{31}), ... (x_{n1}, y_{n1}); (x_{12}, y_{12}), (x_{22}, y_{22}), (x_{32}, y_{32}), ... (x_{n2}, y_{n2}); ... and so on. However, if the JIK modifier is present, then it is assumed that the input data is in the order x_{jik}. The I and J values are then transposed internally to the ACRi x_{ijk} 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_n, 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^- and that at Face number 4 in the R^+ direction. Further details are given in Section 3.5 and the **CONN**ECTIVITY 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 'XRTHETA'
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] [V_{frq}] [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, $\mathbf{\Phi}^n$ its value at n^{th} time (or iterative) step, then its 1st and 2nd 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:

$$R_{11} = \langle \mathbf{\Phi}^2 \rangle - \langle \mathbf{\Phi} \rangle \langle \mathbf{\Phi} \rangle$$

$$C_{11} = \frac{R11}{\langle \mathbf{\Phi} \rangle \langle \mathbf{\Phi} \rangle}$$

$$D_{11} = \mathbf{\Phi} - \langle \mathbf{\Phi} \rangle$$

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, 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 V_{frq} specification.

V_{frq} 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 **CORR**ELATION commands for the specified variable and subregion are disabled. New commands may be subsequently specified.

EXAMPLES

CORRelation for variable U for the SELEcted subregion at the end of simulations
CORRelation for variable U for the ID=LOC_AUTO every 25 steps
CORRelation OFF for variable U for the ID=LOC_AUTO

MODE 2: **Cross Correlation for Two Variables**

SYNTAX **CORR { Φ_1, Φ_2 } [subrgn] [fname] [TIME] [NOW] [V_{frq}] [OFF]**

Φ_1, Φ_2 **Two** symbols that denote the variables for which correlation is desired. Valid symbols are listed in Table 2.7.1. If Φ_k denotes the instant value of the k^{th} variable at a given location, Φ_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:

$$R_{12} = \langle \Phi_1 \Phi_2 \rangle - \langle \Phi_1 \rangle \langle \Phi_2 \rangle$$

$$C_{12} = \frac{R12}{\sqrt{\langle \Phi_1^2 \rangle - \langle \Phi_1 \rangle^2}\ \sqrt{\langle \Phi_2^2 \rangle - \langle \Phi_2 \rangle^2}}$$

$$D_{12} = (\Phi_1 - \langle \Phi_1 \rangle)(\Phi_2 - \langle \Phi_2 \rangle)$$

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 **V_{frq}** specification.

V_{frq} 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 **CORR**ELATION commands for the specified variable and subregion are disabled. New commands may be subsequently specified.

EXAMPLES

CORRelation for variable U and V for the SELEcted subregion at the end of simulations
CORRelation for variable U and T for the ID=LOC_AUTO every 25 steps
CORRelation OFF for variable U and T for the ID=LOC_AUTO

MODE 3: **Two Point Correlation for One or Two Variables**

SYNTAX **CORR {TWO} { Φ_1 } [Φ_2] [subrgn] [fname] [TIME] [NOW] [V_{frq}] [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 CORR**ELATION command.

Φ_1, Φ_2 **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 **Φ_1** and **Φ_2.** The **Φ_1** 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 **Φ_2** is taken to be the values at the 2nd set of paired elements. If **two** symbols are specified then **Φ_2** 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 CORR**ELATION 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, **V_{frq}** 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 **V_{frq}** specification.

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.

OFF Any previously specified **CORR**ELATION commands for the specified variable and subregion are disabled. New commands may be subsequently specified.

EXAMPLES

CORRelation is TWO point type for variable U at ID=LOC_CORR2 at the end of simulations
CORRelation is TWO point type for variables U and V at ID=LOC_CORR2 output on file 'TWOPCORR.UV'
CORRelation is TWO point type for variables U and V at ID=LOC_CORR2 at the end of simulations
CORRelation 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

COMMAND **DATUM**

PURPOSE To specify datum coordinates, x, which are used to define the total hydraulic head, $\tilde{H}$. 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, **θ)** 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 **GRAV**ITY 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.

$$\alpha_f = \mathrm{Cos}^{-1}\frac{\sum_{i=1}^{N23} A_i \delta x_i}{A_f \delta S}$$

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 {Φ} [fname] [subrgn] [V_{frq}] [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.

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.

TIME By default, **V_{frq}** is the computation (and output) frequency in terms of number of steps. If this modifier is present, then **V_{frq}** 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_{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 acr_MATRXxxxx.TMP where "xxxx" are replaced by the non-blank characters of the 1^{st} 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 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 ($-A_{ij}$, $i \neq j$).

N_{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 FIELD 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] [C_D] [α] [N_1, N_k] [N_{k+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, S_Φ, 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**.** $\mathbf{C_D}$ and $\mathbf{C_\Phi}$ are dimensional constants such that $\mathbf{S_\Phi}$ has appropriate units [e.g. M L T^{-2}]. For example, if N=1, and C_Φ is an area, then $\mathbf{C_D}$ is non-dimensional.

option Options selected for implementation of the source.

option	Interpretation
VOLU	The coefficient C_Φ in the S_Φ term is set equal to the volume **(δV)** of the element.
AREA	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.
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.
NORM	The coefficient C_Φ in the S_Φ term is computed as: $C_\Phi = \sum_i A_i \bullet V_i$ 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 **NORM**AL 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, $\mathbf{C_D}$, 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 **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.

N_{k+1} The density value that multiplies the computed source, if the **DENS**ITY modifier is present. There is no default values 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

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 DEFI $\{X_1=V_1\}$ $[X_2=V_2]$, ..., $[X_n=V_n]$ [OFF]

$X_1, X_2,...X_n$ A list of symbolic variables that at run-time is replaced by the corresponding numerical value, $V_1, V_2,...V_n$ 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.

$V_1, V_2,...V_n$ The numerical values that replaces every occurrence of the $X_1, X_2,...X_n$ 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** = **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.

The symbolic variable appearing on a **DEFI**NE 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.

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

MODE 3: **Multiple Simulations of a Given Input for a Series of Assigned Values**

SYNTAX **DEFI {variable} {LIST} {V_1, V_2, .., V_n}**

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 **DEFI**NE 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 **DEFI**NE **LIST** command must not appear if a metafile for input is specified (see **META** command).

V_1, V_2, .., V_n 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 **OUTP**UT 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
```

```
!
!*****************************************************************************
! 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 120
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 130
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 LIST of values: 1., 2., 3., 4

MODE 4: **Multiple Simulations of a Given Input for a Series of Assigned Values**

SYNTAX **DEFI {variable} {DO} {V_1, V_2, V_3}**

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 **DEFI**NE 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.

DO A DO Loop is specified to generate a sequence of inputs from the assigned values. A **DEFI**NE **DO** command must not appear if a metafile for input is specified (see **META** command).

V_1, V_2, V_3 The numerical values that generate a sequence of values to replace the **variable** in each data set. **V_1** is the starting value, **V_2** the ending value, and **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.

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 **OUTP**UT 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 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
```

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:

```
!************************************************************************
! 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
!
!*************************************************************************
! 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]} {N_1, N_2, .., N_n | 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.

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.

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 $\partial\rho/\partial t$ 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] [ρ*] [α] [β] [γ]**

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 1st phase of the fluid. This modifier is available only for the multi-phase versions of the **PORFLOW™** and **ANSWER™** Software Tools.

ρ* Reference density for the fluid, **ρ***

α The exponent for the **POWE**R law or the coefficient for the **POLY**NOMIAL and **LINE**AR relations. The default value is 0.2 for the **POWE**R law equation and 0 otherwise

β The critical temperature for the of the **POWE**R law, the coefficient for the **POLY**NOMIAL relation or the reference concentration for the **LINE**AR relation. The default value is 374.15 for **POWE**R law and 0 otherwise

γ The coefficient in the **POLY**NOMIAL and **LINE**AR 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 **POWE**R law: rho* = **1.**, Exponent = **0.25**, Tc = **374.15** K
DENSITY **POLY**NOMIAL law: rho* = **1000**, a=**1000**., b=**0.05**, c=**0**., d=**3.E-5**
DENSITY **LINEA**R function: **997**, Beta=**1.0E-4**
DENSITY **LINEA**R function **789**, Beta=**1.0E-4** for **SECO**ND 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:

$$\rho = \frac{p + p^*}{R_u\,(T+T_a)\sum_j \frac{m_j}{M_j}}$$

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 Mj 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:

$$\rho = \frac{(p + p^* + A)(1 - B\,\rho)}{R_u\,(T+T_a)\sum_j \frac{m_j}{M_j}}$$

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 **INCO**MPRESSIBLE mode

MODE 4: **Density of Brine as a Function of Salt Concentration**

SYNTAX **DENS {SAND} [ρ*] [α] [ρ_{max}] [ρ_{salt}] [C_{S_Sat}]**

SAND Density varies according to the exponential law correlation:

$$\frac{\rho}{\rho^*} = \min\{ \exp(\alpha C_s), \rho_{max}\}$$

,

Where C_S is the mass concentration of salt ($0 \le C_S \le 1$) 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 **SAND**IA function
DENSITY **SAND**IA function; rho* = **998.2**, alfa=**0.6995**, rho_max=**1209**
DENSITY **SAND**IA function; rho* = **998.2**, alfa=**0.6995**, rho_max=**1209**, rho_salt=**2165**, C_{sat}=**0.2643**

MODE 5: **Density of Solid or Particle Material**

SYNTAX **DENS {SOLI|PART} {func[ξ]} {N_1, N_2, .., N_n|fname} [ALWA] [subrgn]**

SOLI|PART The solid material or particlulate 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.

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 **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 **SOLI**D is = **1**
DENSITY of **SOLI**D 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 [Φ] [NOW|OFF] [ELEM] [OPEN] [HIGH] {N_1,...., N_n} [N_{Freq}] [N_{File}] [fname] n=1 for unstructured, n = 2 for 2D and n = 3 for 3D input mode

Φ 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 **SCREEN** command) by default. All 9 variables are directed to the screen if the **WIDE** modifier is present on the **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 **N1,..,Nn** specifies the grid indices. If this modifier is present, then N1 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 **N1,..,Nn**) that is located in a blocked region (**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,...,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 **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_{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_{File} The frequency of output to the extended diagnostic file described by **fname** below. If no value is specified, then the default value is set equal to **N_{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 **CONV**ERGENCE 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 (**CONV**ERGENCE **REFE**RENCE 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
DIAGnostic output: TIME, U, BP & 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

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)

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:

$$\Gamma_{ij} = \varphi_D \, \tau_{ij} \, \Gamma_M + \varphi_E \, D_{ij} \quad , \tag{1}$$

$$\mathbf{D_{ij}} = \alpha_T \, \delta_{ij} \, \underline{\mathbf{V}} + (\alpha_L - \alpha_T) \frac{|\mathbf{V_i} \, \mathbf{V_j}|}{\underline{\mathbf{V}}} \quad , \tag{2}$$

Where:

Γ_{ij}	is the effective diffusivity tensor,
φ_D	saturated diffusional porosity,
τ_{ij}	is the tortuosity,
Γ_M	is the molecular diffusivity,
φ_E	saturated effective porosity,
D_{ij}	is the hydrodynamic dispersion,
δ_{ij}	is the Kronecker delta,
V_i	the particle velocity vector, and
$\underline{V}$	the magnitude of the particle velocity.

EXAMPLES

DISPERSION for **C 5** and **1** meters
DISPERSION for **C LONG**itudenal coef **5** ; **TRAN**sverse value = **1** meters for **ID**=**SAND**
DISPERSIVITY for **C LONG**itudenal coef **5** meters **ID**=**SAND**
DISPERSION for **C TRAN**sverse value = **1** meters for **ID**=**SAND**

MODE 2: **Dispersion Coefficient as a General Function**

SYNTAX **DISP {Φ} {LONG|TRAN|xyz} {func[ξ]} {N_1, N_2, .., N_n|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 **ZY**. 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.

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.

COMMENTS

The implementation proceeds in the manner above except that if the **xyz** modifier is present, then the corresponding component of the $\mathbf{D}_{ij}$ 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 **DISP {Φ} {STRA} {α_{LH}, α_{TH}, α_{LV}, α_{TV}} [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.

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 $\alpha_{LH} = \alpha_L$; $\alpha_{TH} = \alpha_T$ and α_{LV} and α_{TV} are ignored.

α_{LH} The horizontal longitudinal dispersion coefficient. The default value is 0.

α_{TH} The horizontal transverse dispersion coefficient. The default value is 0.

α_{LV} The vertical longitudinal dispersion coefficient. The default value is 0.

α_{TV} The vertical 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 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 $\mathbf{D}_{ij}$ tensor, assuming that the vertical direction is z, are then given by:

$$\mathbf{D_{xx}} = \alpha_{LH}\frac{\mathbf{V_x^2}}{\mathbf{V}} + \alpha_{TH}\frac{\mathbf{V_y^2}}{\mathbf{V}} + \alpha_{TV}\frac{\mathbf{V_z^2}}{\mathbf{V}} \quad , \tag{3a}$$

$$\mathbf{D_{yy}} = \alpha_{TH}\frac{\mathbf{V_x^2}}{\mathbf{V}} + \alpha_{LH}\frac{\mathbf{V_y^2}}{\mathbf{V}} + \alpha_{TV}\frac{\mathbf{V_z^2}}{\mathbf{V}} \quad , \tag{3b}$$

$$\mathbf{D_{zz}} = \alpha_{TV}\frac{\mathbf{V_x^2}}{\mathbf{V}} + \alpha_{TV}\frac{\mathbf{V_y^2}}{\mathbf{V}} + \alpha_{LV}\frac{\mathbf{V_z^2}}{\mathbf{V}} \quad , \tag{3c}$$

$$\mathbf{D_{xy}} = \mathbf{D_{yx}} = (\alpha_{LH} - \alpha_{TH})\frac{\mathbf{V_x V_y}}{\mathbf{V}} \quad , \tag{3d}$$

$$\mathbf{D_{xz}} = \mathbf{D_{zx}} = \{0.5\,(\alpha_{LH} + \alpha_{LV}) - \alpha_{TV}\}\frac{\mathbf{V_x V_z}}{\mathbf{V}} \quad , \tag{3e}$$

$$\mathbf{D_{yz}} = \mathbf{D_{zy}} = \{0.5\,(\alpha_{LH} + \alpha_{LV}) - \alpha_{TV}\}\frac{\mathbf{V_y V_z}}{\mathbf{V}} \quad , \tag{3f}$$

This equation becomes identical to Equation (2) when:

$$\alpha_{LH} = \alpha_{LV} = \alpha_L \quad \text{and} \quad \alpha_{TH} = \alpha_{TV} = \alpha_T \tag{3g}$$

EXAMPLES

DISPERSION for **C STRA**TIFIED 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, ρ_S is the density of solid, S is the fluid phase saturation, Θ_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 **DIST**RIBUTION 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:

$$C_s = \rho_s \, k_d \, C^n ,$$

where ρ_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

$$C_s = \rho_s \, c_{smax} \, \frac{C}{C_{lang} + C} ,$$

where c_{smax} is the maximum concentration per unit mass in the solid phase and C_{lang} is the Langmuir constant. It is seen that when $C << C_{lang}$, the relation become equivalent to a linear isotherm with $k_d = c_{smax} / C_{lang}$.

subrgn See Mode 1 specification.

N1 The distribution coefficient, k_d, for the Freundlich Isotherm or the c_{smax} for the Langmuir equation.

N2 The power exponent, n, for the Freundlich Isotherm or the Langmuir constant, C_{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 **DIST**RIBUTION and **RETA**RDATION commands) and by the **REAC**TION 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_{smax} 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_{lang} has units of pressure, P.

EXAMPLES

DISTribute C as FREUndlich Isotherm with kd=0.22, n = 0.8 for ID=CLAY
DISTribute C as LANGmuir equation with C_smax=1.89, C_langmuir = 0.2 for ID=CLAY

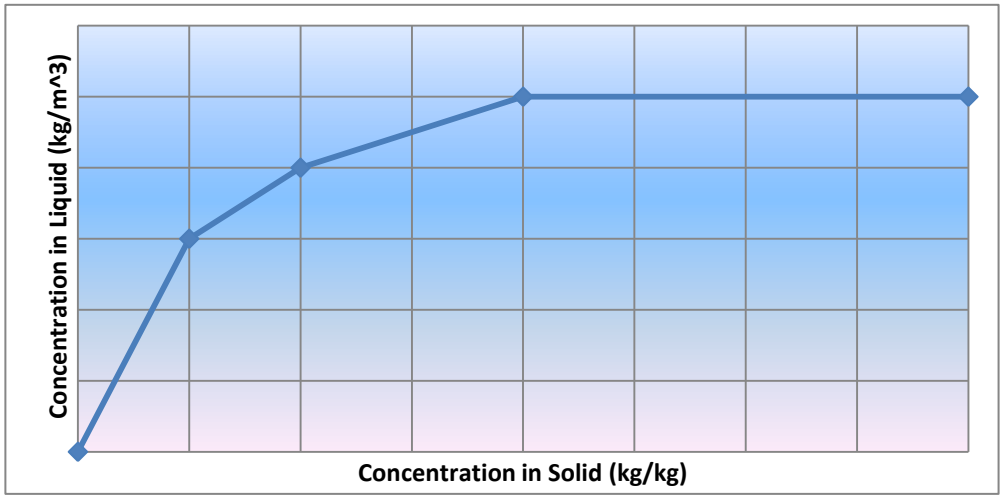
MODE 3: **Distribution Coefficient from Fluid & Solid Phase Concentrations**

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 **INVE**NTORY 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.



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 **DIST**RIBUTION and **STOR**AGE commands) and by the **REAC**TION 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} {Φ_1, Φ_2, .. Φ_k} {TABL} [STEPILINE|SECO|CUBI] [subrgn] {N_{sets}} [N_1,..., N_n | 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 **INVE**NTORY 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:

$$C_{solid} = \frac{\sum_k m_k - \sum_k \phi_k \theta S_f \delta V}{\rho_s (1-\theta) S_s \delta V}$$

Where, k denotes the species, m and Φ are, respectively, the computed mass and liquid concentration, θ is the porosity, S_f is the saturation of the liquid phase, ρ_s is the particle density of solid and δV is the volume of the element for which the computation is being performed. The quantity S_s in the denominator 1 if the **TOTA**L 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:

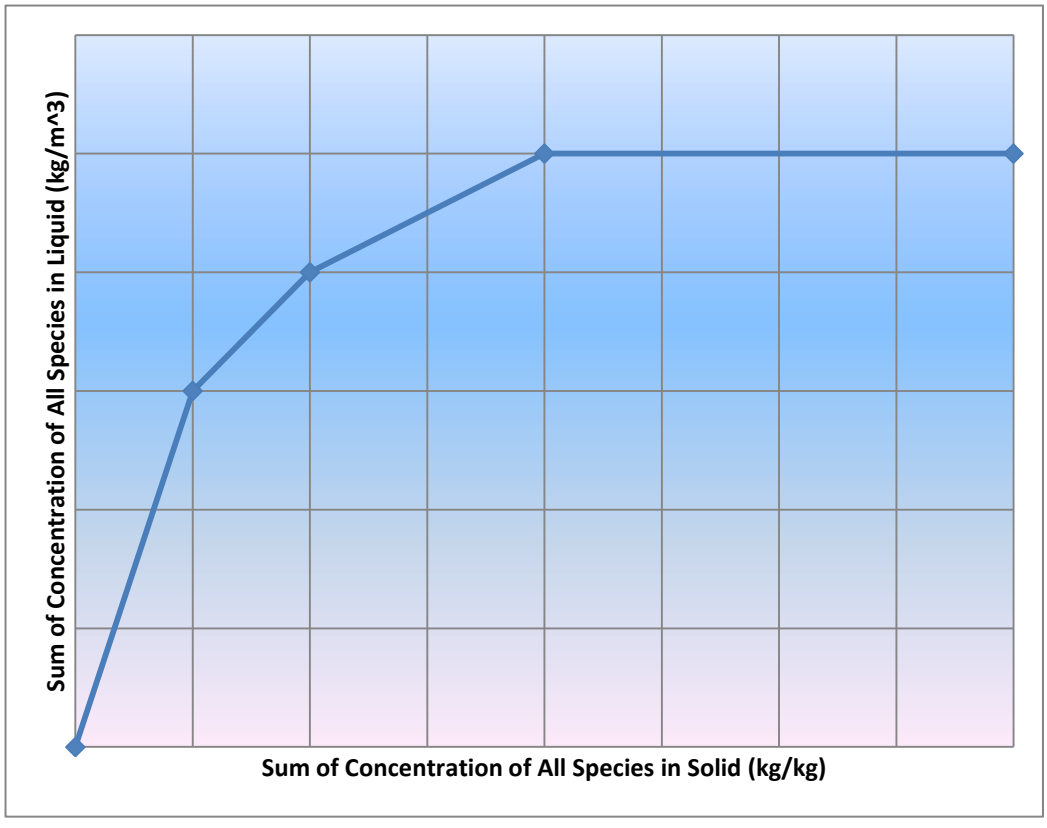
$$k_d = \frac{C_{solid}}{C_{liquid}};\ \text{if } C_{liquid} > 0, \quad k_d = \frac{\partial C_{solid}}{\partial C_{liquid}};\ \text{if } C_{liquid} = 0$$

Finally a new value for each of the species in the chain is computed as:

$$\phi_k^{corrected} = \frac{m_k}{\theta S_f \delta V + \rho_s k_d (1-\theta) S_s \delta V}$$

Φ_1, Φ_2, .. Φ_k 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.

N_{sets} Number of sets of data in the table.

N1, .., 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 **DIST**RIBUTION and **STOR**AGE commands) and by the **REAC**TION 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 **DIST {CONCRETE} {CAL} {CAS} {TABL} [LINE|SECO|CUBI] {N_{Set}} {N_1 ..., N_n|fname} {S_{si}}, [subrgn]**

CONCRETE This modifier triggers the solution of a CEA developed algorithm for degradation of concrete which is incorporated in the governing equation:

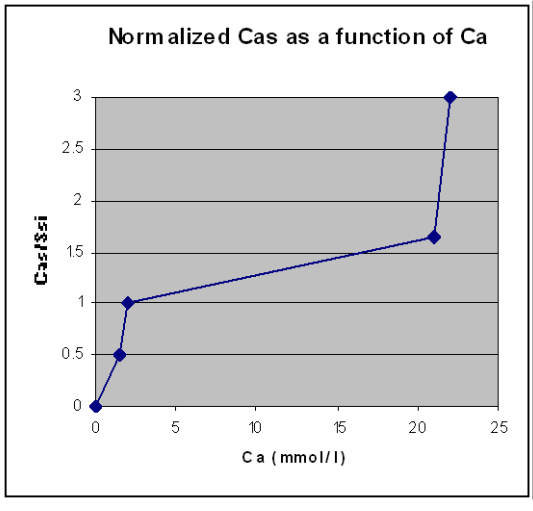
$$\frac{\partial}{\partial t}(\theta Ca + Ca_s) + \frac{\partial}{\partial x_i}(V_i Ca) = \frac{\partial}{\partial x_i}(\Gamma_{ca} \frac{\partial Ca}{\partial x_j}) + S_{ca} - \gamma_{ca}$$

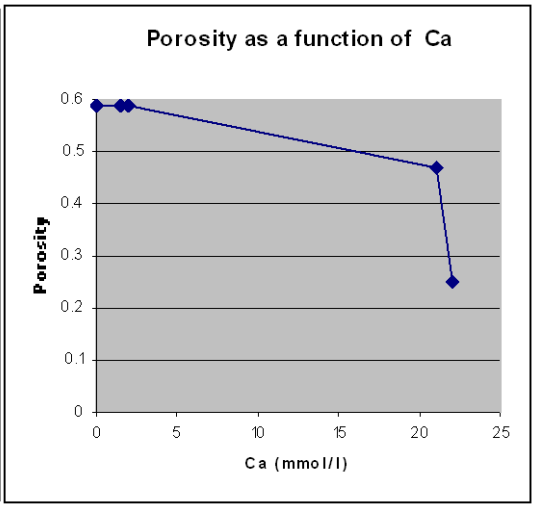
Where Ca and Ca_s are the concentrations of Calcium in the liquid and the solid phase respectively (The default symbolic name of Ca is CAL and that of Ca_s is CAS). In this equation (x_i,t) denote the space and time, Vi is the Darcy velocity, θ is the porosity, Γ is the diffusivity, S and γ are the source and sink (reaction) terms and the subscript Ca denotes the Ca species. The diffusion coefficient for the governing concentration equations is typically an exponential function of porosity:

$$\Gamma = \Gamma_o \exp(\frac{\theta}{\theta_o})$$

The diffusion coefficient must be specified by an appropriate **DIFF**USION command. Tognazzi (1998) and Torrenti et al. (1999) quote $\Gamma_o = 2.3 \times 10^{-13}$ and $\theta_0 = 0.100503$. 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 (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 (Ca_s) are tabulated functions of the calcium concentration in solution (Ca) (Please see References 1, 2 and 3 below for fuller details). The typical variation of Ca_s and porosity with Ca is as shown in the figures below.





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, Ca_s.

TABL Specifies that a tabular function for the normalized Ca_s/S_{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.

N_1, .., N_n N_{Set} set of values for the characteristics. Each set consists of 3 values: Ca, normalized Ca_s/S_{Si} ratio, and porosity (θ), 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_s/S_{Si} ratio above. The specified values will be multiplied with this number to obtain the actual Ca_s 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 (**ALLO**CATE) and appropriate distribution coefficients (see Mode 1 of **DIST**RIBUTION and **STOR**AGE commands) and by the **REAC**TION command.

EXAMPLES

DISTRIBUTION characteristics for CONCRETE given by 5 sets of values in a TABLE:

CAL	CAS	POR	
0.	0.	0.59	
1.5	0.5	0.59	
2.0	1.0	0.59	
21.0	1.65	0.47	
22.0	3.0	0.25	S_{si} = 4900

MODE 6: **Distribution Coefficient for Two Equation Concrete Degradation Model**

SYNTAX **DIST {CONCRETE} {CARB} {CAL} {CAS} {TABL} [LINE|SECO|CUBI] {N_{Set}} {N_1 ..., N_n|fname} {S_{si}}, [k], [Ca_{eq}] [θ_{Lim}] [$V_{mol\_calcite}$] [subrgn] [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:

$$\frac{\partial}{\partial t}(\theta Ca + Ca_s) + \frac{\partial}{\partial x_i}(V_i Ca) = \frac{\partial}{\partial x_i}(\Gamma_{ca} \frac{\partial Ca}{\partial x_j}) + S_{Ca} - \gamma_{Ca} - R_{Calcite}$$

$$\frac{\partial}{\partial t}(\theta CO_3) + \frac{\partial}{\partial x_i}(V_i CO_3 a) = \frac{\partial}{\partial x_i}(\Gamma_{co3} \frac{\partial CO_3}{\partial x_j}) + S_{CO3} - \gamma_{CO3} - R_{Calcite}$$

The reaction rate of Calcite formation, $R_{Calcite}$ and the evolution of porosity are given by:

$$R_{Calcite} = k(\theta - \theta_{lim}) \max\{\min[(Ca - Ca^*), (CO_3 - CO3^*)], 0.\}$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial W_{Ca}}{\partial t} - R_{Calcite} V_{mol\_Calcite}$$

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, θ_{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 CO3* are the corresponding equilibrium concentration of the species. The rest o 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:

$$\Gamma = \Gamma_o \exp(\frac{\theta}{\theta_o})$$

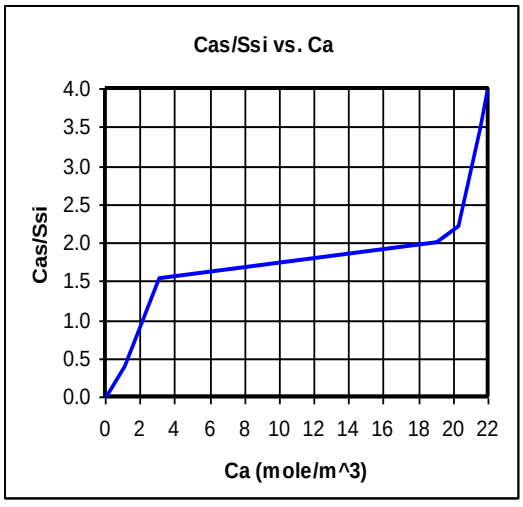
The diffusion coefficient must be specified by an appropriate **DIFF**USION command. Tognazzi (1998) and Torrenti et al. (1999) quote $\Gamma_o = 2.3 \times 10^{-13}$ and $\theta_0 = 0.100503$. Alternative diffusion coefficients may also be specified.

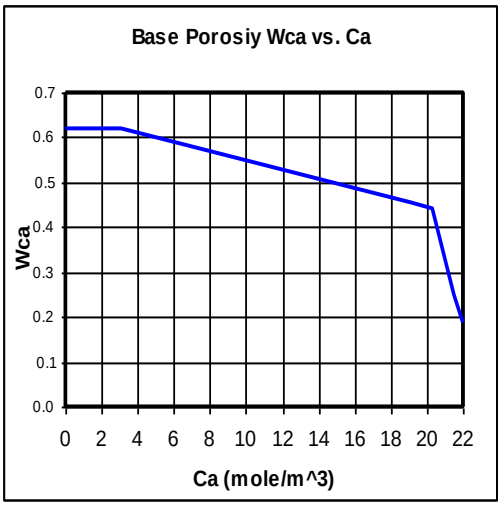
This degradation model is based on the assumption that the major mechanism of degradation is leaching of Calcium (Ca) from the concrete components from the solid state into solution and that the primary calcification reaction is given by:

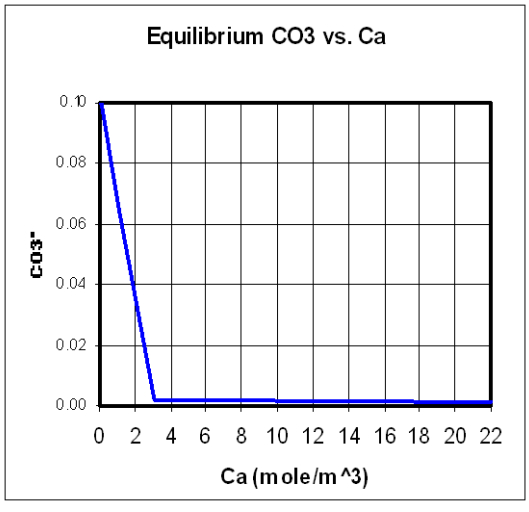
$$Ca^{2+} + CO_3^{2-} = CaCO_3$$

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 Buil (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, CO3*, 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, Ca_s.

TABL Specifies that a tabular function for the normalized Ca_s/S_{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.

N_1, .., N_n N_{Set} set of values for the characteristics. Each set consists of 4 values: Ca, normalized Ca_s/S_{Si} ratio, W_{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_s/S_{Si} ratio above. The specified values will be multiplied with this number to obtain the actual Ca_s value. The default value is 4900.

k Reaction rate for the Ca and CO_3 reaction. Typical values are in units of [s^{-1}] but any consistent units may b used. The default value is 1

Ca_{eq} The equilibrium value of Ca. The default value is 0.11

θ_{Lim} The minimum value of porosity. The default value is 0.01

$V_{mol\_calcite}$ The molar volume of Calcite. The default value is 3.69 x10^{-5} [m^3/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 **CONV**ERGENCE **COUP**LED **SPEC**IES 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 **CONV**ERGENCE 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 (**ALLO**CATE) and appropriate distribution coefficients (see Mode 1 of **DIST**RIBUTION and **STOR**AGE commands) and by the **REAC**TION 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 **CONV**ERGENCE **COUP**LED **SPEC**IES 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 **CONV**ERGENCE 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:

CAL	CAS	POR	CO3*
0.0	0.0000	0.6210	0.100
0.11	0.0000	0.6210	0.100
1.10	0.4000	0.6210	0.066
3.09	1.5200	0.6210	0.002
19.08	2.0100	0.4539	0.001
20.31	2.2100	0.4410	0.001
21.54	3.4900	0.2480	0.001
22.00	3.9687	0.1862	0.001

SSI = 4900
Reaction Rate = 1
Equilibrium Ca = 0.11
Limiting Porosity = 0.01
Calcite Molar Volume: = 3.69E-5 !m^3/mol

MODE 7: **Distribution Coefficient for Gas Phase**

SYNTAX **DIST {GAS} {Φ} {func[ξ]} {N_1, N_2, .., N_n | fname} [subrgn]**

GAS The species is partitioned in equilibrium between the liquid and gas phases. The partitioning concentration, Cg, in the gas phase is given by:

$$C_g = \rho_g k_g C$$

Where ρ_g is the gas density, k_g is a distribution coefficient and C is the concentration in the liquid phase. This k_g 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 **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 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 **DIST**RIBUTION and **STOR**AGE commands) and by the **REAC**TION 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 Transient Term 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 **REAC**TION command that is limited by the eddy breakup (EBU) limit. To activate this limit, the modifier EBU must also appear in the corresponding **REAC**TION command. The EBU reaction rate is computed from:

$$R_{EBU} = C_{EBU}\,\rho\,\frac{\varepsilon}{k}\,\Phi_{ebu}^{rms},$$

$$\Phi_{ebu}^{rms} = \min\left(\Phi_1,\ \alpha\Phi_2,\ \beta\Phi_3\right).$$

If R_{KIN} is the kinetic reaction rate (see **REAC**TION command), then the actual EBU-limited reaction rate for the **idreac** is defined by one of the following two options:

$$R_{Actual} = \min\left(R_{KIN},\ R_{EBU}\right), \text{ or}$$

$$R_{Actual} = \frac{R_{KIN}\,R_{EBU}}{\gamma R_{KIN} + (1-\gamma)R_{EBU}}.$$

The first equation is used for the default mode of the EBU-limiter whereas the second equation is used if the **HARM**ONIC modifier is specified.

Φ One or more of the symbols in Table 2.8.1-3 which identify the EBU limiting species (**Φ_1**, **Φ_2**, or **Φ_3**). If no symbol is specified then the species participating in the corresponding **REAC**tion 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, **α** and **β**, in the EBU relation given above. The default value is unity.

γ The constant **γ** 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 **idreac** 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 is10.

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

COMMAND ENDIF

PURPOSE To define an IF construct to control which, if any, of one or two blocks of user input statements are executed.

SYNTAX ENDI

COMMENTS

This command is part of the IF-ELSE-ENDIF construct; please see the IF command

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 **CLOS**E modifier is present.

attribute	Interpretation
FORM	File is opened in the FORMATTED mode. This is the default option.
UNFO	File is opened in the UNFORMATTED mode
UNKN	File status is defined as UNKNOWN. This is the default option.
NEW	File status is defined as NEW. An error will occur if the file already exists.
OLD	File status is defined as OLD. An error will occur if the file does not exists..
BOTH	File is available for both READ & WRITE operations. This is the default option.
READ	File is available only for READ operations.
WRIT	File is available only for WRITE operations.

filetype **One** of the modifiers below that identify the file to be opened or closed.

filetype	Interpretation
DEBU	Debug output file (**DEBU**G), Unit 17, is selected for the operation.
FLUX	Flux output file (**FLUX**), Unit 14, is selected for the operation.
HIST	Time History file (**HIST**ORY), Unit 13, is selected for the operation.
SAVE	The default Archive file (**SAVE**), Unit 11, is selected for the operation.
TRAC	Particle track file (**TRAC**K), Unit 18, is selected for the operation.

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 **BOUN**DARY command). Multiple commands may be used to fix values in an arbitrary manner. The **INIT**IAL, **READ** or **SET** commands may be used to define the variable values. Once specified, these values remain unchanged unless modified by a subsequent **INIT**IAL, **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 **FIX [Φ] [subrgn] {N_1, ... , N_n}; n=6 for 2D and 8 for 3D input mode**

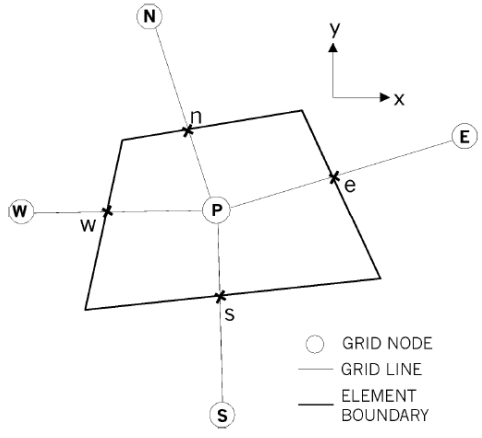
Φ A symbol that denotes the dependent variable for which input is specified. The valid symbols are listed in Table 2.7.1. There is no default value.

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

N_1, .., N_n 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:

$$\Phi_P^n = N1 + N2\,\Phi_P^o + N3\,\Phi_W^n + N4\,\Phi_E^n + N5\,\Phi_S^n + N6\,\Phi_N^n$$

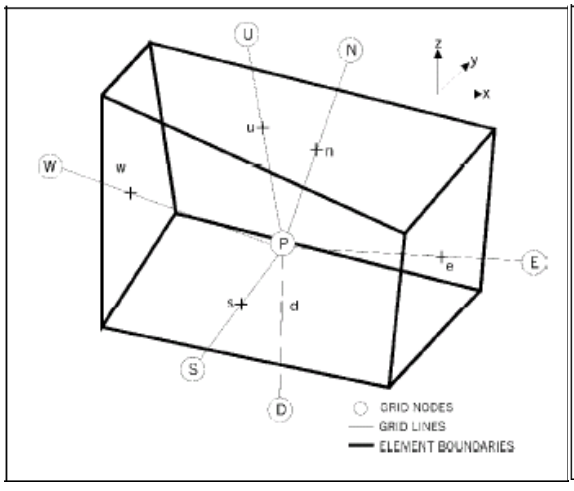
where superscript 'o' denotes the existing value and 'n' denotes the new computed value. The subscripts P, W, E, S and N denote the node being computed and the nearest neighboring nodes in the X-, X+, Y- and Y+ directions, respectively.

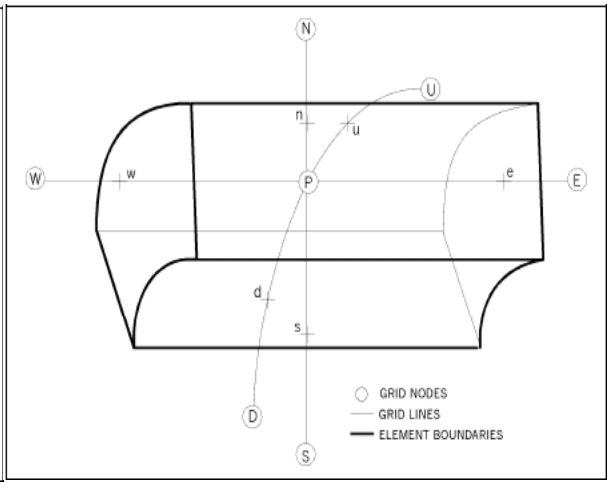


For 3D simulation, the formula is:

$$\Phi_P^n = N1 + N2\,\Phi_P^o + N3\,\Phi_W^n + N4\,\Phi_E^n + N5\,\Phi_S^n + N6\,\Phi_N^n + N7\,\Phi_D^n + N8\,\Phi_U^n$$

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

COMMAND FLOW

PURPOSE To specify the flow rate and other dependent variables at a boundary.

MODE 1: Flow Injection or Withdrawal with Fixed Variable Values

SYNTAX FLOW [TOTA [option] [func[ξ]] {N_1, N_2, .., N_n|fname} [Φ_1 =N_{n+1}, .., Φ_m = N_m] [N_{m+1}, N_k] [ρ_B] [subrgn] {dir}

TOTA By default, the amount of flow 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.

option Options selected for implementation of the source.

option	INTERPRETATION
VOLU	In the absence of the TOTAL modifier, the flow for each element is computed as: **Q = q δV.** Here **q** is the amount specified by the user and **δV** 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 δV /V**, where **V** is the volume of the total **subrgn**.
AREA	In the absence of the TOTAL modifier, the source for each element is computed as: **Q = q δA,** where **δA** 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 δA /A**, where **A** is the total area of the **subrgn** in the **dir** direction.
INTE	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.
NORM	In the absence of the TOTAL modifier, the source, **Q**, is computed as: $Q = q \sum_i A_i \bullet V_i$ 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.
DENS	The computed source, **Q**, is further multiplied by density. The density may be specified as the last value, ρ_B, 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.

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.

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.

Φ_1, .., Φ_m The dependent variables for the properties that are injected along with the flow such as heat(enthalpy or temperature) and concentration of species, etc.

N_{n+1}, .., N_m The corresponding values of Φ_1, .., Φ_m that are injected with the flow. Each of these values

must follow the symbol for the corresponding **Φ**.

N_{m+1}, .., N_k The normalizing vector components, V_i, if the **NOR**MAL 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.

ρ_B The density value that multiplies the computed source. It can only be specified if the **DENS**ITY modifier is present and then it must be the last value on the command. If no value is specified but the modifier **DENS**ITY is present, then default value is the boundary value at the node indicated by the **dir** modifier.

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.

COMMENTS

The **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 **SOUR**CE **FLOW** command may be more appropriate.The injection at an exterior domain boundary is more appropriately accounted for by the **INLE**T 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 **INLE**T 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 **INTE**RNAL modifier should be used.

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 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 TABLe 3 sets SELEcted (0, 0), (100, 1), (200, 0) U=1, V=0.1, W=0, T=10, K=0.001, L=1
FLOW: EXPOnential series with TIME 7 sets from 'SOURCE' T=100, C=0.
FLOW q=10 X- direction T=100, U=20. NORMalized velocity 0., 1.5, 2.5 ID=VSOURce;
FLOW q= -10 in X- dir with NORMalized vel 1., 1.5, 2.5 and DENSity for ID=VSOURce
FLOW q=10 X- dir variable values: U=10, V=0, W=-20, T=100, K=0.03, L=0.5 INTErnal with NORMalized vel 1., 1.5, 2.5 and DENSity for ID=VSOURce:
FLOW q=10 per unit VOLUme injected variables: U=10, V=0, W=-20, T=100, K=0.03, L=0.5 multiply by DENSity = 5 for SELEcted region

MODE 2: **Flow Injection with Fixed Variable Values and Computed Momentum Components**

SYNTAX **FLOW {MOME} [TOTA] [option] [func(ξ)] {N_1, N_2, .., N_n | fname} [$\Phi_1=N_{n+1}$, .., $\Phi_m=N_m$] [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 ρ_B, is the density, A is the area of the element boundary specified by the **dir** modifier, and n_j is a normalizing vector. If the **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.

TOTA See Mode 1 specification

option See Mode 1 specification. Unless the **NORM**AL modifier is present, it is assumed that the **AREA** modifier is in effect. Any specification of the **VOLU**ME 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_{n+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 **VOLU**ME modifier, are applicable provided that the modifier **MOME**NTUM is added. Some illustrative examples specific to this mode are given below.

FLOW with 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 SERIes TIME 7 sets 'SOURCE' T=100, C=0. NORMal 1. –1 SELEcted
FLOW 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 3: **Flow Injection at Fixed Spherical Angles with Computed Momentum Components**

SYNTAX **FLOW {ANGL} [TOTA] [func[ξ]] {N_1, N_2, .., N_n | fname} [Φ_1=N_{n+1}, .., Φ_m =N_m] [N_{m+1}, …, N_{m+5}] [DENS|SPEE] [ρ_B|V_S] [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 ρ_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.

TOTA 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.

Φ_1, .., Φ_m See Mode 1 specification.

N_{n+1}, .., N_m See Mode 1 specification.

N_{m+1} 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.

N_{m+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.

N_{m+3}, ..,N_{m+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.

ρ_B See Mode 1 specification.

SPEE The injection speed, V_S, is specified as the last value on the command.

V_S 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.

EXAMPLES

All examples cited for Mode 1 are applicable provided that the modifier **ANGL**E 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 **FLOW {Φ} {TABL} {MULT} [option] {N_{sets}} {N1,..,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

Time	Flow	U	V	T
0.	0.001	1.00	0.02	100
1.	0.002	0.50	0.01	200
2.	0.004	2.00	0.01	500
5.	0.010	5.00	0.02	600

FLOW with MULTiple TABLe: 4 sets per unit VOLUme

Time	Flow	U	V	T
0.	0.001	1.00	0.02	100
1.	0.002	0.50	0.01	200
2.	0.004	2.00	0.01	500
5.	0.010	5.00	0.02	600

MODE 5: **Flow Injection or Withdrawal at a Boundary**

SYNTAX **FLOW {ONLY} [option] [func[ξ]] {N_1, N_2, .., N_n | fname} [subrgn]**

ONLY By default the injected (or withdrawn) flow is assumed to 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.

N_1,...,N_n 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 comptue the storage term in the continuity eqution. **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.

$$\alpha_f^n = \frac{1}{\rho^n}\left(\frac{\partial \rho^n}{\partial P^n}\right)$$

In this equation, α_f is the fluid compressibility, ρ 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 is **α** is user input value to set a minimum threshold for the computed phase saturation compressibility, α_S. S is the phase saturation and pc is the corresponding capillary pressure.

α_f The compressibility of the fluid; **α_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 **SPEC**IFIC 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 **COND**UCTIVITY 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 **DENS**ITY 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] [$V_{Frq-File}$, V_{Frq}] [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 name 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, $V_{Frq-File}$ and V_{Frq} are interpreted as the frequency of output in terms of number of steps. If this modifier is present, then $V_{Frq-File}$ and V_{Frq} are interpreted to be the time interval between successive outputs.

$V_{Frq-File}$ 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.

V_{Frq} 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 $V_{Frq-File}$. 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 recommende**d; 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 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, **Φ**, the units of the cumulative flux are the units of **Φ** multiplied by the units of the density (ρ) 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 **ANSWER™** 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

#	Term and Notation	Description
1.	Active Subdomain:	Particulars of the Sub-domain for which Flux Balance is given
2.	Subdomain ID:	ID assigned to the Sub-domain by the user or the default ID automatically assigned if none given by User
3.	Time:	The simulation Time at which the flux summary is computed
4.	Net flux disparity (Qin-Qout-Qa-Qdecay)	The total "disparity" or "error" in the subregion. It is a sum of the total inflow minus the total outflow for the system
5.	Total inflow (Qin = Qc_in+Qd_in+Qsor):	Total inflow into the subregion by convective flux (Item 11), diffusive flux (item 12) and incoming (or positive) Sources (Item 13)
6.	Total outflow (Qout = Qc_out+Qd_out+Qsnk):	Total outflow from the subregion by convective flux (Item 14), diffusive flux (Item 15) and Sinks or outgoing (or negative) Sources (Item 16)
7.	Net accumulated gain (Qa = Qn-Qo)	Net increase in the amount of property (storage) in the subregion from the start of simulations.
8.	Decay from start (Qdecay)	Net accumulated decay in the property in the subregion from the start of simulations.
9.	Total initial property in region (Qo)	Initial amount of property present in the subregion at start of simulations
10.	Total property in region now (Qn)	Amount of property currently present in the subregion.
11.	Convective influx (Qc_in):	Net inflow of property due to convection from all boundaries of the subregion from the start of simulations.
12.	Diffusive influx (Qd_in):	Net inflow of property due to diffusion or dispersion from all boundaries of the subregion from the start of simulations.
13.	Source influx (Qsor):	Net inflow of property due to sources in the subregion from the start of simulations.
14.	Convective outflux (Qc_out)	Net outflow of property due to convection from all boundaries of the subregion from the start of simulations.
15.	Diffusive outflux (Qd_out)	Net outflow of property due to diffusion or dispersion from all boundaries of the subregion from the start of simulations.
16.	Sink outflux (Qsnk):	Net outflow of property due to sources or sinks in the subregion from the start of simulations
17.	Flux disparity due to mass balance (div*F)	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.
18	Convective Influx from Blocks	The inflow from the blocked areas of computational domain that were defined by the **BLOCK** or **LAND** command.
19	Diffusive Loss to Blocks	The diffusive/conductive outflow to the blocked areas of computational domain that were defined by the **BLOCK** or **LAND** command.
20	Influx due to Sub-domain Movement	The inflow due to movement of regions that evolve or move during simulation and change their nature of position.
21.	Change from last time step	Change in the amount for property from the last time step
22.	Instantaneous convective flux (in-out):	The current net inflow of convective flux at all boundaries of the subregion.
23.	Instantaneous diffusive flux (in-out):	The current net inflow of diffusive flux at all boundaries of the subregion.
24.	Instantaneous source-sink:	The current net inflow of property due to sources in the subregion.

MODE 2: **Convective Flux and Flux-Average Value of a Variable**

SYNTAX **FLUX {AVER} [Φ] [option] [subrgn] [dir] [fname] [TIME] [V_{Frq}] [NOW] [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.

option	INTERPRETATION
INLE	Boundaries specified by the **INLE**T command are selected.
OUTL	Boundaries specified by the **OUTL**ET command are selected.
OPEN	Boundaries specified by the **OPEN** command are selected.
IO	All boundaries specified by **INLE**T, **OUTL**ET or **OPEN** command are selected.
WALL	Walls specified by **WALL** or **BLOCk** command are selected.
EXTE	All external (or outer) boundaries of the computational domain are selected.
ALL	All of the above boundaries are selected.

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_{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_{Frq} specification.

OFF Any previously specified **FLUX AVER**AGE commands for the specified variables and subregion are disabled. New commands may be subsequently specified.

EXAMPLES

FLUX AVERage for ALL boundaries ! All active variables by default
FLUX AVERage for T (temperature) at IO boundaries ! All INLEt, OUTLet & OPEN boundaries
FLUX AVERage for T (temperature) at INLEt and OPEN ! INLEt & OPEN boundaries
FLUX AVERage for T at INLEt and BOUNdaries ! INLEt & domain 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 **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 ID=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 **HYDR**AULIC, **MULT**IPHASE, **ROCK**, **SOIL**, **THER**MAL and **TRAN**SPORT 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} {W_{frac}} [func[ξ]] [N_1, N_2, .., N_n | 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**.

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 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.

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.

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 correcpoding properties that apply to the porous matrix are not available for Fracrtures. 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

MODE 2: **Specification of a Fracture Aligned with Principal Axis**

SYNTAX **FRAC {ID=subrgn} {W_{frac}}} [func[ξ]] [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.

ξ 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], {C_{f1}}, [C_{f2}]**

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.

$$C_f = g \{\frac{C_{f1}}{C_{f2}}\}^2 \frac{1}{H^{1/3}}$$

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.

$$C_f = \frac{g}{C_{f1}^2}(C_{f2} + \frac{1}{\sqrt{H}})^2 ,$$

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.

$$C_w = C_{w1} + C_{w2} \{ \max [0 , (1 - \frac{w_o}{w})^2] \} ,$$

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_o 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_o = 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

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** **{[Φ_1=N1, Φ_2=N2, ..., Φ_n=Nn]}**

Φ_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 **REAC**TION 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

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 **OPTI**ON command).

GAMM γ, 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 **OPTI**ON command).

V1 The reference sonic speed or γ for the gas. The default value is 300 for the sonic speed and 1.4 for the ratio of specific heats (γ).

EXAMPLES

GAS SONIC speed is 275 m/s
GAS GAMMA is 1.2

MODE 4: **Universal Gas Constant**

SYNTAX **GAS {CONS} [func[ξ]] [N_1, N_2, .., N_n | fname]**

CONS The universal gas constant, R_u 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.

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.

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 θ 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} {dir_1} {dir_2} [φ_1, φ_2]**

ROTA The coordinates in the two directions specified by **dir_1** and **dir_2** are rotated in the plane defined by dir_1 and dir_2 by **φ_1** and **φ_2** degrees, respectively, according to the following equations:

$$X_{New} = X_{Old} \text{ Cos } \phi_1 + Y_{Old} \text{ Cos } \phi_2$$

$$Y_{New} = X_{Old} \text{ Sin } \phi_1 + Y_{Old} \text{ Sin } \phi_2$$

dir_1, dir_2 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 dir_1 and dir_2.

φ_1 The angle **φ_1** (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.

φ_2 The angle **φ_2** (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 ROTAte X and Y by 45 degrees
GEOMetry ROTAte X by 45 and Y by 135 degrees!! same as above
GEOMetry ROTAte X and Y by -45 deg.
GEOMetry ROTAte X and Y 30 and Z by 115 degrees from old x-axis

MODE 3: **Scale Previously Specified Coordinates**

SYNTAX **GEOM {SCAL} {dir} { V_{Mult} } [V_{Add}]**

SCAL The coordinates in the direction(s) specified by **dir** are scaled according to the following equation:

$$X_{New} = X_{Old} * V_{Scale} + V_{Add}$$

dir One or more of the **X**, **Y**, **Z**, **R** or **THETA** modifiers that, respectively, denote the x, y, z, r or θ coordinates each of which is scaled according to the equation given above.

V_{Mult} The multiplication factor for the transformation defined above. There is no default value; a value must be specified.

V_{Add} 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} [θ_1, θ_0]**

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.

Θ_1, The angle of the cylinder circumference in degrees. The default value is 180 degrees.

Θ_0 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 - θ Plane**

SYNTAX **GEOM {ANNU} {R_o} [R_i, e, θ_1, θ_0]**

ANNU Generates an annular geometry for the computational domain in the **r -θ** plane.

R_o The outer radius of the annulus. There is no default vale; a value must be specified.

R_i The inner radius of the annulus. The default vale 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. The default vale is 0.

θ_1 The total angle for the outer arc of the cylinder in degrees. The default value is 180 degrees.

θ_0 The starting angle from the origin for the cylinder in degrees. The default value is 0 degrees.

COMMENTS

Currently this command is available only if the computational domain is located in the 1st or 2nd quadrant.

EXAMPLES

GEOMetry is ANNUlar with radius = 1.
GEOMetry is ANNUlar with rin=1, rout=0.5
GEOMetry is ANNUlar with rin=1, rout=0.5, epsilon=0.1
GEOMetry is ANNUlar with rin=1, rout=0.5, epsilon=0.1, theta = 90
GEOMetry 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:

$$x_1 = r \, \mathrm{Cos}\,\theta$$

$$x_2 = r \, \mathrm{Sin}\,\theta$$

RADI Convert existing Cartesian coordinates to cylindrical radial coordinates according to the transformation:

$$r = \mathrm{sqrt}\,(x_1^2 + x_2^2)$$

$$\theta = \tan^{-1}(x_2 / x_1)$$

dir_1, dir_2 Two of the **X**, **Y**, **Z**, **R** or **THET**A modifiers that, respectively, denote the x_1 and x_2 directions in the Cartesian framework to be transformed to or from the **r** and **θ** directions of the cylindrical coordinate system. By default r direction is assumed to be aligned with the y direction and the θ with the z direction.

COMMENTS

Transformation from Cartesian to radial framework is possible only for a 3-dimensional grid since in the 2-dimensional mode only (x, r) coordinate system is available. For the transformation to a cylindrical system the resulting **r** is stored at the same location as x_1 and **θ** at x_2. For transformation to a Cartesian system the resulting x_1 is stored at the same location as **r** and x_2 at **θ**.

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

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 is -9.81 for 2D flow and g_z is -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 **PORFLW™** 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:

$$B_i^n = \frac{\rho^n}{\rho^*}\frac{g_i}{g}$$

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 ρ* 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:

$$B_i^n = \frac{\rho^n - \rho^*}{\rho^*}\frac{g_i}{g}$$

The pressure equation is solved for the Total head, H^n. This is the default option for the **PORFLOW™** Software Tool.

This **RELA**TIVE 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 **PROB**LEM **ATMO**spheric or **REFE**RENCE **HYDR**aulic 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 **GRAV**ITY **ABSO**LUTE 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 (**GRAV**ITY **RELA**TIVE) by default. For saturated flow, if no **GRAV**ITY 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 are: 0., -9.81RELATIVE mode                ! Orientation against y-axis
GRAVity constants are: -6.937, -6.937, 0.          ABSOLUTE mode    ! 45 deg to x & y
GRAVity constants are: 0., 0., -9.81               ! Orientation against z-axis
GRAVity constants are: 0., 0., -32.2, 32.2                  ! Orientation against z-axis
GRAVity constant is 9.81
```

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] {N_X} [N_Y, N_Z]

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 N_X, N_Y and N_Z 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.

N_X 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.

N_Y 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.

N_Z 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 N_Z is not specified, then the 2Dsolution 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 **COOR**DINATE command. The connectivity of the vertices to the elements is specified on a file through the **CONN**ECTIVITY 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 **CONN**ECTIVITY command is not required. The coordinates of the vertices must be specified on a file through the **COOR**DINATE command.

VERTEX The **VERT**EX mode of the **CONN**ECTIVITY command is invoked. Please see the **CONN**ECTIVITY command for further details. This is the default option.

HYBRID The **HYBR**ID mode of the **CONN**ECTIVITY command is invoked. Please see the **CONN**ECTIVITY 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 CONNectivity of VERTices to elements on file “VERT2ELM.CNC”
GRID CONNectivity for HYBRID elements on file “MIXED_ELEMENTS.CNC” THREE D problem

COMMAND **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] [V_{Frq}] [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 **LOCA**TE command must be specified with an **ID=subrgn** or a **SELE**CT/**LOCA**TE 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.

V_{Frq} 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, **V_{Frq}** is interpreted as the frequency of output in terms of number of steps. If this modifier is present, then **V_{Frq}** 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 **HIST**ORY 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, .., N_n} [fname]**
N=m in unstructured mode, = 2m in 2D and =3m in 3D mode

N_1, .., 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] [V_{Frq}] [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.
V_{Frq}	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] [LINE|SQUA] [N1,..Nn] [V_{Frq}] [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.

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 present, this must be last value on the command. By default the time history is generated at every step.

TIME By default, **V_{Frq}** is interpreted to be the frequency in terms of number of steps. If this modifier is present, then **V_{Frq}** 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 SQUAre 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 COOR (1.35, 0.796, 0.0975) TIME interval 0.235; SQUARE method 'HISTORY.XYZ'

MODE 5: History of Source for a Variable

SYNTAX HIST {SOUR} {Φ} [subrgn] [fname] [TABL] [OFF] [V_{Frq}] [TIME]

SOUR Output for the source term for **Φ** is required.

Φ 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 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 "**_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 φ and **subrgn** is deactivated.

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 time history is generated at every step.

TIME By default, **V_{Frq}** is interpreted to be the frequency in terms of number of steps. If this modifier is present, then **V_{Frq}** 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 **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

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_{Frq}] [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 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 "_**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_{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 time history is generated at every step.

TIME By default, **V_{Frq}** is interpreted to be the frequency in terms of number of steps. If this modifier is present, then **V_{Frq}** 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

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:

$$S_e^n = R^n S^n \alpha_s + R^n \theta_E \left(S^n \alpha_f^n + \alpha_{Sat}^n \right)$$

α_S, the compressibility of the matrix, is assumed to be a constant that is specified from empirical data. The superscript "n' denotes the n^{th} fluid phase, R is the density ratio, S is the saturation, α_f, is the fluid compressibility and α_{Sat} is the compressibility due change of saturation with pressure. For a liquid α_f is generally small and is specified by the user as input. For a gas, the fluid compressibility is calculated from the perfect gas law as:

$$\alpha_f^n = 1/P^n$$

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 ($i \neq j$) 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_j are the reference values of the hydraulic conductivity tensor for a reference fluid (usually water) of density ρ* and viscosity μ* . The K_j 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 **STOR**AGE or **DIST**RIBUTION commands and those for hydraulic conductivity can be specified by the **COND**UCTIVITY command.

EXAMPLES

HYDRAULIC properties: ss = **0.2**, Kx* = **2,** Ky* = **0.2**, Kz* = **0.2** ft per day
HYDRAULIC properties: ss = **0.2**, Kx* = **2,** Ky* = **0.2**, Kz* = **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

1st block of FREEFORM statements

[ELSE

2nd block of FREEFORM statements]

ENDIF

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.

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 1st block of statements is executed and the 2nd block, if present, is ignored. If the status is false then the 1st block of statements is ignored and the 2nd 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.**

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 1st block of statements is executed and the 2nd block, if present, is ignored. If the status is false then the 1st block of statements is ignored and the 2nd 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 2nd block is optional. However, if the 2nd 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 **INCL**UDE command provides for unlimited nesting in that the file being incorporated may itself contain embedded **INCL**UDE 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 **INCL**ude 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 **INCL**UDE 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

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 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)
    &                                                    to (1.0,
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]

Φ 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.

Φ_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

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

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_{Elaps}][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 defaults, values of **V_{Start}**, **V_{Elaps}**, **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.

STAR 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 **TEMP**ERATURE) 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 Introduce 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, **TINJ**ection=280. Kelvin, **QINJ**=10 kg/s, **HIST**ory 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 **INJE {CURTAIN} [ID=subrgn] {QINJ=V_{Qinj}} [DIAM=V_{Diam}] [TIME] [TEMP] [STAR=V_{Start}|STAR NOW] [COOR=V_X, V_Y [V_Z]] [STOP=V_{Stop}|STOP NOW] [ELAP=V_{Elaps}] [HIST=V_{Hist} [fname]]**

subrgn The subregion for which the input is specified. **This subregion must be defined with LOCATE INJECTION command**. See Section 3.4 for additional details.

QINJ Introduces the mass rate of water in the film. There is no default value; a positive value must be specified.

V_{Qinj} Mass rate of water in the film

DIAM Introduces droplet diameter of water curtain

V_{Diam} Droplet diameter. There is no default value; a positive value must be specified.

TIME By defaults, values of **V_{Start}**, **V_{Elaps}**, **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.

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.

STAR Introduces the start time of the film. By default this is defined by **INJE FREQ** for all injections.

V_{Start} Step or Time (if modifier **TIME** is present) or Temperature (if modifier TEMP is present) 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.

COOR If modifier **TEMP** is present then this keyword must be added to define coordinates of the point at which film temperature monitored.

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, a history file is written.

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 "**_CURTAIN.TMP**". For example, if the Standard Output file is "**PROBLEM.OUT**", then the file is named "**PROBLEM_CURTAIN.TMP**".

EXAMPLES

INJE CURTain ID=ZCURT QINJection=10. kg/s DIAMeter=0.001 m
STARt NOW and STOP at TIME 180 seconds
HISTory every 0 second, file is 'CURTain.his'

MODE 3 **Location and Properties for Condensation**

SYNTAX **INJE {COND} {subrgn} [dir] [option] [TIME] [HIST=V_{Hist} [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.

option

option	INTERPRETATION
DROP	The droplet condensation model is activated. This is the default option.
FILM	The film condensation model is activated.

TIME By defaults, values of V_{Hist} (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.

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 "**_CONDENSE.TMP**". For example, if the Standard Output file is "**PROBLEM.OUT**", then the file is named "**PROBLEM_CONDENSE.TMP**".

COMMENTS

If **FILM** model is activated, the water film falling direction is defined the **GRAV**ITY 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} {N_1} [N_2, N_3]**

FREQ The spray computation frequency parameters are specified.

N_1 The frequency of droplet computations in terms of computational steps. The default value is 10.

N_2 The first computational step at which the droplet computations are performed. The default value is 1.

N_3 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 **INJE**CTION 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

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 **INIT**IAL, **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

INLEt at X- boundary at left (minimum x)
INLEt at Y- boundary for the most recently SELEcted subregion
INLEt at X+ boundary for subregion ID = INFLow
INLEt 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 **INTE [Φ] {HYBR | BOUN | CENT | QUIC | ACRI | UPWI}**

Φ 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^{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^{nd} order central-difference scheme is used for integration. The scheme uses 2^{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^{st} order upwind scheme is used computing convective fluxes whereas the diffusive fluxes are still computed by the 2^{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.

$$\mathbf{Pe = U\,\delta L / \Gamma}$$

where **U** is the flow speed, **δL** is the grid interval and **Γ** 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

COMMAND LAGRANGIAN TRANSPORT

PURPOSE To select the Lagrangian Random-Walk algoritm for transport of species.

MODE 1: Specification of Maximum Number of Particles

SYNTAX LAGR {PART} {N_{Part}} [q_{Part}] [MASS|[LOCA|[DENS=ρ]|[RADI=β]]] [OFF]

PART The number of Lagrangian particles to be tracked for transport of a species.

N_{Part} 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 they can be eliminated and consolidated based on specified criteria. There is no default value.

q_{Part} The mass of the Lagrangian particle at time of release in to 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.

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 **OUTP**UT 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 purpose.

COMMENTS

A **LAGR**ANGIAN **PART**ICLE command must be present to initiate the solution of the transport equation by the stochastic **RADM** (**RA**ndom Walk **D**ispersion **M**ethod) 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 PART**CLES.
LAGRANGIAN transport with **10000 PART**CLES and mass of each as **0.002** kg with RADIus factor as **10.**

LAGRANGIAN transport with **10000 PART**CLES and mass of each as **0.002** kg concentration **OFF.**

MODE 2: **Specification of Particle Release Rate**

SYNTAX **LAGR {RELE} [Φ] {func[ξ]} {N_1, N_2, .., N_n | fname} [NUMB=N_{Part}] [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.

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.

NUMB By default the mass of each particle is assumed to be that specified as **q_{Part}** 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 **N_{Part}** and the mass of each is equal to the toal 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.

N_{Part} 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 reelased 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 **LAGR**ANGIAN **RELE**ASE 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 RAND**OM numbers.

MODE 3: **Specification of a Receptor for Concentration Computations**

SYNTAX **LAGR {TABL} [TIME] [V_{frq}] [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, **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 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 **OUTP**UT command must be given ot obtain the output of the concentration field.

EXAMPLES

LAGRANGIAN **RECE**PTOR at **ID**=**STATION1** at end of simulations.
LAGRANGIAN **RECE**PTOR 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 RAND**OM 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

COMMAND **LAND**

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

COMMENTS

This command is identical to the **BLOCK** command. Please see the **BLOCK** command for details.

COMMAND LIMIT

PURPOSE To specify the limiting values for field variables

SYNTAX LIMI {Φ} {Φ_{Min} , Φ_{Max} | OFF} [MATR]

Φ A symbol that denotes the variable for which the limits are being set.

OFF All previously set limits for the selected variable are deactivated.

Φ_{Min} The minimum permissible value for the variable. Any computed value that is less than Φ_{Min} is set to Φ_{Min}.

Φ_{Max} The maximum permissible value for the variable. Any computed value that is greater than Φ_{Max} is set to Φ_{Max}.

MATR 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.

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 **LOCA**TE or **SELEct** on the command can make a generic reference to the specified subregion until the next **LOCA**TE or **SELE**CT command. See Section 3.4 for additional details.

FIEL If the **LOCA**TE 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 **FIEL**D 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 FIEL**D **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 (**BLOC**K command) are excluded from the selected set of elements.

SOLI If this modifier is present then only the solid or blocked (**BLOC**K 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 assume dto 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] {N_1, ..., N_n} [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 **FIEL**D 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 **INTE**RSECTION 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 **BOUN**dary modifier is present, then only the external boundary nodes are selected. Any elements interior to the computational domain are excluded.

N_1, .., N_n 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 **SCAL**E command is specified immediately preceding this command, then the input coordinate values are scaled as described in the **SCAL**E 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] {N_1, ..., N_n} [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 **FIEL**D and **BOUN**DARY 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 **BOUN**DARY 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.

N_1, .., N_n The grid coordinates (x, y) or (x, y, z) for the vertices of the polygon. The number of values must equal N23D * N_{vertex} where N23D is 2 for 2D and 3for 3D geometry and * N_{vertex} 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 **SCAL**E command is specified immediately preceding this command, then the input coordinate values are scaled as described in the **SCAL**E command.

EXAMPLES

LOCAte POLYgonal region (x, y) coordinates are: (0, 0) (1,0) (1,1) (0,1) !2D rectangle
LOCAte POLYgon (x, y) coordinates are: (0, 0) (1,-1) (2,0) (1,1) !Diamond shaped region
LOCAte POLYgon (x, y): (0, 0) (0.5,-0.866), (1.5,-0.866) (2,0) (1.5,0.866) (0.5,0.866) !Hexagon
LOCAte 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
LOCAte region ID=DIAMOND POLYgon (0, 0) (1,-1) (2,0) (1,1) output on “FILE.LOC”
LOCAte 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}} [N_1,.... N_n] [IJK|ELEM] [N_{n+1},..N_m], [N_{m+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 **FIEL**D modifier is present.

idsub See Mode 1 specification.

FIEL See Mode 1 Specification.

BOUN If the **BOUN**DARY 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.

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 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_1]** specifies the element which is at the center of the cylinder. Only 1 value must be specified.

N_{n+1},...N_m 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.

N_{m+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 than 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 **LOCA {SPHE} [ID=idsub] [FIEL] [FLUI|SOLI] {R_{sphere}} [N_1, . 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 **FIEL**D 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, . N_n The (x,y) or the (x,y,z) coordinates of the center of the sphere.

fname See Mode 1 Specification.

EXAMPLES

LOCAte SPHEre radius=0.4, center coordinates (2., 0.5) !2D
LOCAte SPHEre radius=0.4, center coordinates (2., 0.5, 0.5)
LOCAte SPHEre radius =0.4, center coordinates (2., 0.5, 0.5) FIEL node only
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 **FIEL**D 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_1** specifies the element which is at the center of the cylinder. Only 1 value must be specified.

Nn+1, ... Nm See Mode 4 Specification.

Nm+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=idsub] {N_{mat}} [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.

N_{mat} The material type or zone number that previously appeared in a **MATE**RIAL (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**TE 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] {N_1 | N_1, …, N_n}**

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 **FIEL**D 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 (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 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 **SCAL**E command is specified immediately preceding this command, then the input coordinate values are scaled as described in the **SCAL**E 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 COOR LIST 500 as ID=BIG from file 'XYZ.LST' only FIELD ! Read file; only field
LOCAte COOR 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 **EXTE**RIOR 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] {N_1|N_1, …, N_n}**

LIST Explicit list of element numbers is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the **FIEL**D 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 (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 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, 22, 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] {N_1, N_2} [N_3]**

SEQU A sequence of elements is specified. Only the internal elements can be specified. Associated boundary nodes are automatically included unless the **FIEL**D 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.

N_1, N_2, N_3 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 **N_3** is not specified, it is assumed to be 1.

EXAMPLES

LOCAte ID=lLISTSEQ 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 $\Phi_{Min} \leq \Phi \leq \Phi_{Max}$ 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_1, ..., 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**.

N_1, .., N_n 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. **CORR**LELATION) 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 **LOCA**TE or **SELE**CT on the command can make a generic reference to the specified subregion until the next **LOCA**TE or **SELE**CT 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] {N_1|N_1, N_2, N_3, … , N_n]**

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 (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 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 N_1, N_2 below. If the file input mode is not **activated, then N_1 is interpreted as given below.**

N_1, N_2 N_1 is the element number and N_2 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.

N_3,..,N_n The element number and a surface number for the rest of the elements which comprise current subregion in the manner N_1 and N_2.

EXAMPLES

LOCAte (element, surface) PAIRs: (35,1), (53,3), (77,2), (13,4)
LOCAte PAIR : (35,1), (53,3), (77,2), (13,4) as boundary ID=BNDRy
LOCAte PAIR : 500 sets as ID=BNDRy from file 'BOUNDARY.BIG'
LOCAte PAIR : (35,1), (53,3), (77,2), (13,4) as boundary ID=BNDRy
LOCAte PAIR : (35,1), (53,3), (77,2), (13,4) as boundary ID=BNDRy
LOCAte PAIR : (35,1), (53,3), (77,2), (13,4), (28,5), (33,3), (35,6)
LOCAte 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_1, …, 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

option	INTERPRETATION
ANY	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.
ONE	A boundary element is included if at least one of its vertices is included.
TWO	A boundary element is included if at least two of its vertices are included.
THRE	A boundary element is included if at least three of its vertices are included.
FOUR	A boundary element is included if at least four of its vertices are included

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 **SEQU**ENCE modifier, these numbers identify the vertices that define the boundary of interest. In the presence of the **SEQU**ENCE 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 **FORT**RAN DO loop.

REMARKS

The complementary operation cannot be performed on regions that are defined by **MATC**HED **PAIR** or **CORR**ELATED type of element sub-domains or on previous **LOCA**TE commands defined with a **FIEL**D modifier.

EXAMPLES

LOCAte: VERTices 1,3,7,8,10,20,55,99,203,105,77
LOCAte VERTices: in SEQUence from 23 through 231 in steps of 3 as boundary ID=BNDRy
LOCAte VERTices: 500 values as ID=BNDRy from file 'BOUNDARY.BIG'
LOCAte 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 **LOCA**TE commands which identify a boundary (**LOCA**TE **PAIR**, **LOCA**TE **VERT**ex, **LOCA**TE **COOR**DINATE **BOUN**DARY and **LOCA**TE **POLY**GON **BOUN**DARY 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

MODE 19: **Specification of a General Second Order Surface**

SYNTAX **LOCA { SURF} { BOUN } {N_1, N_2, , N_n} [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.

ε The tolerance for judging the proximity to the surface. This numerical value must be present if the modifier **TOLE**RANCE 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. +1. TOLErance=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 **LOCA**TE **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 **LOCA**TE **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 **INTE**RIOR 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 LOCA **{UNIO|INTE} {ID=id1} {ID=id2} {ID=….} {ID=idn} [NOT] [EXCL] [ID=idsub] [FIEL] [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 **INTE**RSECTION 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 nth 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 **INTE**RSECTION 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 **MATC**HED **PAIR**, **CORR**ELATED or I**NJE**CTION modifiers.

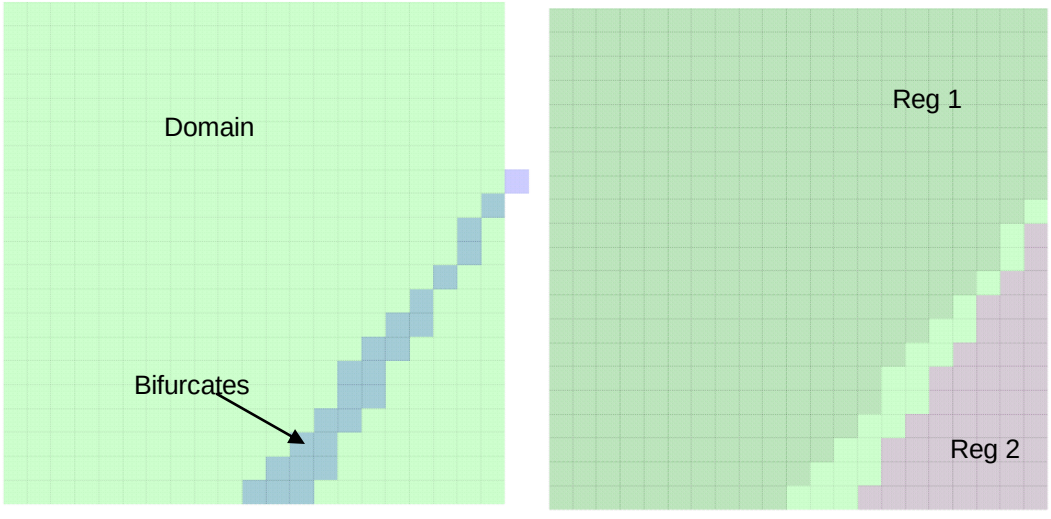
EXAMPLES

LOCAte UNIOn of ID=DMN1 and ID=DMN2
LOCAte UNIOn of ID=DMN1 and ID=DMN2 as ID=DMN3
LOCAte INTErsection ID=DMN1 and ID=DMN2
LOCAte UNIOn of subregions ID = DMN1 and ID=DMN2 EXCLude selection only FIELd elements
LOCAte UNIOn of ID=DMN1 and ID=DMN2; EXCLude selected and name ID=DMNM12
LOCAte ID=DMN1 plus ID=DMN2 select INTErsection & EXCLude
LOCAte ID=DMN1 plus ID=DMN2 select NOT INTErsection & EXCLude output on file ‘DMN12.LOC’

MODE 23: **Subregion Contiguous to a Boundary or Surface**

SYNTAX **LOCA {CONT} {ID=idsub1} {ID=idsub2} {x_0,y_0, [z_0]} [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 **x_0,y_0, [z_0].** 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 **x_0,y_0,,z_0** 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.

x_0,y_0, [z_0] 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 **LOCA {ID=idsub1} [EXCL] [ID=idsub] [FIEL] [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

LOCAte ID=DMN1 as new subdomain called ID=DMN2
LOCAte EXCLude ID=DMN1 and define new complimentary set as ID=COMPDMN1
LOCAte EXCLude ID=DMN1 and define new complimentary FIELd only set as ID=COMPDMN1
LOCAte EXCLude ID=DMN1 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 **LOCA**TE **LIST** command) or boundary type of sub-domains (such as **LOCA**TE **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 **BOUN**DARY 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 **FIEL**D 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] {N_1, …, N_n} [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 "**CURT**AIN mode" (see **INJEC**TION **FILM** and **INJEC**TION **CURT**AIN 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.

N_1, .., N_n **N_1** through **N_n** 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 **N_1, …, N_n** 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:: $\overline{AB} \wedge (\overline{AB} \wedge \bar{g})$.

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=WCURTAIN
with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
LOCAte INJEction on ID=WALLRIGHt and define ID=WFILM
with injection from (2.0, 2.7, 0.0) to (5.0,2.7,2.0)
LOCAte INJEction on SELEcted surface and define ID=WFILM
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] {N_1, ..., N_n} [STOR = N_{add}] [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.

N_1, .., N_n 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.

N_{add} 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 **MOVI**NG region ID=MOVE_FRAC with initial **COOR**dinates (0.,40.0,4.40) to (45.,60.0,4.70)
LOCAte **MOVI**NG ID=MOVE_FRAC **COOR**dinates (0.,40.0,4.40) to (45.,60.0,4.70) **STOR**=1000

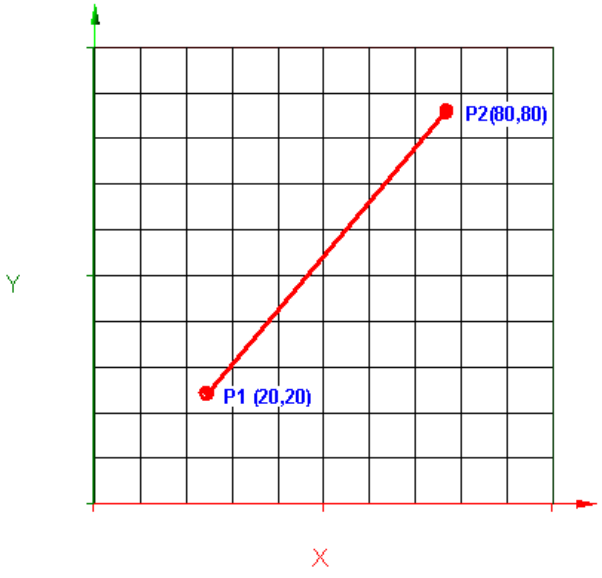
MODE 28: **Stationary or Evolving Embedded Planar Fracture**

SYNTAX **LOCA {FRAC} [MOVE|MOVI] {ID=idsub} {N_1, ..., N_n}**

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.

N_1, .., N_n 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 **FRAC**TURE ID=FRAC2D from (20,20) to (80,80) ! 2D fracture
LOCAte **MOVI**ng **FRAC**TURE ID=FRAC3D from (15,15,25), (35,15,25),(35,35,25),(15,35,25) !3D fracture

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] {ρ_S} [Θ_E, Θ_T, Θ_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.**

ρ_S The density of a dry, solid component, ρ_S (> 0). The default value is 1.

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.

APPLICABILITY

This command is currently available only for the **PORFLOW™** Software Tool.

COMMENTS

This mode of the command has been superseded by the 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] {N_{Mat}} [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.**

N_{Mat} 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 mare than 100 material types are required, then the **ALLOCATE MATE**RIAL 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 **FIEL**D 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 idensity to each material type. It is used primarily only for output pruposes. 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 =N_1, Φ =N_2, ..., Φ =N_n] [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.

N_1,..., N_n 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 (**CONV**ERGENCE 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 =N_1, Φ =N_2, ..., Φ =N_n]**

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.

N_1,..., N_n Number of times the matrix is "swept" for the variable denoted by the symbol immediately preceding the value. This input is ignored if the **EXPL**ICIT 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 **EXPL**ICIT 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 **MATR {Φ} {solver} [precon] [NORM] [N_{Degree} | N_{Block}]**

Φ 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.

solver

- **BICG** Matrix is solved by the bi-conjugate gradient stabilized method.
- **BICO** Matrix is solved by the bi-conjugate gradient stabilized method.
- **CONJ** Matrix is solved by the conjugate gradient method. To be used for symmetric matrices only.
- **CG** Matrix is solved by the conjugate gradient method. To be used for symmetric matrices only.
- **CGNR** Matrix is solved by the conjugate gradient for normalized equations method. This method may be inferior to the BICG method.
- **LUDE** Matrix is solved by sparse direct LU decomposition method. This method can be slow and memory intensive if the problem size exceeds 20000 elements. **MATR**IX **ITER** mode of the command is ineffective with this option.
- **BLOC** 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.
- **USER** Matrix is solved by an algorithm supplied by the user. See Section 4.7.

precon

- **NEUM** 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.
- **SSOR** The symmetric SOR pre-conditioner for the BICG, CG, and CGNR methods.

NORM See Mode 1 specification.

N_{Block} The size of the block if **BLOC** modifier is present; the specified value must be greater than 99. The default value is 2000.

N_{Degree} The degree of the polynomial if **NEUM** pre-conditioner is specified. The default value is 4.

COMMENTS

Currently, the **CONJ**ugate gradient and **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

MATRix for T USER option 5! Matrix Solver supplied by User
MATRix for T accelerator: BICOnjuate gradient preconditioner: NEUMann degree 7
MATRix for T accelerator: BICOnjuate gradient preconditioner: SSOR
MATRix for P by sparse LUDEcomposition (only for less than 20000 elements)
MATRix for P by BLOCk size=1000 elements
MATRix for P accelerator: CONJugate gradient preconditioner: SSOR (symmetric matrices only)

MODE 4: **Number of Inner Matrix Iterations**

SYNTAX **MATR {ITER} [MAX |MIN] {N1|Φ =N_1, Φ =N_2, ..., Φ =N_n} [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 **MATR**IX **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 **CONV**ERGENCE 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 **CONV**ERGENCE command for the variable.

Φ Symbols that denote the variable(s) for which the **N_1**, **N_2,** ..., 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.

N_1,..., N_n 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 (**CONV**ERGENCE 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] [N_{degree}]**

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.

precon	INTERPRETATION
NEUM	Neumann matrix polynomial. This is the default option.
LEAS	Least squares matrix polynomial.
DEGR	Degree of NEUMann or LEASt squares polynomial (integer) default: 3
REDU	Reduced System preconditioner.
CHOL	Incomplete Cholesky Factorization.
JACO	The point Jacobi preconditioner.
SOR	The Successive Over-Relaxation preconditioner and accelerator

accel Accelerator Component of the Matrix Solver

accel	INTERPRETATION
CONJ	Conjugate Gradient accelerator.
BCGS	The Biconjugate Gradient Squared accelerator.
GMRE	GMRES accelerator. This is the default option.
ORTH	ORTHOMIN accelerator.
CGNR	Conjugate Gradient applied to Normal Equations.
LANC	Lanczos with ORTHOMIN accelerator.

option Modifier for the specification or matrix or solver method

option	INTERPRETATION
MODI	If CHOLESKY preconditioner is selected, then modified incomplete Cholesky decomposition is used; otherwise this input is ignored.
PERM	If CHOLESKY preconditioner is selected, then matrix is red-black permuted; otherwise this input is ignored.

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.

N_{degree} The degree of the polynomial if **NEUMANN** modifier is present.

EXAMPLES

MATRIX for **P** by **NSPCG** (**PERMUTED CHOLESKY**).
MATRIX for **P** from **NSPCG** with **JACOBI** preconditioner and **BCGS** accelerator
MATRIX U V W P use **NSPCG** preconditioner: **NEUMANN** poly of **DEGREE** 3 **GMRES** accelerator
MATRIX P NSPCG NEUMANN DEGREE 3 GMRES
MATRIX NSPCG P NEUMANN DEGREE 2 **TRUNcated GMRES ELIMINATE** equations below threshold.
MATRIX 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_{Vector}] [NORM]**

HYPR One of the parallelized matrix solvers from the HYPRE package of the Lawrence Livermore National Laboratory (University of California), Livermore, California is used. A recent summary of the HYPRE library is described in: **"Falgout, R.D. and Yang, U. M., "HYPRE: A Library of High Performance Preconditioners," in *Computational Science - ICCS 2002 Part III,* P.M.A. Sloot, C.J.K. Tan. J.J. Dongarra, and A.G. Hoekstra, Eds., Lecture Notes in *Computer Science,* vol. 2331, pages 632-641, 2002, Springer-Verlag. Also available as Lawrence Livermore National Laboratory technical report UCRL-JC-146175.** The source code and manuals are available at http://www.llnl.gov/CASC/hypre/. A special agreement is required for use of this solver package.

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.

precon	INTERPRETATION
AMG	Algebraic Multi-Grid Preconditioner. This is the default option.
CHOL	Incomplete Cholesky Factorization.
DIAG	Diagonal Scaling Preconditioner
SPAR	The Sparse Approximate Inverse Preconditioner.

accel Accelerator Component of the Matrix Solver

accel	INTERPRETATION
AMGA	The AMG accelerator.
BICG	The BI-Conjugate Gradient accelerator
CONJ	Conjugate Gradient accelerator.
GMRE	GMRES accelerator. This is the default option.

option Modifier for the specification of matrix or solver method

option	INTERPRETATION
SYMM	By default the matrix is assumed to be non-symmetric**.** If this modifier is present, then the matrix is assumed to be symmetric.
INDE	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 **INTE**GRATION Command)
STAT	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 **STAT**ic modifier will lead to a more efficient set up strategy. This modifier is ignored if any preconditioner other than AMG is specified.

VECT This modifiers defines the number of vectors in the Krylov space that are saved.

N_{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_{Coef}] [ZERO=V_{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_{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_{Zero} The numerical value for the machine zero. The default values are given in the table below.

1.192×10^{-7}	IEEE real with 32-bit precision.
2.22×10^{-16}	IEEE real with 64-bit precision. This is the default.
7.1×10^{-15}	Cray XMP.
1.49×10^{-8}	Dec 10 (single precision)
4.768×10^{-7}	IBM 370 / 158 (single precision)

NORM See Mode 1 specification.

EXAMPLES

MATRix COEFficient 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, COEFficient=1.E-30.

MODE 8: **Tolerance Threshold for Minimum Value of Matrix Elements**

SYNTAX **MATR {TOLE} {V_{Tole}|Φ=V_{Tole1}, Φ =V_{Tole2}, ..., Φ =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 **HYPR**E 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 **CHOL**ESKY 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.

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 the **CHOL**ESKY, **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}|Φ=N_{Level1}, Φ=N_{Level2}, ..., Φ=N_{Leven}} [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.

Φ 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} {N_0|Φ=N_{01}, Φ=N_{02}, ..., Φ=N_{0n}} [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 **CHOL**ESKY Preconditioner of the **HYPR**E package.

N_0 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 effecitvie if no symbol is specified, and it is then applied to all variables for which the **CHOL**ESKY, method has been selected.

N_{01}, N_{02},, N_{0n} As for **N_0** above except that the input is effecitvie if one or more variable (**Φ**) is specified.

Φ Symbols that denote the variable(s) for which the **N_{01}, N_{02},, N_{0n}** 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 **NSPC**G solvers, by default the specified convergence tolerance (**CONV**ERGENCE 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 **MATR**IX 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

COMMAND META

PURPOSE To Generate Multiple Simulations form 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:

%metacomand1% <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>
END
%metacomand1% <valid ACRi FreeForm™ Command>
%metacomand3%<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 **THET**A modifiers that, respectively, denotes the x, y, z, r or θ 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 (**BLOC**K 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 at the moving boundary 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 **ABSO**lute velocity mode is recommended for most applications. In general it depicts better numerical behavior. The **RELA**tive 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.

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 **ABSO**LUTE velocity mode is recommended for most applications. In general it depicts better numerical behavior. The **RELA**TIVE 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**

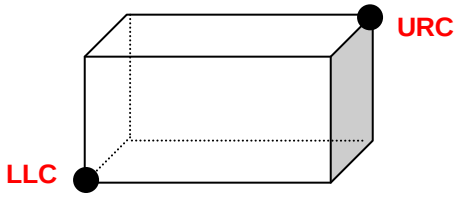
SYNTAX **MOVE {ID=subrgn} {LLC|URC} {X|Y|Z} {func [time]}**

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]}**

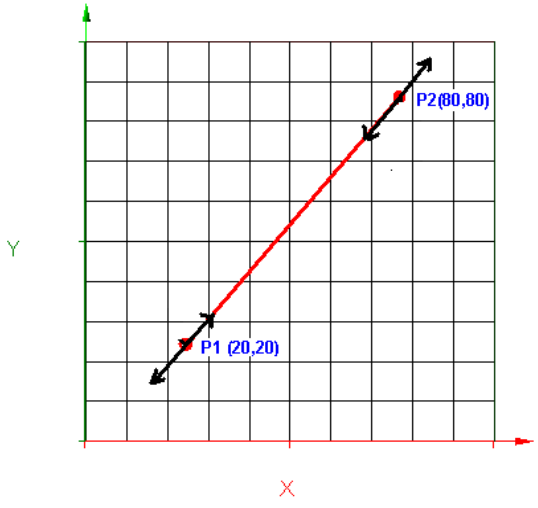
ID The modifier to indicate that the input is for a previously defined subregion.

subrgn The fracture subregion for which the input is specified. The subregion must have been previously specified with a **LOCATE MOVE FRAC** command.

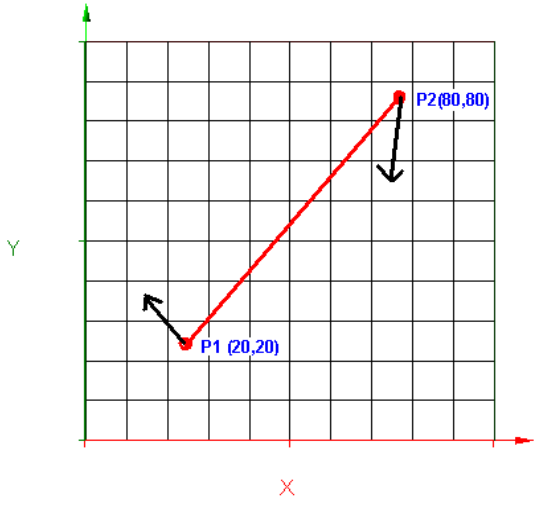
N1 The input pertains to the N^{th} point defining the plane in order in which the points are specified by the **LOCATE MOVE FRAC** command. N1 can only be 1 or 2 for a 2D fracture. For 3D, N1 is between 1 and the number of points defining the fracture plane.

X| Y| Z The input is specified for the corresponding x, y or z coordinates of the **N1** 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.)

COMMAND **MULTIPHASE**

PURPOSE 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.

MODE 1: **The Brooks & Corey Soil Characteristic**

SYNTAX **MULT {BROO}[SATU | COND] [BURD | MUAL] [COMP] [phase] {λ, Ψ_a} [S_r,, S_g, k_{rmin}] [subrgn]**

BROO The fluid phase saturation and the capillary pressure are related according to the Brooks and Corey expression given below.

$$\hat{S}^n = (\psi_a / \psi^n)^{\lambda} \; ; \; \psi > \psi_a$$

$$\hat{S}^n = 1 \; ; \; \psi \le \psi_a$$

$$\hat{S}^1 = \frac{S^1 - S_r}{1 - S_r - S_g} ; \quad \hat{S}^2 = \frac{S^1 + S^2 - S_r}{1 - S_r - S_g} ; \quad \hat{S}^3 = 1$$

$$\psi^n = P^n - P^{n+1}$$

$$\sum_{n=1}^{N} S^n = 1$$

In these relations, the superscript "n" denotes the n^{th} fluid phase, $\hat{S}$ is the normalized satuation, Ψ is the capillary pressure, P is the computed fluid pressure, and Ψ_a, λ, 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 appliy to a 2 phase system except that the 2^{nd} (rather than the 3^{rd}) 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 equqtions given below. This is the default option.

$$k_r^n = (\hat{S}^n - \hat{S}^{n-1})^2 \, [\, (\hat{S}^{n-1})^{(1+2/\lambda)} - (\hat{S}^n)^{(1+2/\lambda)} \,] ; \quad n > 1$$

$$k_r^1 = (\hat{S}^1)^{(3+2/\lambda)} ; \quad n = 1$$

MUAL The relative conductivity, k_r, is computed from the Mualem (1976) model which leads to:.

$$k_r^n = (\hat{S}^n - \hat{S}^{n-1})^{1/2} \, [\, (\hat{S}^{n-1})^{(2+2/\lambda)} - (\hat{S}^n)^{(2+2/\lambda)} \,] ; \quad n > 1$$

$$k_r^1 = (\hat{S}^1)^{(5/2+2/\lambda)} ; \quad n = 1$$

COMP If the modifier **SECO**nd is also present then k_r for the second phase is computed from the complimentary function:

$$k_r^2 = 1 - k_r^1$$

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.

S_r An empirical fitting constant (≥ 0) sometimes also called the residual saturation for the porous matrix.The default value is 0.

S_g 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.

$$\hat{S}^n = \frac{1}{\left[1+\left(\alpha\,\psi^n\right)^N\right]^M} \quad ; \quad \psi^n > 0 \quad ,$$

$$\hat{S}^n = 1 \quad ; \quad \psi^n \le 0$$

$$\hat{S}^1 = \frac{S^1 - S_r}{1 - S_r - S_g}; \quad \hat{S}^2 = \frac{S^1 + S^2 - S_r}{1 - S_r - S_g} \quad ; \quad \hat{S}^3 = 1$$

$$\psi^n = P^n - P^{n+1}$$

$$\sum_{n=1}^{N} S^n = 1$$

In these relations, the superscript "n" denotes the n^{th} fluid phase, $\hat{S}$ is the normalized satuation, **Ψ** is the capillary pressure, P is the computed fluid pressure, and **α**, 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 appliy 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.

$$k_r^n = (\hat{S}^n - \hat{S}^{n-1})^{1/2}\,[\,\{1-(\hat{S}^{n-1})^{1/M}\}^M - \{(1-(\hat{S}^n)^{1/M}\}^M\,]^2 \; ; \quad n>1$$

$$k_r^1 = (\hat{S}^1)^{1/2}\,[\,\{1-\{(1-(\hat{S}^1)^{1/M}\}^M\,]^2 \; ; \quad n=1$$

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.

$$k_r^n = (\hat{S}^n - \hat{S}^{n-1})^{2}\,[\,\{1-(\hat{S}^{n-1})^{1/M}\}^M - \{(1-(\hat{S}^n)^{1/M}\}^M\,]^{1/2} \; ; \quad n>1$$

$$k_r^1 = (\hat{S}^1)^{2}\,[\,\{1-\{(1-(\hat{S}^1)^{1/M}\}^M\,] \; ; \quad n=1$$

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 **α** (> 0) of the above equation. There is no default value for this input.

S_r An empirical fitting constant (≥ 0) sometimes also called the residual saturation for the porous matrix.The default value is 0.

S_g 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.

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; Alf=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_1, ..., 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 **COND**UCTIVITY 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 **SCAL**E 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

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_r
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) ! 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

$$\hat{S} = \frac{C}{C + [\exp(\alpha\psi)]^N - 1} \quad ; \quad \psi > 0$$

$$\hat{S} = 1 \quad ; \quad \psi \le 0$$

LOGA Saturation is a logarithmic function of Ψ given in below equation (*) as

$$\hat{S} = \frac{C}{C + [\ln(\alpha\psi)]^N} \quad ; \quad \psi > 1/\alpha$$

$$\hat{S} = 1 \quad ; \quad \psi \le 1/\alpha$$

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 specifciaiton.

EXAMPLES

MULTiphase EXPOnential characteristic: N=2., alpha=0.2
MULTiphase LOGArithmic relation: n = 1.0, alpha = 1, C=200, sr=0.05, sg=0.

MODE 5: **Capillary Pressure as a Polynomial Function of Saturation**

SYNTAX **MULT {POLY} [phase] {A, B, C, D, E} [S_r, S_g, k_{rmin}] [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, S_r in the definition of the normalized of satuation (see Mode 1)

E The residual saturation, S_g of the above equation (≥ 0), for the exponential or logarithmic relations, or 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_{rmin} The minimum value of k_r. The default value is 10^{-6}.

subrgn See Mode 1 specifciaiton.

EXAMPLES

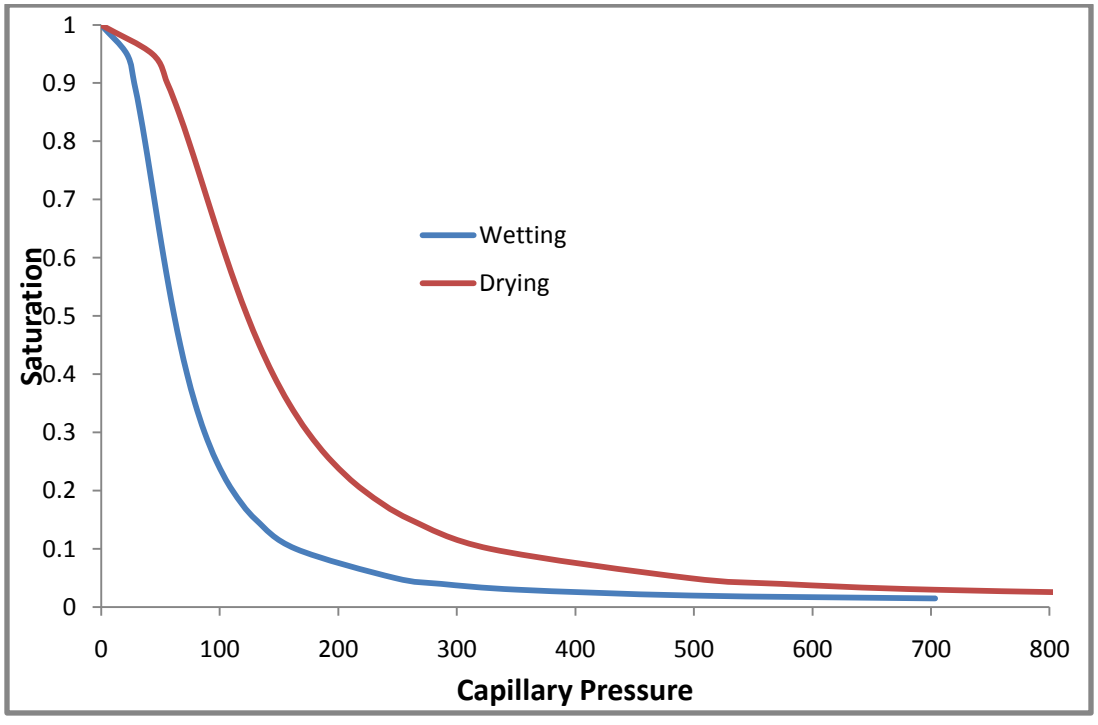
MULTiphase POLYnomial: a = 1., b = -1.
MULTiphase POLYnomial: a=10, b=-5., c=-2.5, d=-1.5, e=-1, sr=0.1, sg=0.05

MODE 6: **Tabulated Saturation Characteristic with Hysteresis**

SYNTAX **MULT {TABL} [HYST] {N_{sets}} {fname | N_1, ..., N_n | fname} [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, **Ψ**. **See comments below.**



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 Ψ and drying Ψ).

N_1 The first value of S (≥0) for the S- Ψ characteristic.

N_2 The first value of ψ 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 ψ for drying cycle.

N_4,..., N_n The sets of values of S, Ψ_{wet}, Ψ_{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}**.

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.

COMMENTS

Capillary pressure as defined in ACRI Software Tools is the negative of the commonly sued soild moisture potential that is defined as a negative quanity. 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 separta4ely specified. Care must be taken that if an analytical form (such as van Genuchten) realtion is specified, then it must specify the modier COND on the command and that the characteristic curve speciied here uis not overwritten.

EXAMPLES

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_r
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) ! Ψ vs. k_r
MULTi COND vs HEAD: TABLe of 40 sets from file 'SVSKRH'

MODE 7: **Saturation as a Function of Temperature**

SYNTAX **MULT {WHEE} {λ, T_d} [S_r, S_g] [subrgn]**

WHEE Saturation relation is that of Wheeler (1973) equation as shown below

$$\hat{S} = \frac{1}{\left[1+\left(T_F - T\right)/T_D^{\lambda}\right]} \quad ; \quad T \le T_F$$

$$\hat{S} = 0 \quad ; \quad T > T_F$$

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 λ is an empirical power-law exponent. The normalized saturation is deinfed in Mode 1 of this command.

λ The exponent, **λ**, 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 specifciation)

S_g An empirical fitting constant S_g in the definition of the normalized saturation (see Mode 1 specifciation)

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

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 specifciaiton.

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_{rmin}] [COMP] [phase] [subrgn]**

COND The input is for the relative hydraulic conductivity, k_r.

POLY k_r is a 4^{th}-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_{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 specifciaiton.

EXAMPLES

MULTiphase POLYnomial: a = 1., b = -1., C=0.5, D=-0.5

MODE 10: **Relative Hydraulic Conductivity as a Function of Capillary Pressure.**

SYNTAX **MULT {COND} {EXPO | LOGA | INVE} [COMP] [phase] {N, α} [C] [S_r, S_g, k_{rmin}] [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

$$k_r = \frac{C}{C + [\exp(\alpha\psi)]^N - 1} \quad ; \quad \psi > 0$$

$$k_r = 1 \quad ; \quad \psi \le 0$$

LOGA Relative conductivity is a logarithmic function of Ψ as defined by the below equation

$$k_r = \frac{C}{C + [\ln(\alpha\psi)]^N} \quad ; \quad \psi > 1/\alpha$$

$$k_r = 1 \quad ; \quad \psi \le 1/\alpha$$

INVE Relative conductivity is an inverse power law function of Ψ as shown by below equation

$$k_r = \frac{C}{C + [\alpha\psi]^N} \quad ; \quad \psi > 0$$

$$k_r = 1 \quad ; \quad \psi \le 0$$

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_{rmin} 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

MULTiphase EXPOnential CONDuctivity characteristic: N=2., alpha=0.2
MULTiphase LOGArithmic CONDuctivity: n = 1.0, alpha = 1, C=200.
MULTiphase CONDuctivity INVErse power law: N=2., alpha = 0.05, C=1.
MULTiphase 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] {Q_m} [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.

Symbol	Description of Corresponding Option
DISA	The specified option(s) listed below is (are) deactivated
EVAP	The droplets evaporate during move. The option is active by default.
DRAG	The droplets undergo drag during move. The option is active by default.
OUTP	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.

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 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 **ABSO**LUTE 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 **ABSO**LUTE 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_{Set} and N_{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_{Sets} value.

N_{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_{Sets} value.

T_{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_{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_{Sets} value.

N_{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_{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_{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.

Symbol	Description of corresponding datatype
X	The X-coordinate location of the droplet is specified
Y	The Y-coordinate location of the droplet is specified
Z	The Z-coordinate location of the droplet is specified
M	Element number for the location of the droplet is specified
I	Grid index I for the location of the droplet is specified
J	Grid index J for the location of the droplet is specified
K	Grid index K for the location of the droplet is specified
N	The corresponding field is not processed
Skip	The corresponding field is not processed
Dia	The diameter of the droplet, in microns, is specified
Φ	The property denoted by the symbol **Φ** is specified. Any of the properties listed in Table 2.8.1-3 may be specified.

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, 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, or 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_{Set} sets is assumed to be the same. The number of droplets in the n^{th} set, N_n, is computed as:

$$N_n = \frac{Q_m}{\rho_l \sum_{n=1}^{N_{Set}} \frac{\pi}{6} d_n^3}$$

Here Q_m is the injected mass, N_{Set} is the number of sets, ρ_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_{Set} sets and the number of droplets in the n^{th} set is computed as:

$$N_n = \frac{Q_m}{N_{Set}\, \rho_l \frac{\pi}{6} d_n^3}$$

fname The name of the file containing the droplet location and properties. The file must contain N_{Set} records. Each record must have then same number of values in the same order as the **datatype** symbols on the command.

N_1,.., N_n The data for the droplets if a file name is not specified. N_{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.

REMARKS

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} m).

EXAMPLES

NOZZle DROPlets q_fuel= 0.02, 500 records; data order: N I J K DIA U V W T file 'Droplets.NZL'
NOZZle DROPlets q_fuel= 0.02, 500 sets. ELEMents N I J K DIA U V W T file 'Droplets.NZL'
NOZZle with WATEr DROPlets q=0.02, 500 sets. ELEMents N I J K DIA U V W T file 'Droplets.NZL'
NOZZle DROPlets data on 'Nozz2D.FIL' q_fuel= 0.02, 500 records Data order is: DIA J I V U T
NOZZle DROPlets 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 DROPlets 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 DROPlets 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 DROPlets 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.

MODE 2: Nozzle Location and Injection Parameters (3D Geometry)

SYNTAX NOZZ {LOCA|DEGR} [FUEL|WATE] {X_o, Y_o, Z_o} {Q_m} {Rad, φ } {n_X, n_Y, n_Z,} {Θ_0, Θ_F} {d_{SMD}} {N_{Ray}} [option] [[ABSO] RATE=Q_{Evap}] [STAR=t_{Start}] [STOP=t_{Stop}] [STOR=N_{Stor}] [TEMP=T_{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.

φ 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_0, 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 **NOZZ**LE command with **DIST**RIBUTION 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 **NOZZ**LE command with **DIST**RIBUTION modifier. There is no default value.

The location of each of these droplets is computed so as to cover the total discharge area of the nozzle in a uniform manner. The droplet velocity of each droplet is computed in succession for each sub-ray from the **N_{Vel}** values of spray velocity distribution.

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 **ABSO**LUTE 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 **ABSO**LUTE 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 **STAR**T 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 N_{Ray} but before the location of N_{Vel}.

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 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 N_{Set} and N_{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 N_{Ray} but before the location of N_{Vel}.

N_{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 applications; a warning is printed if droplets remain unevaporated even at the end of N_{Stor} 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 N_{Ray} but before the location of N_{Vel}.

T_{NZL} 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.

N_{Vel} The number of values ($\geq$**I**) in the spray velocity distribution. There is no default value.

$V_1,..V_{nvel}$ Spray velocity distribution; the specified number of values must equal N_{Vel}**.** 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.

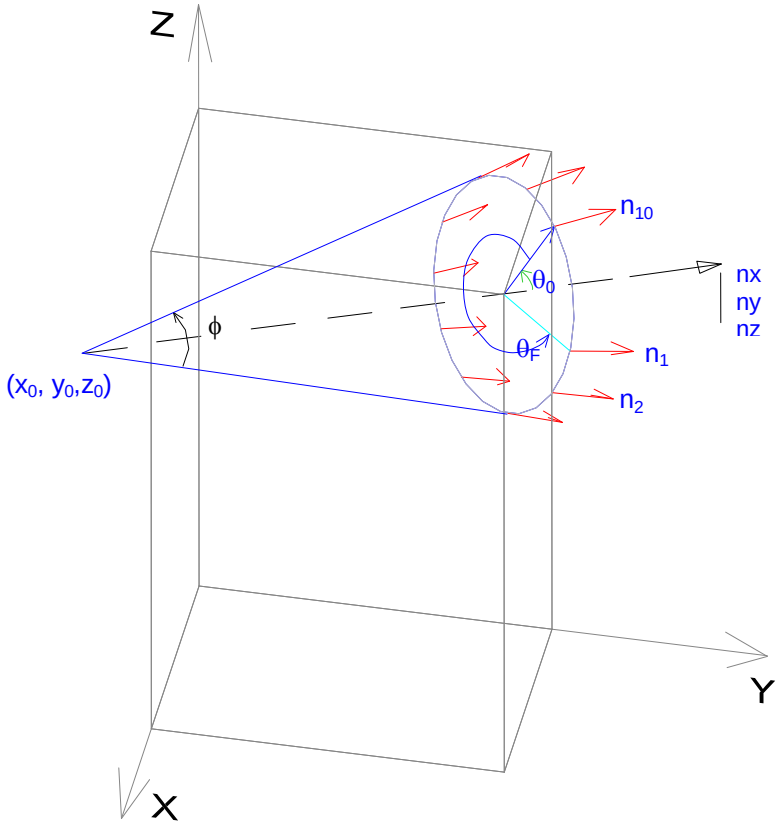
COMMENTS

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 **DISTR**IBUTION 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 **DISTR**IBUTION command and 10 rays (N_{Ray}) 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 (d_{SMD}) 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 $1/70^{th}$ of the total injected fuel (Q_m).

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 (Θ_0, Θ_F) are 45 and 315, then the 1^{st} through the 10^{th} 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 is determined by the N_{Vel} values of velocity distribution ($V_1,..V_{nvel}$), the N_{Ray} values of the number of rays and the N_{subray} values on the NOZZLE **DISTR**IBUTION command. The starting velocity of each droplet is computed from the logic given below.

```
IV   = 0
do n = 1, NRay
     do ns = 1, Nsubray
          IV  = MOD(IV, NVel) +1
          Vdroplet(n,ns) = Vspecified(IV)  !Vspecified ()= V1,..Vnvel
     enddo
enddo
```



Schematic of the Nozzle and Corresponding Input Parameters

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] {X_o, Y_o} {Q_m} {H_0, φ} {n_X, n_Y} {d_{SMD}} {N_{Ray}} [option] [[ABSO] RATE=Q_{Evap}] [STAR=t_{Start}] [STOP=t_{Stop}] [STOR=N_{Stor}] [TEMP=T_{NZL}] {N_{Vel}} {N_1,..N_n}**

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.
X_o, Y_o	The x, and y coordinates of the location of the nozzle. There is no default value.
Q_m	The mass flow rate injected through the nozzle. There is no default value.
H_0	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.
n_X, n_Y	Direction cosines of nozzle orientation in the X and Y directions, respectively). There is no default value.
d_{SMD}	Same as Mode 2.
N_{Ray}	Same as Mode 2.
option	Same as Mode 2.
ABSO	Same as Mode 2.
RATE	Same as Mode 2.
Q_{Evap}	Same as Mode 2.
STAR	Same as Mode 2.
T_{Start}	Same as Mode 2.
STOP	Same as Mode 2.
T_{Stop}	Same as Mode 2.
STOR	Same as Mode 2.
N_{Stor}	Same as Mode 2.
TEMP	Same as Mode 2.
T_{NZL}	Same as Mode 2.
N_{Vel}	Same as Mode 2.
N_1,.., N_n	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 **NOZZ**LE command with **LOCA**TION or **DEGR**EE 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 (d_{SMD} specified by **NOZZ**LE command with **LOCA**TION or **DEGR**EE 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 **NOZZ**LE command that precedes this command will use the previously supplied (or default) droplet distribution. Thus each Mode 2 or 3 **NOZZ**LE 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_{Biegin}, 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 **NOZZ**LE 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 **NOZZ**LE 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_NOZLLE.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 **NOZZ**LE **FREQ**UENCY 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=α_{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, α_{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.

α_{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=δ_{Tmax}]** **[EVAP=δ_{qmax}]** **[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.

δ_{Tmax} 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.

δ_{qmax} 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 **INIT**IAL, **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:

$$Q_f = C_D \rho \sqrt{\frac{2 (P_B - P)}{\rho}} A_B$$

Where Q_f 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_f is the computed pressure in the flow field interior to the boundary and ρ 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_j as its vector components, the velocity components, v_j, at the element face are computed from:

$$v_j = \frac{Q_f}{\rho} \frac{|A_j|}{A}$$

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|PRESS 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

COMMAND **OPTION**

PURPOSE To select or modify built-in default options.

MODE 1: **Geometry, Interpolation and Solver Options**

SYNTAX **OPTI [NEW|OLD] [QUAD|VOLU] [INTE] [ROBU]**

NEW 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. This is the default option.

OLD **Use of this modifier is not recommended.** 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.

QUAD 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. This modifier is effective only if the **OLD** modifier is not present..

VOLU The values of a field variable at the element interface are computed as a volume-weighted function of the two nearest element values. This modifier is effective only if the **OLD** modifier is not present.

INTE 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.

ROBU 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.

EXAMPLES

OPTIon NEW geometry computations with QUADratic interpolation

MODE 2: Mach Number Computation Options

SYNTAX OPTI {MACH} {SONI|GAMM|T|GAS} [V_1]

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 SONI**C command. This is the default option unless **COMP**RESSIBLE or **REAC**TION command is specified.

GAMM The Mach number is computed from the relation:

$$Ma = \frac{V}{\sqrt{\gamma C_p \frac{P}{\rho}}}$$

Here V is the fluid speed, **γ** 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 ρ is the gas density. The **γ** can be specified by **N1** or the **GAS GAMM**A 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:

$$Ma = \frac{V}{\sqrt{\frac{R}{C_p - R} C_p T}}$$

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:

$$Ma = \frac{V}{\sqrt{\frac{C_p}{C_p - R} \frac{P}{\rho}}}$$

Here V is the fluid speed, R is the gas constant, C_p is the specific heat, P is the pressure and ρ is the gas density. R is computed from the mass fractions and molecular weights of the gas components. This is the default option if **COMP**RESSIBLE or **REAC**TION command is specified.

V_1 The sonic speed if the **SONI** modifier is present; the default value is 300. The specific heat ratio **γ** if the **GAMM** modifier is present; the default value is 1.4.

EXAMPLES

OPTIon MACH number from GAMMA

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

OPTIon 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 10^6 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 **ENTHaply** 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 **OPTI [OUTL] [OFF|VELO]**

OUTL *For all incompressible flow simulations and for steady state compressible flow simulations, the flow at **OUTL**ET 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 **OUTL**ET 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 **OUTL**ET modifier for the **ANSWER™** Software Tool.

VELO By default the corrections relating to the **OUTL**ET 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 **OUTL**ET modifier for the **ANSWER™** Software Tool. **The use of this modifier is not generally recommended.**

EXAMPLES

OPTIon OUTLET VELOCITY from convective flux

MODE 6: **Salt Dissolution Options**

SYNTAX **OPTI {SALT} [FORC|CONS|VELO|OFF] [Z_{min}] [Z_{max}] [α] [β]**

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 Nu_e, Nu_{fc} and Nu_{nc}, respectively, the effective, the forced convection and the natural convection Nusselt numbers, the forced convection enhancement is based on the correlation:

$$(Nu_e)^3 = (Nu_{fc})^3 + (Nu_{nc})^3$$

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 Nu_{fc} is given by:

$$Nu_{fc} \propto [V\ R]^{0.8}$$

We may further assume that the characteristic velocity, V, is related to the injection velocity, **β**, and the radius, R as:

$$V \propto \frac{\beta}{R^2}$$

From these equations, we obtain:

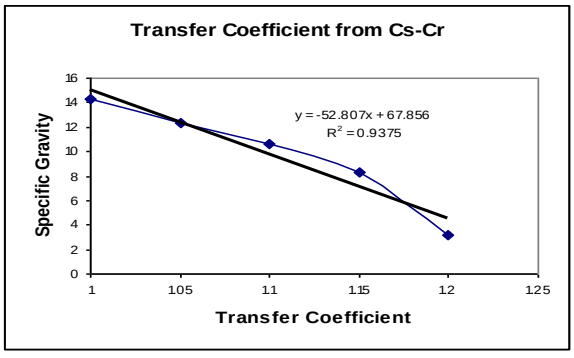
$$\frac{Nu_e}{Nu_{nc}} = \left[1+\left(\frac{C\,V^{0.8}}{R^{0.8}\,Nu_{nc}}\right)^3\right]^{1/3}$$

We write the Nu_{nc} as:

$$Nu_{nc} = \frac{h_{nc}\,L}{\Gamma} = \frac{q\,L}{\Gamma\,\Delta C_s};\quad h_{nc} = \frac{q}{\Delta C_s}$$

Where, h_{nc} is a transfer coefficient, L is a characteristic length, **Γ** is a diffusivity, q is the mass transfer rate and ΔC_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:

$$Nu_{nc} = \frac{L}{\Gamma}(67.856 - 52.807C_s)$$



Therefore the forced convection enhancement factor, f_{fc}, can be written:

$$f_{fc} = \frac{Nu_e}{Nu_{nc}} = \left[1+\left(\frac{\alpha\ \beta^{0.8}}{R^{0.8}\ L\ (67.856-52.807C_s)}\right)^3\right]^{1/3}$$

The constant of proportionality,**α**, 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 representatives cavern velocity. The enhancement factor is computed from:

$$f_{fc} = 0.98077 - 5.15405V + 74.73588V^2 - 108.98371V^3; \quad V > 0.008467; \quad f_{fc} \le 4$$
$$= 1; \quad V \le 0.008467$$

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**.

α The forced convection enhancement constant if the modifier **FORC** or **CONS** is present.

β 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

OPTIon SALT FORCed convection with Zmin=0. Zmax = 200, alpha=100, beta=5
OPTIon SALT CONStant enhancement factor for Zmin=0. Zmax = 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|Q_f] [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 COOR**dinate or **LOCATE LIST** command). Volume type of subregions specified with a **LOCATE** command with **FIELd**, **STATion** or **CORR**elation 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** boundayf, 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 m^{th} port, Q_m is computed from:

$$Q_m = Q_{out} \frac{\sum_{n=1}^{N}\sum_{i=1}^{3}(\rho\, u_i\, A_i)_m}{\sum_{m=1}^{M}\sum_{n=1}^{N}\sum_{i=1}^{3}(\rho\, u_i\, A_i)_m}$$

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 area vectors, u and A, and the density, ρ, 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:

$$Q_m = Q_{out} \frac{\sum_{n=1}^{N} A_{n,m}}{\sum_{m=1}^{M}\sum_{n=1}^{N} A_{n,m}}$$

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: $Q_m = Q_f$.

Q_f 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:

$$Q_m = Q_{out} \frac{Q_f}{\sum_{m=1}^{m=N} Q_f}$$

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

OUTLet at X+ boundary of ID=DOMAIN equal to X- boundary of ID=DOMAIN
OUTLet flow at X+ boundary of ID=OUTLET to be equal to X- boundary of ID=INLET
OUTLet 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 **ρ**, 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

OUTLet SOURCE type at ID=OUTLET divide by VOLUME
OUTLet SOURCE type at X+ of ID=OUTLET divide by FLUX
OUTLet 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

OUTLet OFF at X- boundary for subregion ID = OUTFlow

COMMAND **OUTPUT**

PURPOSE To select the field arrays to be written to the standard output device and to specify the extent, manner and frequency of output.

MODE 1: **Output of Phase Space Variables**

SYNTAX **OUTP [Φ] [plane|TABL] [ADD] [STAN|fname] [subrgn] [STAT|NOST|NOTA] [NARR|WIDE] [TIME] [V_{frq}] [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 **SOLV**E 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., YX, ZX, ZY, RX, RY, RZ and ZR**. The strings **XY, YX, XR** and **RX** all denote the xy plane, **YZ, ZY, RZ** 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 liner columnar table of values ordered by element numbers, the default mode for unstructured grids.

ADD One **OUTP**UT command is activated by default. If the **ADD** modifier is present, then the specified command is added to the list of active **OUTP**UT 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 **OUTP**UT command with an **ADD** modifier, then this file is uniquely attached to a unit for output from that command and any subsequent **OUTP**UT 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 OUTP**UT 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 **STAN**DARD modifier is subsequently specified, then the previous file is closed and all subsequent output from **all OUTP**UT 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 **LOCA**TE command). **If any other type of subregion is specified, then the TABL**E **mode (MODE 2) of the command is automatically invoked.** For **TABL**E 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.

WIDE The output tables are produced in a 132-column (wide) format. This is the default mode.

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 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 **SOLV**E command is given. It then enables the output of the current value of specified variable(s) immediately. After the 1st **SOLV**E 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 **SOLV**E command.

NOW If this modifier is specified before the 1st **SOLV**E 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 **SOLV**E 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 **IMME**DIATE modifier or at the frequency determined by **Vfrq**.

OFF Output for any previous command(s) for the same **subrgn** and type (**plane** or **TABL**E) is subsequently suppressed.

COMMENTS

If no **OUTP**UT 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 OUTPUT 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.

EXAMPLES

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 TABLes 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] [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.

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 **OUTP**UT 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.

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 **IMME**DIATE 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 the1st **SOLV**E 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**E) and

same combination of **COND, DIFF, STOR, SOUR, MATR,** and **RESI** modifiers is subsequently suppressed.

COMMENTS

This mode of the **OUTP**UT 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 (V_{frq} 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

OUTPut: for U and P of DIFFusion coefficients at the final stage
OUTPut: for T DIFFusion, coefficients NOW and the end to file = 'DIFFUSION.T'
OUTPut: for T STORage and MATRix coefficients NOW (at the next step)
OUTPut: for T CONDuction, STORage, SOURce, MATRIx and RESIDUe at step number 52 ONLY
OUTPut: for C: SOURce at step number every 52 steps
OUTPut: in TABLE format of MATRIX for T and P at frequency of 75 steps
OUTPut: of RESIdue for T at the end

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] [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.

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.

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 **IMME**DIATE 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 the1st **SOLV**E 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**E) and same combination of **FLUX, CONV, DIFF** and **TOTA**L modifiers is subsequently suppressed.

COMMENTS

This mode of the **OUTP**UT 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

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, φ_{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, ω, 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 2 D flow.

STRUCTURE Output of a "vorticity" structure variable, Ω, is obtained. It is defined as:

$$\Omega = -\frac{\partial u_1}{\partial x_2}\frac{\partial u_2}{\partial x_1} \quad \text{for 2D}$$

$$= -\frac{\partial u_1}{\partial x_2}\frac{\partial u_2}{\partial x_1} - \frac{\partial u_2}{\partial x_3}\frac{\partial u_3}{\partial x_2} - \frac{\partial u_3}{\partial x_1}\frac{\partial u_1}{\partial x_3} \quad \text{for 3D}$$

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, τ_{ij}, is obtained, where:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\sum_k \frac{\partial u_k}{\partial x_k}\right) - \delta_{ij}\, p$$

Here **μ** is viscosity and p 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 **μ** is the viscosity and **ρ** is the density. There are 3 components for 2D and 6 for 3D flow.

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.

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 **TABL**E) 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] [STAN|fname] [subrgn] [STAT|NOST|NOTA] [NARR|WIDE] [TIME] [V_{frq}] [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:

$$Q_{\Phi S} = Q_{\Phi} - Q_f \Phi$$

Here $Q_{\Phi S}$ 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.
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 **TABL**E) 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 **TRAN**SPORT, **DIST**RIBUTION or **RETA**RDATION 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 N_2 per mole of O_2. 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 **BOUN**DARY command with a corresponding boundary index (X-, X+ or 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 **LOCA**TE 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 **PERI**ODIC command.

option	INTERPRETATION
LINE	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.
CYCL	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**
Φ	**One or more (≤ 54)** symbols that denote the variables, which are periodic (or not periodic if **OFF** modifier is specified) at the θ_1 and θ_2 boundaries. By default all variables are assumed to be periodic.
OFF	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.
PRES	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.

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] [Ψ, 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 **BOUN**DARY command with a corresponding boundary index (X-, X+ or 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 (**θ**) direction of a cylindrical coordinate system. At times a problem which is periodic in cylindrical (x, r, **θ**) 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 **θ**=θ_1 and **θ**=θ_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.

Ψ The angle of periodicity, **Ψ**, 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] [V_1, …, V_9]**

X|Y|Z The boundary conditions for the corresponding x, y or z direction boundaries are determined automatically from the requirement of periodicity. A **BOUN**DARY command with a corresponding boundary index (X-, X+ or Y-, Y+, or 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:

$$\begin{bmatrix} U2 \\ V2 \\ W2 \end{bmatrix} = \begin{bmatrix} n1 & n2 & n3 \\ n4 & n5 & n6 \\ n7 & n8 & n9 \end{bmatrix} \bullet \begin{bmatrix} U1 \\ V1 \\ W1 \end{bmatrix}$$

STAC The velocity vector at the identified periodic boundaries is transformed according to the transformation specified in the most recent **STAC**K **TRAN**SFORMATION command.

option See Mode 1 specification.

V_1,..V_9 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 -1
0 1 0

PERIodic boundaries in Z Velocity TRANsformed by:
1.0 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. 0.00.0 0.995004 -0.09983340.0 0.0998334
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 [L^2]. The SI units are [m^2]. 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[ξ]} {N_1, N_2, .., 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.

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.

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],

θ 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 **CARM**AN relationship diameter =**0.002** meters for the entire domain
PERMEABILITY from **CARM**AN relationship diameter =**0.002** m for **ID=POROUS** subdomain.
PERMEABILITY from **CARM**AN relationship diameter =**0.002** m with Cck= **150**.

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 temepratuire is specified. This is the default mode.

FREE Freezing temepratuire is specified.

T_{phase} The temperature at which phase change occurs. If **FREE** modifier is specified; then it is the freezing remperture with a default value of 0 ^{o}C otherwise it is the evaporation temperature with a default value of 100 ^{o}C.

EXAMPLES

PHASE change at **100** Degrees Celcius
PHASE change is **FREE**ZING 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:

$$T_s = T_0 + \frac{T_1}{A - \ln(P/P_0)} \quad ,$$

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:

$$P_s = P_0 \, Exp\left(A - \frac{T_1}{T - T_0}\right) \quad ,$$

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

T		P_s (pascals x 10^5)	
°C	K	Equation	Steam Tables
0	273.15	0.00594	0.00611
20	293.15	0.02309	0.02337
50	323.15	0.12260	0.12335
100	393.15	1.00539	1.0133
150	425.15	4.72619	4.7597
170	443.15	7.87248	7.9203
200	473.15	15.47723	15.5506
250	523.15	39.54853	39.776
300	573.15	84.61033	85.92
350	623.15	158.7037	165.37

EXAMPLES

PHASE Change according to default CLAPEYRON's relation
PHASE Change CLAPEYRON's equation: T0=45, T1=3841.1954, p0=131.57894, a1=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] [subrgn]**

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.

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 **Θ_T** and **Θ_D**, if specified, are ignored. Also for **ANSWER™** this command automatically triggers the inclusion of Brinkman-Forchheimer terms (**BRIN**K 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 **EFFE**CTIVE 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:

$$R_{\Phi} = \omega (\xi - \Phi) \quad (1)$$

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 **PREC {ELEM} {idreac} {Φ} {Ψ} {ω} {ξ} {C_{Sat}} [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 C_{Sat} as the solubility of the pure element, the solubility, C_S, in the presence of other elements is given by:

$$C_S = C_{Sat} \frac{\left(M_i^{liquid} + M_i^{solid}\right)}{\sum_{j=1}^{n}\left(M_j^{liquid} + M_j^{solid}\right)}$$

where M^{liquid} and M^{solid} 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 **Φ** precipitates to generate species **Ψ** or the species **Ψ** is converted to species **Φ** by uptake . The reaction rate is computed as:

$$Rate = \omega\ (C_S - \Phi)\ .$$

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 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 C_s.

C_{Sat} The solubility limit for the species (units of **Φ**) 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, ξ. If the species concentrations are in terms of mass units, then **SET LINE**AR command must be used to define ξ 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=V_{tol}] [NORM] [BASE=Φ_{basel}] [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.

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 **THET**A modifiers. It denotes the coordinate of locations at which the averages are computed. The **Z**, **R** or **THET**A can only be used for three-dimensional geometry. In this case is **R** = sqrt (y^2 +z^2) and **THET**A = 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: $S_i - V_{tol} \le S < S_i + V_{tol}$ 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}.

V_{tol} 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 the 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:

$$\Phi_{output} = \frac{\Phi_{computed} \quad \Phi_{base}}{\Phi_{norm} \quad \Phi_{base}}$$

where Φ_{base} and Φ_{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 Φ_{base} must be specified and, in this case, only one variable (**Φ**) must be specified on the command.

Φ_{base} The user specified value for Φ_{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 Φ_{norm} is taken to be arithmetic mean of the values for the sub-domain. If this modifier is present, then Φ_{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 Φ_{norm} is the arithmetic mean of the values for the sub-domain. If this modifier is present, then Φ_{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.

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 **Φ** should be the symbol **T** (for Temperature) and the base value, **Φ_{base}**, should be specified as the average inlet temperature (commonly called T3). The **Φ_{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: $S_i - V_{tol} \leq S < S_i + V_{tol}$ 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: **Forces and Moments for a Selected Variable at a Specified Location**

SYNTAX **PRIN [Φ] {FORC|MOME} [subrgn] [dir] [X_i] [Φ_0] [V_{freq}] [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:

$$F_i = \int (\Phi + \Phi_o)\, n_i \, dA$$

$$M_i = F_i \otimes (X_i - Y_i)$$

Where
F_i is the force vector for the **Φ** variable,
Φ_0 is a reference datum for the **Φ** 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 **Φ** variable,
$\otimes$ 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**E 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 elected. 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 **Φ**.If specified this must be the 3rd numerical value for 2D and 4th numerical value for 3D geometry. The default value is zero.

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 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, **V_{frq}** 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 **Φ** 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] [V_{frq}] [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.

option	INTERPRETATION
INLE	Boundaries specified by the **INLE**T command are selected.
OUTL	Boundaries specified by the **OUTL**ET command are selected.
OPEN	Boundaries specified by the **OPEN** command are selected.
IO	All boundaries specified by **INLE**T, **OUTL**ET or **OPEN** command are selected.
WALL	Walls specified by **WALL** or **BLOC**K command are selected.
EXTE	All external (or outer) boundaries of the computational domain are selected.
ALL	All of the above boundaries are selected.

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.

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.

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 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_{frq}** 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] [V_{frq}] [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.

option	INTERPRETATION
INLE	Boundaries specified by the INLET command are selected.
OUTL	Boundaries specified by the OUTLET command are selected.
OPEN	Boundaries specified by the OPEN command are selected.
IO	All boundaries specified by INLET, OUTLET or OPEN command are selected.
WALL	Walls specified by WALL or BLOCK commands are selected.
EXTE	All external (or outer) boundaries of the computational domain are selected.
ALL	All of the above boundaries are selected.

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.

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.

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 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 **V_{frq}** 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:

$$p = p_{computed} + \rho^* \sum_j (x_j^* - x_j) g_j$$

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} {ξ_o}**

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 terms 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:

$$S_i = \beta (\xi - \xi_o) g_i$$

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, **ξ** 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 **ρ** is the density of the fluid. If the working fluid is a gas and the perfect gas law applies, then **β** can be estimated from:

$$\beta = -\frac{\rho_o}{T_o}$$

where T_o is a reference temperature and ρ_o is a reference density. For air at atmospheric pressure and 300K, **β** ≈ -0.004 [Kg/(m^{3}K)]. For water at 300K, **β** ≈ -0.2 [Kg/(m^{3}K)].

ξ_o 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 **ξ** 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 **ALLO**CATE 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:

$$S_i = \{ \beta_1 (T - T_O) + \beta_2 (C - C_O) \} g_i$$

Then the **ALLO**CATE command can be used to specify a composite variable **ξ** with:

$$\xi = \beta_1 T + \beta_2 C; \quad \beta = 1.; \quad \xi_O = \beta_1 T_O + \beta_2 C_O$$

The composite variable, **ξ**, in turn can be defined by an appropriate **SET** command with the **ALWA**YS 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] [N_1, …, N_4]**

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.

N_1, .., N_4 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 [k_r] | 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:

$$K_i^{effective} = S_f K_i^{saturated}$$

where $K^{effective}$ is the hydraulic conductivity used in the governing equations, $K^{saturated}$ is the value specified by the user and S_f 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:

$$K_{dir}^{effective} = k_r K_{dir}^{saturated}; \quad S_f < 1$$

Where k_r is the relative conductivity for the dry soil and the subscript "dir" denotes the direction specified by **dir.**

k_r 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 **MULT**IPHASE 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 MULT**iphase **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

MODE 6: **Phase Change with Freezing and Thawing**

SYNTAX **PROB {FREEZ} [V_1]**

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.

V_1 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 pahse satuation is computed from enthalpy equation.

EXAMPLES

PROBlem with EVAPoration

MODE 8: **Phase Change with Thermodynamic Non-Equilibrium**

SYNTAX **PROB {EVAP} [DYNA] [FIXE] [C_m, δT, α, R_f]**

EVAP The Evaporation/condensation phase-change mode is selected.

DYNA 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),
Θ_E is the effective porosity
S is the saturation fraction of the fluid,
α 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**D 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.

R_f 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 boudns 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 soruce terms may be introduced in the approatie phase equations to control the pahse change.

EXAMPLES

PROBlem DYNAMIC EVAPORATION: Cm=0.01, dt=0.02, power=0.20, RF=0.5

COMMAND PROPERTY

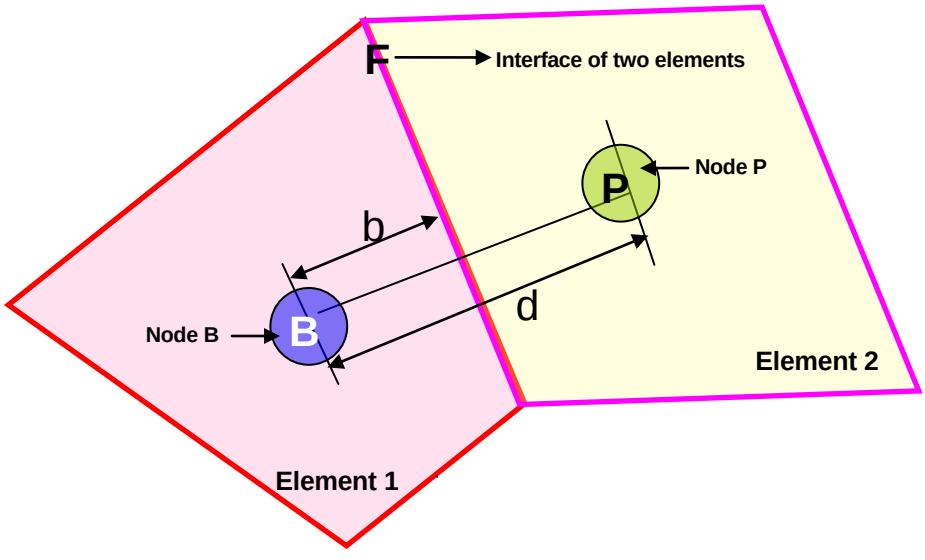
PURPOSE To specify the mode of calculation of fluid or material properties at an interface that lies between two elements where the properties are known at the element nodes.

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 figure below, the interface value of a property, Γ_f, is obtained from the node values, Γ_B and Γ_P, by:



$$\Gamma_F = \alpha \Gamma_P + \beta \Gamma_B$$

$$\alpha = \frac{b}{d}; \quad \beta = 1 - \alpha$$

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:

$$\Gamma_F = \frac{\Gamma_P \Gamma_B}{\alpha \Gamma_B + \beta \Gamma_P}$$

GEOM: The interface value is the weighted geometric mean of the values at nodes B and P which is computed as:

$$\Gamma_F = \Gamma_P^{\alpha} \Gamma_B^{\beta}$$

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 **HARM**ONIC 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:

$$\Gamma_F = \Gamma_P \Gamma_B \frac{\alpha S_P^{1/\lambda} + \beta S_B^{1/\lambda}}{\alpha S_P^{1/\lambda}\Gamma_B + \beta S_B^{1/\lambda}\Gamma_P}$$

λ The inverse of the power exponent of saturation if the **SATU**RATED **HARM**ONIC 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 **COND**UCTIVITY command). In **TIDAL™** software it is effective only for the thermal and species equations.

EXAMPLES

PROPerty at interface for all variables by arithmetic average
PROPerty for U use GEOMetric mean
PROPerty averages for T and C by UPWInd mean
PROPerty for C by MAXImum method
PROPerty 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 **TRAN**SPORT 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 DIST**RIBUTION **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 DIST**RIBUTION **command for interpretation of this modifier.**

COMMENTS

This mode of the PROPERTY **command must be specified before the TRAN**SPORT **command to which it applies; it will then apply to all TRAN**SPORT **commands that follow till the next PROP**ERTY **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 CO_2 and H_2O) 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[ξ]} {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.

MODE 4: **Specification of Surface Emissivity**

SYNTAX **RADI {EMIS} {func[ξ]} {N_1, N_2, .., N_n|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.

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.

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=σ]**

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 ≥ 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

σ 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.

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:

$$C_nH_m \rightarrow C_nH_{m-2} + H_2$$
$$C_nH_{m-2} + 1/2\, n\, O_2 \rightarrow n\, CO + 1/2\,(m-2)\, H_2$$
$$CO + 1/2\, O_2 \rightarrow CO_2$$
$$H_2 + 1/2\, O_2 \rightarrow H_2O$$

If this modifier is present, then the reaction mechanism is assumed to be:

$$C_nH_m + 1/2\ n\ O_2 \rightarrow n\, CO + 1/2\ m\ H_2$$
$$CO + 1/2\, O_2 \rightarrow CO_2$$

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_nH_m, CO, H_2, O_2, H_2O, CO_2, and N_2. For the 4-step system, an 8th species, C_nH_{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 **ARRH**ENIUS command. The EBU constants can be changed by the **EBU** command.

EXAMPLES

REACtive flow with default options
REACtion with TWO-step mechanism default options
REACtion process is KINEtically controlled
REACtion process; use default PRODuct relations; explicit reactions supplied later
REACtion for HYDRocarbon fuel; next commands explicitly supply the reaction details
REACtion 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] {Z_0, E, α, β, γ] [θ]**

idreac A unique identifier for the reaction rate. The reaction rate is computed as:

$$\text{Rate} = Z_0 \exp\left(-\frac{E}{R_u T}\right) \Phi_1^{\alpha} \Phi_2^{\beta} \Phi_3^{\gamma} T^{\theta}$$

where Z_0 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 Z_0 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 Z_o 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

option	INTERPRETATION
MASS	By default it is assumed that the computed **Φ**'s are in mass units and that **Z_0** is given in molar units. Therefore **Z_0** is internally converted to appropriate mass units. If this modifier is present, then no unit conversion is performed. It is assumed that **Z_0**is specified in appropriate units for the computed **Φ**'s.
CGS	By default, **Z_0** and **E** are assumed to be in specified SI (kg-mole - m^3 - J - K) units. If this modifier is present, then **Z_0** and **E** are assumed to be in the cgs (gm-mole – cm^3 - cal - 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.
LIFE	**Z_0** is in units of time [t] representing the half -life of the reaction. In this case **E** must be the activation temperature [T].
DECA	**Z_0** 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].

Z_0 The pre-exponential constant, Z_0. The specified value may be internally converted to appropriate units based on the **option** modifier. For example, in the CGS system, units are $cm^{3n-3}/moles^{n-1}$-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 **γ** 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 4^{th}, 5^{th} or 6^{th} numerical value depending on the order of the reaction (1, 2 ,or 3 reactants). The default value is 0.

EXAMPLES

REACtion R1 preexp=1.960E+18, activ_e=2.48E+04 FU ^ 0 and O2 ^ 0.5
REACtion R1 FU, O2 1.960E21 2.062E8 0.0 0.5 1.07 CGS EBU TEMP SELEcted subregion
REACtion R2 CH, O2, FU: 5.395E16, 2.50E04 0.0 0.9 1.18 -0.57 TEMP for ID=RGN1 active
REACtion R1 MASS based preexp=1.50, activ_T= 600 FU ^ 1 and O2 ^ 1
REACtion R1 MASS FU, O2 1.50 0. 1 0.5 1.07 EBU! No effect of temperature
REACtion R2 DECAy frequency FU: 2.00, 1000 1.0 for SELEcted region
REACtion 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, …., 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,…,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 N1 times N2 values must be specified with the command. There is no default value.

EXAMPLES

REACtion FAST chemistry; lookup table has 1000 rows and 5 columns on file ‘FAST_CHEM’
REACtion FAST chemistry 1000 rows & 5 columns values!!!! 5000 values must be specified)

MODE 4: **Empirical Constants for Fast-Chemistry Reaction**

SYNTAX **REAC {FAST} {CONS} {N_1, N_2}**

FAST The two-parameter PDF fast-chemistry reaction model is used.

CONS The empirical constants required for the fast-chemistry reaction are specified.

N_1 The constant C_{g1} **(>0)** for fast-chemistry reaction (see Jones and Whitelaw, 1982). The default value is 2.

N_2 The constant C_{g2} **(>0)** for fast-chemistry reaction (see Jones and Whitelaw, 1982). The default value is 2.

EXAMPLES

REACtion FAST chemistry CONStants: cg1 = 3.0
REACtion FAST chemistry CONStants: cg1 = 2.0 and cg2 = 3.0
REACtion 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. 3.3 for more information. There is no default file name; a file name must be specified.

fmt The modifier "**FORM**ATTED" or "**UNFO**RMATTED" 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 2.8.1-3 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 **SOLV**E 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 **REST**ART 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, OUTP**UT and **SOLV**E 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 **OUTP**UT 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 **REFE {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 φ 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 FREEZing 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/m^2) 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 (**HYDR**AULIC 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):

$$P = p_{computed} - p_{referencenode}$$

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 **ρ*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} {N_1, .., N_n}**

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:

$$C_p = \frac{P - P_{ref}}{0.5\,\rho\,V^2}$$

In the equation above, P is the computed pressure, P_{ref} is the pressure at the specified location, ρ 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**).

N_1, , N_n 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=N_1, Φ=N_2, ..., Φ=N_n] | [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.

N_1, .., N_n 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.

$$\Phi^{k+1} = \Theta\, \Phi^{computed} + (1-\Theta)\, \Phi^{k}$$

Where:

Φ^{k}	is the value at the k^{th} step (most recent previous value)
$\Phi^{computed}$	is the value computed from the numerical process at the $k+1^{st}$ step, and
Φ^{k+1}	is the value stored as the new value at the k+1th 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 **CONV**ERGENCE 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.

δV is the volume of the element at P

K is the grid node values at E,W,N,S,U and D respectevity.

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 wether 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 **STOR**AGE command

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] [V_{frq}] [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 **OUTP**UT Command) but with the extension changed to "SAV"' for the **BLOC**K and "_TABLE.SAV" for the **TABL**E 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 "**FORM**ATTED" or "**UNFO**RMATTED", 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 **GEOM**ETRY 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 **COMP**ACT modifier takes precedence over the **GEOM**ETRY 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.

REPL If multiple records are written due to the V_{frq} input or the **NOW** 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.

SEQU If **SEQU** modifier is present, then sequential files are written at a frequency determined by the V_{frq} input and the **NOW** 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 **NOW** input. Any extension specified with the file name 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.

subrgn This modifier is effective only for the **TABL**E 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.

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 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 **SOLV**E command is given. It then enables the output of the current value of specified variable(s) immediately. After the 1st **SOLV**E 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 **SOLV**E command.

NOW If this modifier is specified before the 1st **SOLV**E 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 **SOLV**E command. The output is always produced as soon as the command is encountered; this modifier is redundant.

ONLY 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 **NOW** or **IMME**DIATE modifier is present.

OFF Output for any previous command(s) for the same **subrgn** and type (**BLOC**K or **TABL**E) is subsequently suppressed.

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 UNFOrmatted 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 U in TABLe for subregion ID=DMNTable at TIME interval = 0.2 hours
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] [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.

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.

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 **IMME**DIATE 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 the1st **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 (**BLOC**K or **TABL**E)

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 (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 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 SAVE 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

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 **IMME**DIATE 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 the1st **SOLV**E 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 (**BLOC**K or **TABL**E) and same combination of **FLUX, CONV, DIFF** and **TOTA**L modifiers is subsequently suppressed.

COMMENTS

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] [V_{frq}] [IMME|NOW|ONLY|OFF]**

GRAD The tensor components of the gradients of velocity, φ_{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, ω, 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 2 D flow.

STRUCTURE Output of a "vorticity" structure variable, Ω, is obtained. It is defined as:

$$\Omega = -\frac{\partial u_1}{\partial x_2}\frac{\partial u_2}{\partial x_1} \quad \text{for 2D}$$

$$= -\frac{\partial u_1}{\partial x_2}\frac{\partial u_2}{\partial x_1} - \frac{\partial u_2}{\partial x_3}\frac{\partial u_3}{\partial x_2} - \frac{\partial u_3}{\partial x_1}\frac{\partial u_1}{\partial x_3} \quad \text{for 3D}$$

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, τ_{ij}, is obtained, where:

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\sum_k \frac{\partial u_k}{\partial x_k}\right) - \delta_{ij}\, p$$

Here **μ** is viscosity and p 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 **μ** is the viscosity and **ρ** 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.

REPL See Mode 1 specification.

SEQU See Mode 1 specification.

subrgn 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

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] [V_{frq}] [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:

$$Q_{\Phi S} = Q_{\Phi} - Q_f \Phi$$

Here $Q_{\Phi S}$ 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.

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 **TABL**E) 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 **TRAN**SPORT, **DIST**RIBUTION or **RETA**RDATION 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

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] [V_{frq}] [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 **REST**ART modifier to restart the computations for the same identical problem. Only the **SOLV**E command may be modified for the new simulations; all other input data must be identical to the run that generated the file. **REST**ART 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 **OUTP**UT 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 V_{frq} is interpreted to be the frequency 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 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 V_{frq} 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:

$$Q_{in} = a_1 * Q + a_2$$

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 **COOR**DINATE, **LOCA**TE, **SET** and **SOUR**CE 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] [$\Phi=V_1$, $\Phi=V_2$, ..., $\Phi=V_n$]

EFFE If the modifier **EFFE**CTIVE 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.

V_1, .., V_n 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.

COMMETNS

This input is only effective for the **ANSWER™** Software Tool.

EXAMPLES

SCHMidt number for fluid = 1.
SCHMidt number for FF = 0.5, FU = 0.7, CH = 0.7
SCHMidt number EFFEctive value for FF = 0.5

COMMAND SCREEN

PURPOSE To control the echo of diagnostic output obtained from the **DIAG**NOSTIC 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 (**DIAG**NOSTIC 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

COMMAND **SELECT**

PURPOSE To locate and identify a subregion or material type in the domain of computation for later input by one of the other commands.

COMMENTS

This command is identical in all respects to the **LOCA**TE command.

EXAMPLES

See **LOCA**TE 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]] {N_1, N_2, .., N_n | 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 (**ALLO**CATE 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.

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.

operation Available modifiers are **REPL**ACE, **ADD, SUBT**RACT, **MULT**IPLY, **DIVI**DE, **ABS, ABSOLUTE**, **POSI**TIVE and **NEGA**TIVE. 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** modfiiers. 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 **STAC**K **LOCATE** command.

COMMENTS

The primary purpose of the **SET** command is to specify the value of a dependent variable. Combinations of **ALLO**CATE 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 **BOUN**DARY command.

EXAMPLES

Generic examples for this command are given in Section 4.4. The keyword **SET** must replace the keyword used in these examples.

MODE 2: **Specification of a Variable on a Node by Node Basis.**

SYNTAX **SET {Φ} {NODE|STRU|UNST|fname} [V_1,..V_m] [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 **STRU**CTURED mode if the **subrgn** was defined with a **LOCA**TE command in terms of grid indices or in the **UNST**UCTURED 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 **LOCA**TE command which can be examined by including a file name on the **LOCA**TE command.

fname The name of the file for numerical values unless the values are directly specified by **V_1….V_m** below. See Section 3.3 for additional information.

V_1….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 **SOLV**E **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 2.8.1-3 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 **STRU**CTURED mode if the **subrgn** was defined with a **LOCA**TE command in terms of grid indices or in the **UNST**UCTURED 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 **LOCA**TE command which can be examined by including a file name on the **LOCA**TE 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 **SET {Φ_1, …, Φ_n} {NODE|STRU|UNST | fname} {V_1,..V_{nm}} [subrgn] [FIEL] [dir]**

Φ_1, …, Φ_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 (**ALLO**CATE 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.

NODE The **Φ** 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 **STRU**CTURED mode if the **subrgn** was defined with a **LOCA**TE command in terms of grid indices or in the **UNST**UCTURED mode otherwise.

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

Read (NUNIT, *) ((((VAR (L, I, J, K), L=1,n), I=ILO, IHI), J=JLO, JHI), K=KLO, KHI)

Where **NUNIT** is an internally assigned unit number, **VAR** is the set of variables denoted by **Φ**'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 **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 (L, M), L=1,n), M = MLO, MHI)

Where **NUNIT** is an internally assigned unit number, **VAR** is the set of variables denoted by **Φ**'s, **n** denotes the number of variables, 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 **LOCA**TE command which can be examined by including a file name on the **LOCA**TE command.

fname The name of the file (see Section 3.3) from which **V_1** through **V_{nmn}** are read.

V_1….V_{nm} The table of values that pertains to the variable values at each node selected by the **subrgn** and 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.

subrgn See Mode 1 specification.

FIEL See Mode 1 specification.

dir See Mode 1 specification.

EXAMPLES

SET by NODE following variables for ID=SUBRGN1! There are 3 nodes in this region)

U	V	T
10	–5	100
-10	+5	150
-10	+10	200

SET by NODE following variables for ID=SUBRGN1! There are 3 nodes in this region)

SKIP	SKIP	U	V	SKIP	T
0.2	0.2	10	–5	10.20	100
3.5	0.6	-10	+5	12.50	150
10	1.0	-10	+10	2.00	200

SET by NODE for ID=MIDDLE at X- boundary! 3 boundary nodes

(SKIP, SKIP, SKIP)	U	V	T
(0.2, 0.2, 0.2)	10	–5	100
(3.5, 0.6, 1.0)	-10	+5	150
(10., 1.0, 2.0)	-10	+10	200

SET by NODE ID=MIDDLE T, U, V 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** **{Φ} {SUM|LINE} [MASS] {ξ_1, …, ξ_n} [a_1, .., a_n] [a_0] [option] [mod] [ALWA] [subrgn] [FIEL]**

Φ See Mode 1 specification.

SUM The variable **Φ** is computed from:

$$\Phi = \sum_n \xi_n$$

LINE The variable **Φ** is computed from:

$$\Phi = \sum_n a_n \xi_n + a_0$$

MASS By default, the **ξ'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 **ξ's** are replaced by the total mass of the corresponding **ξ** variable. The total mass is equal to the quantity that appears in the accumulation term of the governing differential equation for **ξ** (see Chapter 2) multiplied by the volume of the element. In the presence of this modifier only those **ξ's** can appear on the right hand side for which differential equations are solved.

ξ_1, …, ξ_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 (**ALLOC**ATE 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, …, a_n The numerical constants and coefficients for the linear function. These values must be specified if the **LINE**AR modifier is present. With the **SUM** modifier these values must not be specified. There is not default value; appropriate number of values must be specified.

a_0 The datum for the linear function if **LINE**AR 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** **{Φ} {SQUA|ROOT} {ξ_1, …, ξ_n} [a_1, .., a_n] [a_0] [option] [mod] [ALWA] [subrgn] [FIEL]**

Φ See Mode 1 specification.

SQUA The variable **Φ** 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 **Φ** is computed from:

$$\Phi = \sqrt{\sum_n \xi_n^2} \quad \text{or} \quad \Phi = \sqrt{\max\left[\left(\sum_n a_n \xi_n^2 + a_0\right), 0\right]}$$

ξ_1, …, ξ_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 (**ALLO**CATE 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, …, 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] {Φ_1, …, Φ_n} {Nsets} {V_1,..V_m|fname} [DOMA=V_{domain}|NEAR=V_{near}] [option] [mod] [ALWA] [subrgn] [FIEL]**

DIST The Φ_n variables are computed from a inverse distance based interpolation function (here ξ_i is i^{th} value in the specified table for the corresponding variable, $x_{k,i}$ are its coordinates and **N** is the power to which the distance is raised):

$$\Phi = \sum_i \frac{\xi_i / r_i^N}{1/r_i^N} \quad ; \quad r_i^2 = \sum_k \left(x_k - x_{k,i}\right)^2$$

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).

Φ_1, …, Φ_n 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.

V_1….V_m 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 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 Φ_1 through Φ_n. The number of rows of the table must equal **Nsets**.

fname The name of the file (see Section 3.3) from which V_1….V_m are read.

DOMA The interpolation is restricted to the specified ξ_i that lie within the distance specified by V_{domain}. In the formula above any values where $r_i > V_{domain}$ 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 ξ_i determined by r_i. If this modifier is present and V_{near} is omitted or is < 1, then the nearest specified ξ_i 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

(3.5, 0.6, 1.0) -10 +5 150
(10, 1.0, 2.0) -10 +10 200
SET by 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
(3.5, 0.6, 1.0) -10 +5 150
(10, 1.0, 2.0) -10 +10 200 DOMAIN of influence=0.5
SET by DISTANCE interpolation for ID=MIDDLE from 5 values
(X, Y, Z) U V T
(0.2, 0.2, 0.2) 10 –5 100
(3.5, 0.6, 1.0) -10 +5 150
(10, 1.0, 2.0) -15 +10 200
(10, 2.0, 2.0) -20 +15 250
(10, 5.0, 2.0) -10 +10 300 interpolate from NEAREST 3
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' ALWAYS ADD POSITIVE to existing

MODE 8: Specification of Values from Total Inventory

SYNTAX SET {Φ} {INVENT} [subrgn] {Q} [VOLU | UNIF | SCAL] [ADD]

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 equations a solved. There is no default value; a symbol must be specified.

INVENT The total inventory or amount of the property, **Φ**, is specified. The inventory, Q, for a subregion is defined as:

$$Q = \sum_{subrgn} \alpha_i \ \Phi_i \ \delta V_i$$

Here Q the subscript "i" denotes the values for an element, **α** is the accumulation coefficient for the transport equation, and **δV** 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, **Φ**.

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:

$$\Phi_i = \theta \Phi_i^o + \frac{1}{\alpha_i} \frac{Q}{\sum_{subrgn} \delta V_i}$$

Here Φ_i^o is the existing value of variable, and **θ** = 0 by default but is set to 1 if modifier **ADD** is present.

UNIF The inventory is distributed so that the increment in **Φ** is uniform and constant:

$$\Phi_i = \theta \Phi_i^o + \frac{Q}{\sum_{subrgn} \alpha_i \delta V_i}$$

SCAL The inventory is distributed proportional to the existing value of **Φ**:

$$\Phi_i = \theta \Phi_i^o + \frac{Q \Phi_i^o}{\sum_{subrgn} \alpha_i \Phi_i^o \delta V_i}$$

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.

ADD By default the specified inventory replaces any existing value; that is the constant **θ** = 0 in the above equation. If this modifier is present, then the inventory is added to the existing value; that is **θ** =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 (**ALLO**CATE 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:

$$Q = \lambda \sum_{\substack{\text{subrgn1} \\ \text{(Donor)}}} \alpha_i \, \Phi_i^o \, \delta V_i$$

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:

λ = 1 by default if **β** is not specified.
λ = min (**β,** 1) if **β** is specified but **TIME** is not specified
λ = min (**β δt**, 1) where **δt** is the time step if **β** and **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

$$\Phi_i = \Phi_i^o + \frac{1}{\alpha_i} \frac{Q}{\sum_{\substack{\text{subrgn2} \\ \text{(Receptor)}}} \delta V_i}$$

UNIF The inventory is distributed so that the increment in **Φ** is uniform and constant:

$$\Phi_i = \Phi_i^o + \frac{Q}{\sum_{\substack{\text{subrgn2} \\ \text{(Receptor)}}} \alpha_i \delta V_i}$$

SCAL The inventory is distributed proportional to the existing value of **Φ**:

$$\Phi_i = \Phi_i^o + \frac{Q\, \Phi_i^o}{\sum_{\substack{\text{subrgn2} \\ \text{(Receptor)}}} \alpha_i \Phi_i^o \delta V_i}$$

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.

β A constant (**β** ≥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 **β** specifies the fraction of the current inventory in the donor region that is transferred. Limits are imposed so that ($0 \le \beta \le 1$); 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 **β**.

TIME β specifies the fraction per unit time of the current inventory that is transferred. The actual fraction transferred is equal to **β δt** where **δt** is the time step. Limits are imposed dynamically so that (0 ≤ **β δt** ≤ 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 **ALWA**ys modifier for the same **Φ,** 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 INVEntory of C from ID=DONOR to ID=RECEPTOR! Total amount transferred
SET INVEntory of C from ID=DONOR to ID=RECEPTOR FRACtion=0.5! 50% transferred
SET INVEntory of C from ID=DONOR to ID=RECEPTOR 0.1 TIME ALWAYS! 0.1*dt every time step
SET INVEntory 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 **ALLO**CATE 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

fnc	INTERPRETATION
ABS or **ABSO**	The absolute value for the computed gradient is taken.
POSI	The negative values for the computed gradient are set of zero
NEGA	The positive values for the computed gradient are set of zero
SQUA	The function is computed as the square of the gradient
ROOT	The function is computed as the square root of the gradient; negative values are set to 0.

BLOC If this modifier is present then the value of the gradient at the blocked nodes see (**BLOC**K 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} {Φ_1, …, Φ_n} {V_1,..$V_{(n+1)\,m}$|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.

Φ_1, …, Φ_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 (**ALLO**CATE 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.

V_1….V_{nm} 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 **V_1** 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 **SET {ZALU} {Φ}[ξ] {x_0, y_0, [z_0]} {q_0} {t_{start}, t_{end}} [C_0,C_1,C_2,C_3] [LIMI] [subrgn] [FIEL] [ALWA] [FREQ [NOW]|ONLY] [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:

$$q = \xi \max\left[(C_0 + C_1\, t + C_2\, d + C_3\, U), 0.0\right] \quad \text{if } t_{start} < t \le t_{end} \quad \text{and } S_f \ge 0.99$$
$$= 0 \text{ otherwise}$$

The default values of the constants are: $C_0 = 4.0581\text{x}10^{-2}$, $C_1 = 2.88\text{x}10^{-7}$, $C_2 = -2.294\text{x}10^{-2}$, $C_3 = 19.68013$. 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:

$$Q_{total} = \Sigma q\ (1-\theta)\ \rho_s\ \delta V\ ; \quad Q_{inj} = q_0\ \min\left[(t - t_{start}), (t_{end} - t_{start})\right];\ t > t_{start}$$

In these relations, ρ_s is the particle density of solid, θ is the porosity and δV is the volume of the element; the summation is carried out over all elements of the sub-domain if the modifier **LIMIT** is present then q is corrected according to:

$$q_{final} = q\ \min\left[\frac{Q_{inj}}{Q_{total}}, 1.0\right]$$

If the modifier **LIMIT** is not present, then full correction is applied so that:

$$q_{final} = q\ \frac{Q_{inj}}{Q_{total}}$$

Φ 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.

ξ The independent variable that multiplies the computed value of q. The variable **ξ** can be computed from an equation or specified by other means. If the symbol **ξ** 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_{start}, t_{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.

LIMI 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.

subrgn The subregion for which the colloidal deposition is computed. If no subregion is specified, then entire computational domain is selected.

FIEL See Mode 1 specification.

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.

FREQ The computation is performed at the frequency specified by **V_{frq}**.

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 develop, 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, tstart=10, tend=500 ALWAYS
SET ZALUSKI COLLIOD at (0.1,0.5,0.4) q=0.55, tstart=10, tend=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 **SET {Φ} {OFF} [subrgn]**

Φ See Mode 1 specification.

OFF Previous **SET** commands for the specified variable in the identified subregion are deactivated. A new specification may follow.

subrgn Identifier for the subregion that appeared previously in a **SET** command for the current variable, **Φ**.

EXAMPLES

SET commands for T for OFF for currently SELEcted subregion
SET commands OFF for T for ID=MIDDle

COMMAND **SOLI**D

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 apporparite **COND**UCTIVITY, **DEN**SITY, **PORO**SITY and **SPEC**IFIC 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 [Φ] [ADD] [MANU] [N1, N2, N3, N4, N5]

Φ 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 **BOUN**DARY or **SOUR**CE 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 **Φ** 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 **Φ** 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 **Φ**.

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 **SOLV**E 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 99 999 999.

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.E6 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 **SOLV [Φ] [ADD] {AUTO} [PASS] [N_1, N_2, N_3, N_4, N_5, N_6, N_7]**

Φ See Mode 1.

ADD See Mode 1.

AUTO The time step is automatically determined so that the specified primary convergence constraint is achieved for each time step (See **CONV**ERGENCE 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 **CONV**ERGENCE command with **FLOW** modifier and decreased if it is larger than $4/5^{th}$ of the maximum number of iterations.

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^{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^{-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 **CONV**ERGENCE command. The default value is 2.

N_7 The maximum number of time steps. The default value is 99 999 999.

COMMENTS

The **AUTO**matic 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

SOLVe for 10 days in AUTOmatic mode
SOLVe AUTO 10 days DT=0.2, fac=1.3, mx=1, mn=1.E-5, df=1.1, Nmax=1000
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} [N_1, N_2, N_3, N_4, N_5, N_6, N_7, N_8]**

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:

$$R = \max\left[\frac{\max|A_{ij}|_{i\neq j}}{A_{jj}}\right]_{\text{over all } i} \leq R_{max}$$

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.

N_1 See Mode 1 of command.

N_2 See Mode 1 of command.

N_3 See Mode 1 of command.

N_4 The maximum permissible time step. The default value is 10^{30}.

N_5 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}.

N_6 The cut-off threshold value, R_{max}, for the CFL parameter. If the computed value of R exceeds the threshold value then new time step is computed from:

$$dt_{new} = \frac{dt_{old}}{dt_{fac}}; \quad dt_{fac} = \max\left(\frac{R}{N6}, N7\right)$$

where N7 is defined below. The default value is 0.8

N_7 The minimum geometric ratio divisor (>0) for the time step. The default value is 1.1.

N_8 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} [N_1, N_2, N_3, N_4, N_5, N_6, N_7]**

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.

N_1 See Mode 1.

N_2 The starting value of the time step which will be replaced by the computed value if is larger than the computed value

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^{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^{-10}.

N_6 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 (**N_7** below).

N_7 The maximum number of time steps. The default value is 99 999 999.

COMMENTS

The **AUTO**matic 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 (**N_3** 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 {STEA} [Φ] [ADD] [N_1, N_2]**

STEA 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.

N_1 The maximum number of iterative steps for solution of the matrix. The default value in this instance is 99999999.

N_2 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] [N_1]**

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.

N_1 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 **SOLV**E 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 **SOLV**E 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 [N_1, N_2, N_3, N_4]**

N_1 Soot particle density. The default value is 2000 (kg/m^3).

N_2 Diameter of the smaller soot particles in microns. The default value is 1/40 micron.

N_3 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 **N_2**. The default value is 1 micron.

N_4 Percentage of the smaller soot particles in the total. This input is ignored if **N_3** 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 1.16×10^{31}.

N_2 The Arrhenius activation energy constant divided by the universal gas constant **(>0)** for the soot nuclei equation. The default value is 9.00×10^{4}.

N_3 The 1st exponent **(≥0)** of the soot nuclei equation. The default value is 1,000.

N_4 The 2nd exponent of the soot nuclei equation. The default value is 8.00×10^{-16}.

N_5 The 3rd exponent of the soot nuclei equation. The default value is 1.00×10^{15}.

N_6 The constant **(≥0)** in the soot nuclei equation. The default value is 100.

EXAMPLES

SOOT NUCLei constants: 1.00E31, 1.E5, 1000, 1.E-15, 1.E-15, 100.
SOOT NUCLei constants: 5.00E31, 1.0E4, 900, 8.E-15, 1.E-14, 100.

MODE 3: **Soot Formation Constants**

SYNTAX **SOOT {FORM} [N_1, N_2, , N_7]**

FORM Soot formation constants are specified.

N_1 The Arrhenius prefactor **(>0)** for the soot formation equation. The default value is 1.5626×10^{13}.

N_2 The Arrhenius activation energy constant divided by the universal gas constant **(>0)** for the soot nuclei equation. The default value is 1.60×10^{4}.

N_3 The 1st exponent **(≥0)** of the soot formation equation. The default value is 1.81.

N_4 The 2nd exponent of the soot formation equation. The default value is –0.50.

N_5 The 3rd exponent of the soot formation equation. The default value is –1.94.

N_6 The incipient carbon-to-oxygen ratio at which the soot formation starts. The default value is 0.1.

N_7 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} [N_1]**

FREQ Frequency of soot computations is specified.

N_1 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.

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]] {N_1, N_2, .., N_n | fname} [option] [subrgn] [dir] [N_{n+1}, N_k], [ρ_B]

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 **VOLU**ME 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.

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.

option Options selected for implementation of the source.

option	INTERPRETATION
VOLU	If the **TOTA**L modifier is not present, the source for each element is computed as: **Q = q δV.** Here **q** is the amount specified by the user and **δV** is the volume of the element. The **q**, in turn, is computed from **func(ξ)** and **N1** through **Nn**. If the **TOTA**L modifier is present, the amount for each element is computed as: **Q = q δV /V**, where **V** is the volume of the total **subrgn**.
AREA	If the **TOTA**L modifier is not present, the source for each element is computed as: **Q = q δA,** where **δA** is the area of the element boundary indicated by **dir**. If the **TOTA**L modifier is present, the source for each element is computed as: **Q = q δA /A**, where **A** is the total area of the **subrgn** in the **dir** direction.
INTE	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 **INTE**RNAL modifier is present then the wall treatment and wall diffusive flux are retained.
NORM	In the absence of the **TOTA**L modifier, the source, **Q**, is computed as: $Q = q \sum_i A_i \bullet V_i$ 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 **TOTA**L modifier, **Q** is computed in a manner identical to that for the **AREA** modifier.
DENS	The computed source, **Q**, is further multiplied by density. The density may be specified as the last value, **ρ_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 **NORM**AL 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.

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

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}, .., N_k The normalizing vector components, V_i, if the **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.

ρ_B The density value that multiplies the computed source. It can only be specified if the **DENS**ITY modifier is present and then it must be the last value on the command. If no value is specified but the modifier **DENS**ITY is present, then default value is the boundary value at the node indicated by the **dir** direction if the **AREA** or **NORM**AL 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 (**SOUR**CE) 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]] {N_1, N_2, .., N_n | fname} [option] [subrgn] [dir] [Φ =N_{n+1}, .., Φ =N_m] [N_{m+1}, N_k] [ρ_B]**

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.

N_1, .., N_n See Mode 1 specification.

N_{n+1}, .. N_m Each of these represents the value of injected variable denoted by the symbol immediately preceding the value.

N_{m+1}, .., N_k The normalizing vector components, V_i, if the **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.

ρ_B See Mode 1 specification.

COMMENTS

The **SOUR**CE **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 **INLE**T 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 **INLE**T 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 **INTE**RNAL modifier should be used with the command.

EXAMPLES

All examples cited for Mode 1 are applicable provided that the modifier **FLOW** is added. Some illustrative examples of the use of attributes specific to this mode are given below.

SOURce with FLOW injection: amount = 0.001 with T=50, C=1.
SOURce with FLOW per unit AREA of X- face: = 0.001 with T=50, C=1.
SOURce with FLOW withdrawal: amount =-0.001 per second
SOURce FLOW: TABLe 3 sets SELEcted (0, 0), (100, 1), (200, 0) U=1, V=0.1, W=0., T=10, K=0.001, L=1
SOURce for FLOW: EXPOnential series with TIME 7 sets from 'SOURCE' T=100, C=0.
SOURce FLOW q=10 X- direction T=100, U=20. NORMalized velocity 0., 1.5, 2.5 ID=VSOURce;
SOURce FLOW q= -10 in X- dir with NORMalized vel 1., 1.5, 2.5 and DENSity for ID=VSOURce
SOURce FLOW q=10 X- dir variable values: U=10, V=0, W=-20, T=100, K=0.03, L=0.5 INTErnal with NORMalized vel 1., 1.5, 2.5 and DENSity for ID=VSOURce:
SOURce FLOW q=10 per unit VOLUme injected variables: U=10, V=0, W=-20, T=100, K=0.03, L=0.5 multiply by DENSity = 5 for SELEcted region

MODE 3: **Flow Injection with Fixed Variable Values and Computed Momentum Components**

SYNTAX **SOUR {MOME} [func[ξ]] {N_1, N_2, .., N_n | fname} [TOTA] [option] [Φ=N_{n+1}, .., Φ=N_m] [N_{m+1}, N_k] [ρ_B] [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 , ρ_B is the density, A is the area of the element boundary specified by the **dir** modifier, and n_j is a normalizing vector. If the **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.

N_1, .., N_n See Mode 1 specification.

fname See Mode 1 specification.

TOTA See Mode 1 specification

option See Mode 1 specification. Unless the **NORM**al modifier is present, it is assumed that the **AREA** modifier is in effect. Any specification of the **VOLU**me modifier is ignored. All other modifiers can be used as for Mode 1 Specification.

Φ See Mode 1 specification.

N_{n+1}, .. N_m These values represent the value of injected variable denoted by the symbol immediately preceding the value.

N_{m+1}, .., N_k The normalizing vector components, V_i, if the **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.

ρ_B The density value to compute the velocity components. It can only be specified if the **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 **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 **SOUR**CE **MOME**TUM command is similar to the **SOUR**CE **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 **SOUR**CE **FLOW** command.

EXAMPLES

All the examples cited for Mode 2, except those with **VOLU**me modifier, are applicable provided that the modifier **MOME**ntum 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]] {N_1, N_2, .., N_n | fname} [TOTA] [Φ =Nn+1,.., Φ =Nm] [Nm+1, …, Nm+5] [DENS | SPEE] [ρ_B | V_S] [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 ρ_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.

N_1, .., N_n See Mode 1 specification.

fname See Mode 1 specification.

TOTA See Mode 1 specification

Φ See Mode 1 specification.

N_{n+1}, .. N_m The values of injected variables denoted by the symbols immediately preceding the values.

N_{m+1} The spherical angle, **Θ** 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.

N_{m+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.

N_{m+3}, N_{m+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.

ρ_B See Mode 3 specification.

SPEE The injection speed, V_S, is specified as the last value on the command.

V_S The value V_S if the **SPEE**D 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**E 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, .., 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, ..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

Time	Flow	U	V	T
0.	0.001	1.00	0.02	100
1.	0.002	0.50	0.01	200
2.	0.004	2.00	0.01	500
5.	0.010	5.00	0.02	600

SOURce with FLOW MULTiple TABLe: 4 sets per unit VOLUme

Time	Flow	U	V	T
0.	0.001	1.00	0.02	100
1.	0.002	0.50	0.01	200
2.	0.004	2.00	0.01	500
5.	0.010	5.00	0.02	600

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 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 (Nn+1 and Nn+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 **Φ** in appropriate units, **H** is a transfer coefficient and Φ_{eq} is an equilibrium value of **Φ**. The **H** and Φ_{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.

Φ_{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. **NORM**al and **DENS**ity 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 EQVAlu! EQVA is a symbol
SOURce for T: RADIation VARI COEF as function HVALu, value=15! HVAL is a symbol
SOURce for T: RADI VARI COEF HCOEf & 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 **Φ**, λ is the decay rate and Ψ is the fluid density if the variable **Φ** is defined in terms of mass units and unity if it is defined in terms of volumetric units.

LIFE Half-life of the property **Φ** is specified. The decay rate is computed from the half life, σ:

$$\lambda = -\frac{\log(0.5)}{\sigma}$$

subrgn See Mode 1 specification.

λ The decay rate, λ, for the variable **Φ**.

σ The half-life, **σ**, for the variable **Φ**.

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_1, .., N_n}[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 **REAC**TION command, which comprise the source. Up to 9 reactions may be specified.

N_1, .., N_n 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 REACtion type FU LINEar -1. * R1
SOURce REACtion type CH LINEar -1. * R2 + 0.9586 * R1 in SELEcted subdomain.
SOURce REACtion type CH LINEar -1. * R2 + 0.9586 * R1 for ID=RRGN

MODE 10: Flux Transfer between Adjacent Elements

SYNTAX SOUR {FLUX} {Φ} {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:

$$Q = q \; F_{\Phi} \; F_V \; F_{\rho}$$

Here, q is the amount specified by the user (**func (ξ)** and **N1** through **Nn**). The factors $\mathbf{F_\Phi}$, $\mathbf{F_V}$ and $\mathbf{F_\rho}$ 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 $\mathbf{F_\Phi} = \mathbf{\Phi_0}$, where $\mathbf{\Phi_0}$ 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 $\mathbf{F_\Phi} = \mathbf{\Phi_B - \Phi_F}$, where $\mathbf{\Phi_B}$ and $\mathbf{\Phi_F}$ 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 $\mathbf{F_\Phi} = (\mathbf{\Phi_B - \Phi_F})/\mathbf{L}$, 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 $\mathbf{F_V}$ 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 $Fv = \sum A_i V_i$, 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, $\mathbf{N_{n+1}}$ through $\mathbf{N_k}$. 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 $\mathbf{F_\rho}$ is equal to ρ_B. In the absence of this modifier, $\mathbf{F_\rho}$ is equal to unity.

ρ_B The density value that multiplies the computed source. It can only be specified if the **DENS**ITY modifier is present and then it must be the last value on the command. If no value is specified but the modifier **DENS**ITY is present, then default value is the boundary value at the node indicated by the **dir** direction if the **AREA** or **NORM**AL 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.

MODE 11: **Disable Previously Specified SOURce commands**

SYNTAX **SOUR {OFF} {Φ} {subrgn}**

Φ See Mode 1 specification.

OFF Previous **SOUR**CE 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]} {N_1, N_2, .., N_n | 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.

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.

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 (**SPEC**IFIC) 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.

MODE 2: **Pre-Defined Specific Heat Function**

SYNTAX **SPEC {GORD} [fname]**

GORD The specific heat is computed from the 4th order polynomial relation of Gordon & McBride for multi-species gases. **(S. Gordon and B.J. McBride, 1971.** *Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations,* NASA SP-273).

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] {N_1, .,N_n}

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.

N_1, .., N_n 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 **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 **STAC**k 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 $\mathbf{x_i} = \mathbf{T_{ji}}\ \mathbf{X_j}$. The index **j** varies the fastest. Each row of the transformation matrix is interpreted as a unit vector directed along the $\mathbf{x_i}$ 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 $\mathbf{x_1}$ to be the unit normal to the plane, $\mathbf{x_2}$ is computed by intersecting the plane with the bounding box of the domain, and $\mathbf{x_3}$ is computed as the cross product of $\mathbf{x_1}$ and $\mathbf{x_2}$. The user has no control over the directions of $\mathbf{x_1}$ and $\mathbf{x_2}$. 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 2nd point and the normal points from the 1st to the 2nd point. The transformation is computed in the same way as the previous option.

N_1, .., N_n The 1st through 3rd components of the transformation matrix if the **MATR**IX 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 **PLAN**E modifier is present and the coordinates of the 1st point if the **POIN**T modifier is present. There is no default value.

N_{n+1}, .,N_m The 4th through 6th components of the transformation matrix if the **MATR**IX modifier is present, a vector (or direction cosines) to specify the normal to the plane of transformation if the **PLAN**E modifier is present and the coordinates of the 2nd point (on the plane of transformation) if the **POIN**T modifier is present. There is no default value.

N_7, .,N_9 The 7th through 9th components of the transformation matrix if the **MATR**IX modifier is present; otherwise this input is ignored. There is no default value.

EXAMPLES

STACk TRANsformation between local & global grid is:

1	0	0
0	0	-1
0	1	0

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

STACk TRANsformation for PLANE at (0.12, 0.55) normal vector as: (1, -1)
STACk TRANsformation for PLANE at (0.12, 0.55, 0.012) normal vector as: (1, -1, 0)
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} {Φ|OFF} {a} [b]**

WRIT The output produced by the WRITE command for the specified variable is scaled by **a** and **b** according to:

$$\Phi_{out} = a\ \Phi + b$$

Φ 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 (**ALLO**CATE command) and the real type variables defined in the initialization file (xxxINIT.ACR). There is no default value; a symbol must be specified.

OFF Any previous **STAC**K **WRIT**E 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 **STAC**K **WRIT**E commands each with its own **Φ** may be active at any given time.

EXAMPLES

STACk WRITE T by scaling with 1.8 and add 32 to convert deg Celsius to Fahrenheit.
STACk WRITE P by scaling with 1.00E5 and add 0.

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] [V_{frq}] [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.

V_{frq} 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, **V_{frq}** is interpreted to be the frequency of computations in terms of number of steps. If this modifier is present, then **V_{frq}** 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]} {N_1, N_2, .., N_n | 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 **α** is the storage coefficient, **ρ** is the fluid density and **Φ** 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 **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 independent variable is specified, the 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.

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:

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:

$$C_e^k = \theta_E S^n C^k + (1-\theta_E) S_s \rho_s C_s^k. \qquad (1)$$

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 [M/L^3] (e.g.kg/m^3),
C is the concentration of the species in the fluid phase in units of [M/L^3] (e.g.kg/m^3),
C_s is the concentration of the species in the solid phase in units of [M/M] (e.g.kg/kg of solid),
θ_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,
ρ_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 **PREC**IPITATION and **TRAN**SPORT commands). However, a

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:

$$C_e^k = \varphi_E \left(1 + \frac{\mathbf{S_s}}{\mathbf{S^n}} \frac{1-\theta_E}{\theta_E} \rho_s k_d^k \right) C^k .$$

$$= \varphi_E R_D^K C^k \tag{3}$$

The saturated porosity, φ_E, and the retardation coefficient, R_D, are defined by:

$$\varphi_E = \mathbf{S^n}\ \theta_E . \tag{4}$$

$$\mathbf{R_D^k} = 1 + \frac{\mathbf{S_s}}{\mathbf{S^n}} \frac{1-\theta_E}{\theta_E} \rho_s k_d^k . \tag{5}$$

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 (**STOR**AGE) must replace the keyword used in these examples.

MODE 2: **Dynamic Computation of Storage or Accumulation Term**

SYNTAX **STOR {Φ} {DYNA}**

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.

DYNA A typical storage term, S_Φ, 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 **α, ρ** and **Φ** or the product (**α ρ Φ**) can be stored at the end of n^{th} time step and re-used at the $n+1^{th}$ step. When **α** and **ρ** are constants, the two procedures lead to identical results. However, if **α** and **ρ** are functions of other variables, then depending on the method and sequence of solution of equations, **α** and **ρ** may be revised after Φ^n was computed. That is the prevailing values of **α** and **ρ** may have been used to compute Φ^n at the n^{th} time step and then modified by subsequent operations. For strict compliance with balance equations the product of (**α ρ Φ**) 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 **α** and **ρ**. However, the strict mass balance of the **Φ** variables may not be achieved if **α** and **ρ**. 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 **STOR {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 **α** and **ρ** vary with time, then product (**α ρ Φ**) 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

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 **α** 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 **ω** 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 **ρ** 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 **ρ** 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 **SOUR**CE 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 **LOCA**TE **MATC**H 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 **LOCA**TE **PAIR** or **LOCA**TE **MATC**H command.

N_1 The vane angle, **α**, in degrees if the **ANGL**E modifier is specified or the angular velocity of rotation, **ω**, if the **SOLI**D modifier is specified. The numerical value of **α** 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.

$R_{swirler}$ 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

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] {N_1} [N_2, .,N_n|fname] [N_{n+1},..,N_m] [$R_{swirler}$]**

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.

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 from which numerical values **N_2** through **N_n** 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.

N_{n+1}, ..,N_m 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.

$R_{swirler}$ 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}.

EXAMPLES

Generic examples for this command are given in Section 4.4. The command keyword (**SWIR**L) 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

MODE 3: **Swirl Profile or Mapping from a data file**

SYNTAX **SWIR [PROFile] [RADIal] {subrgn} {dir} {N_1,N_2,N_3,N_4} {fname} [SCALe [NONE] N_5,N_6] [AXIS N_7,N_8,N_9] [ALWA] [FUEL=N_{10}] [DIAG] (Φ_1.. Φ_n)**

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**

N_1 **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.

N_2, N_3, N_4 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.

N_5, N_6 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**.

N_7, N_8, N_9 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.

Φ_1.. Φ_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 **SOLV**E command. This behavior is analogous to the **SET** vs. **SET ALWA**ys 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 **DIAG**nostics 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 PROFline 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+ **ALWA**ys 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:

r	u	Ur	Ut	T	K	L	FU
End Header							
0	-0.1	0	0.1	300	0.001	0.1	0.01
0.1	-0.2	0	0.2	350	0.002	0.15	0.02
0.2	-0.3	0	0.3	400	0.003	0.2	0.03
0.3	-0.4	0	0.4	450	0.004	0.25	0.04
0.4	0.0	0	0.5	500	0.0001	0.3	0.05
0.5	0.6	0	0.6	550	0.006	0.35	0.06
0.6	0.7	0	0.7	600	0.007	0.4	0.05
0.7	0.8	0	0.8	400	0.008	0.45	0.04
0.8	0.9	0	0.9	300	0.009	0.5	0.03
0.9	1.0	0	1.0	300	0.01	0.55	0.02
1.0	1.0	0	0.0	300	0.01	0.6	0.01

SWIRler PROFile RADIal mdot=50.0 kg/s center=(0.5,0.5,0.5)
AXIS=(1,0,0) file='swirl2-r.dat'
additional variables in file: T K L 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 **ALWA**ys detailed DIAGnostics on.

The contents of file 'swirl3-r.dat':

Swirler mapping file for radial swirler:

X	U	Ur	Ut	T	K	L	FU
End Header							
0	-0.5	-0.0	0.0	300	0.005	0.1	0.01
0.1	-0.4	-0.1	0.1	350	0.004	0.15	0.02
0.2	-0.3	-0.2	0.2	400	0.003	0.2	0.03
0.3	-0.2	-0.3	0.3	450	0.002	0.25	0.04
0.4	-0.1	-0.4	0.4	500	0.001	0.3	0.05
0.5	0.0	-0.5	0.5	550	0.0001	0.35	0.06
0.6	0.1	-0.4	0.4	600	0.001	0.4	0.05
0.7	0.2	-0.3	0.3	650	0.002	0.45	0.04
0.8	0.3	-0.2	0.2	700	0.003	0.5	0.03
0.9	0.4	-0.1	0.1	750	0.004	0.55	0.02
1.0	0.5	-0.0	0.0	800	0.005	0.6	0.01

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_S, K_{Ts}, α_L, α_T] [subrgn]**

Cp_S Specific heat of the dry solid, C_{ps}(≥ 0), with typical units as [J/(kg ^oK)]. The default value is 1000 if **GAS** or **DENS**ITY **GAS** command is given otherwise it is 1.

K_{Ts} Thermal conductivity of the dry solid, K_{Ts} (≥ 0), with typical units as [J/(m-s ^oK)]. The default value is 0.

α_L Longitudinal dispersivity, α_L. (≥ 0) with typical units as. [m]. The default value is 0.

α_T Transverse dispersivity, α_T. (≥ 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 **COND**UCTIVITY command and for the dispersivyt by the **DISP**ERSIVITY 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

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} {τ_1, a_1, φ_1} [τ_n, a_j, φ_n]**

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:

$$\eta = \sum_{n=1}^{n} \eta_o^n \cos(f^n t + \phi^n) ,$$

SINE The tide is a sine function given by:

$$\eta = \sum_{n=1}^{n} \eta_o^n \sin(f^n t + \phi^n) ,$$

N Number of sets of harmonic tidal components that follow. The default value is 0.

τ_1 The time period of the 1st component of the tide. The default value is 0.

a_1 The amplitude of the 1st component of the tide. The default value is 0.

φ_1 The phase of the 1st component of the tide. The default value is 0.

τ_n, a_j, φ_n Triplets of period, amplitude, phase lag for the 2nd through **N**th 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, η_1} [t_n, .., η_n]**

dir One of the character strings: **EAST**, **WEST**, **NORT**h, or **SOUT**h. 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. The default value is 0.

t_1 The time at which the first tide height is specified. The default value is 0.

η_1 The tide height at time **t_1.** The default value is 0.

t_n, .., η_n Pairs of time and tide height for one complete tidal cycle

APPLICABILITY

This command is available only for the **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_1, η_{11}, η_{12}} [] {ξ_{start},, ξ_{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**, **NORT**h, or **SOUT**h. 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_1 The time at which the first tide height is specified.

η_{11} The value of the tide at the first location (**Nn+1** below) on the specified boundary.

η_{12} The value of the tide at the second location (**Nn+2** below) on the specified boundary.

t_n, η_{n1}, η_{n2} Triplets of time, and tide at the first and second locations in the manner of **t_1, η_{11}, η_{12}**.

ξ_{start},, ξ_{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, **η**, 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**, **NORT**h, or **SOUT**h. 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

COMMAND **TIME**

PURPOSE To set the initial simulation time for a problem.

SYNTAX **TIME** **{N1}**

N1 The starting time **(≥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 **TORTU**OSITY

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 [V_1, V_2, V_3] [subrgn]**

V_1, V_2, V_3 The x, y and z direction components, respectively, of the tortuosity factor τ_{ij} 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.

$$\Gamma_{ij}^{T} = (1-\theta_T)k_S + \theta_T \tau_{ij} S\, k_f + \theta_E S\, \rho D_{ij}$$

$$\boldsymbol{\Gamma_{ij}^{\varphi}} = \boldsymbol{\theta_D}\, \boldsymbol{\tau_{ij}}\, S\, \boldsymbol{\rho}\, D_M^{\varphi} + \boldsymbol{\theta_E}\, S\, \boldsymbol{\rho}\, D_{ij}$$

$$\mathbf{D_{ij}} = \boldsymbol{\alpha_T}\boldsymbol{\delta_{ij}}\underline{\mathbf{v}} + (\boldsymbol{\alpha_L} \quad \boldsymbol{\alpha_T})\frac{|\mathbf{v_i v_j}|}{\underline{\mathbf{v}}},$$

Where the superscript “n” denotes the nth fluid phase and::

$\boldsymbol{\Gamma_{ij}^{T}}$, $\boldsymbol{\Gamma_{ij}^{\varphi}}$	are the diffusion coefficients for thermal and species equations,
$\boldsymbol{\Theta_E}$, $\boldsymbol{\theta_T}$, $\boldsymbol{\theta_D}$	are the effective, total and diffusional porosities of the material
k_S, k_f,	are the solid and fluid thermal conductivities,
$\mathbf{D_M}$	is the molecular diffusivity of the species
$\mathbf{D_{ij}}$	is the dispersion tensor
$\mathbf{v_i}$, $\underline{\mathbf{v}}$	are the components of particle velocity and the modulus of velocity,
S	is the saturation of the fluid phase
$\boldsymbol{\alpha_L}$, $\boldsymbol{\alpha_T}$,	are the longitudinal and transverse dispersion coefficients
$\boldsymbol{\rho}$	is the density of fluid
$\boldsymbol{\tau_{ij}}$	is the tortuosity or constrictivity tensor

APPLICABILITY

This command is currently available only for the **PORFLOW™** Software Tool.

EXAMPLES

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] {N_1, ..N_n} [V_{stop}, τ_0, N_{frq}]

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.

option	INTERPRETATION
X	Particle tracking stops if its x-coordinate exceeds the Nn+1th numerical value.
Y or **R**	Particle tracking stops if its y-coordinate exceeds the Nn+1th numerical value.
Z or **THETA**	Particle tracking stops if its z-coordinate exceeds the Nn+1th numerical value.
DIST	Particle tracking stops when its distance from the point of release exceeds the Nn+1th numerical value. This is default option if **STOP** modifier is specified.
TIME	Particle tracking stops when the time exceeds the Nn+1th numerical value.
ELAP	Particle tracking stops when the elapsed time from its moment of release exceeds the Nn+1th numerical value.
FREE	Particle tracking stops if it reaches a free surface or zone of saturation.

N_1, .., N_n The coordinates of the starting location of the particle. Two values are required for the 2D and 3 for 3D input modes.

V_{stop} 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.

τ_0 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.

N_{frq} The frequency index for providing the output in the particle track file. The output is obtained every **Nn+3** ($\geq$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

COMMAND **TRANSFER**

PURPOSE To specify the transfer of mass flux and fluid properties from one subregion to another.

MODE 1: **Direct Transfer of Computed Flux**

SYNTAX **TRANSFER** **[FLUX] [LOCA] [subrgn]**

FLUX The flux of mass is transferred from one surface to another. This type of transfer can only be defined by a **LOCA**TE command with **MATC**hed pair option. The purpose of this command is to simulate embedded objects in the flow field such as pipes, pumps, fans, 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 **LOCA**L 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 **LOCA**L 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 **LOCA**TE **MATC**H 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)] {N_1, N_2, .., N_n|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.

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.

LOCA See Mode 1 Specification.

subrgn The sub region for flux or source transfer. If the **SOUR**CE modifier without **AREA** is present, then the sub region must have been previously defined by a **LOCA**TE **MATC**h or a **LOCA**TE **CORR**elated command. Otherwise the sub region must have been previously defined by a **LOCA**TE **MATC**h 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 **VOLU**me or **AREA** modifiers are present.

VOLU If the **TOTA**L modifier is absent, the source for each element is computed as: Q=q**δV**. Here **q** is computed from **func (ξ)** and **N1,…, Nn** and, **δV** is the volume of the element. If the **TOTA**L modifier is present, the amount for each element is equal to: Q=q**δV**/V, where **V** is the volume of the total **subrgn**.

AREA If **TOTA**L modifier is absent, the source for each element is computed as: Q=q**δA**, if **TOTA**L modifier is present, the source is computed as: Q=q**δA/**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 **INTE**rnal 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 **TRAN**SFER 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:

$$q = \rho\, \delta A \left[\frac{1}{2\, C_D} \frac{P_{in} - P_{out}}{\rho} \left(\frac{\rho D}{\mu} \right)^{\beta} \right]^{\frac{1}{2-\beta}},$$

In the equation above:

ρ is the fluid density
δA 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,
μ is the dynamic viscosity, and
β is an exponent that represents the dependence of the drag on Reynolds number (For laminar flow **β** is unity; for turbulent flow **β** 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 **β** is 0.25. Often for fully turbulent flow, the effect of Reynolds number on **β** 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 **β** is specified. There is no default value for this input.

β The exponent **β** for the drag coefficient. The default value is zero.

COMMENTS

This mode of the **TRAN**SFER command is automatically selected if the **DRAG** modifier is present and there are no more that 3 numerical values on the command.

EXAMPLES

TRANsfer DRAG C_drag = 0.10 for subregion ID=Q_TRANSFER
TRANsfer as FLUX DRAG C-drag = 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] { C_D, 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:

$$q = \rho N \frac{\pi D^2}{4} \left[\frac{1}{2 C_D} \frac{P_{in} - P_{out}}{\rho} \left(\frac{\rho D}{\mu} \right)^{\beta} \frac{D}{L} \right]^{\frac{1}{2-\beta}},$$

In the equation above:

ρ is the fluid density
N is the number of holes,
D is the diameter of holes,
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,
μ is the dynamic viscosity,
L is the length of each hole, and
β is an exponent that represents the dependence of the drag on Reynolds number (For laminar flow **β** is unity; for turbulent flow **β** 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 **β** is 0.25. Often for fully turbulent flow, the effect of Reynolds number on **β** 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.

C_D The drag coefficient, **C_D**, 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.

β The exponent **β** for the drag coefficient. The default value is zero.

COMMENTS

This mode of the **TRAN**SFER command is automatically selected if the **DRAG** modifier is present and there are at least 4 numerical values on the command.

EXAMPLES

TRANsfer DRAG C_drag= 0.10 dia= 0.001, number=200, Length= 0.005, for subregion ID=Q_TRANSFER
TRANsfer DRAG C_drag= 0.10 dia= 0.001, number=200, L= 0.005, beta=0.25 ID=Q_TRANSFER
TRANsfer DRAG C_drag= 0.10 dia= 0.001, n=200, L= 0.005, distribution by VOLUme ID=Q_TRANSFER
TRANsfer DRAG C_drag= 0.10 dia= 0.001, n=200, L= 0.005, distribution by AREA ID=Q_TRANSFER
TRANsfer DRAG C_drag= 0.10 dia= 0.001, n=200, L= 0.005, Allow REVErse flow; ID=Q_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 **TRAN {Φ} {α} [D_M, α_L, α_T] [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.:

α The partition coefficient, k_d (≥ 0), that relates the species concentration in the solid to that in the fluid phase. However, if a **PROP**ERTY command with the same symbol and **EFFE**CTIVE 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 **STOR**AGE command (**COMMENTS** Section) for a full discussion of the interpretation of k_d and R_D

D_M Molecular diffusivity, D_M (≥ 0) for the species. The default value is 0.

α_L The coefficient of longitudinal dispersivity: α_L (≥ 0). The default value is 0.

α_T The coefficient of transverse dispersivity: α_T (≥ 0). The default value is 0.

SECO By default the species transport occurs in the 1st phase of the fluid. If **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 eqution for the 2nd phase must be solved for this modifier to be effective.

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:

$$\frac{\partial}{\partial t}\left[(1-\theta_E)\rho_S C^k\right] = \frac{\partial}{\partial x_i}\left(\rho_S \Gamma_{ij}^c \frac{\partial C^k}{\partial x_j}\right) + S_c^k - (1-\theta_E)\rho_S \gamma^k$$

WET The modifier is effective only if the **SOLI**D 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.

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 **α** can be specified by the **DIST**RIBUTION command, those for the diffusivity by the **COND**UCTIVITY command and for the dispersivity by the **DISP**ERSIVITY 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 propertie vary as functions of other variables, then the individual components of the input can be specified (or overwritten) by the **STOR**AGE, **COND**UCTION and **DISP**ERSION commands.

EXAMPLES

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 foer 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} [D_M, 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:

$$\Gamma = D_M \beta \exp(\gamma S \Theta_D),$$

where **S** is the phase satuation and Θ_D is the diffusional porosity. Other symbols are described below.

α See mode 1 of command.

D_M 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

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.

model	INTERPRETATION
CHIE	Chien (1982) low Reynolds number model is used.
CUBI	Cubic **k-ε** model of Shih et al. (1997) is employed.
LRR	Launder, Reece and Rodi (1975) Reynolds stress model is used.
LS	Launder-Sharma (1974) low Reynolds number model is used.
MENT	Menter (1996) two layer blended **k-ε/ k-ω** model is employed.
QUAD	Quadratic **k-ε** model of Shih et al. (1997) is employed.
RNG	RNG enhancements to the **k-ε** model are employed.
RSM	Reynolds stress model of Craft et al. (1996) & Iocovides et al. (1996) is used
SSA	So and Sarkar (1997) low Reynolds number model is used.
SST	Menter (1996) low Reynolds number shear-stress transport model is used.
WILC	Wilcox (1993) **k-ω** model is employed.
YSM	Yang and Shih (1993) low Reynolds number model is used.

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 **QUAD**ratic and **CUBI**C models, the Yang and Shih (1993) low Reynolds option is used.

SECO This modifier is effective only in the presence of the **CUBI**C 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-e
TURBulence model k-e with LOWReynolds number extensions
TURBulence model k-e 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 **TURB {LES} [SMAG | DEDU|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 **SMAG**orinsky 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 Cs=0.04

MODE 3: **Empirical Constants for Turbulent Flows**

SYNTAX **TURB [κ, E, C_μ, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$]**

κ	The constant κ (>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_μ	The constant **C_μ** (>0) of the **k-ε** model. The default value is 0.09.
$C_{\varepsilon 1}$	The constant **$C_{\varepsilon 1}$** (>0) of the **k-ε** model. The default value is 1.44.
$C_{\varepsilon 2}$	The constant **$C_{\varepsilon 2}$** (>0) of the **k-ε** model. The default value is 1.92.

COMMENTS

The default values are for the 'standard" k-ε 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 **UPTA**KE

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 **PREC**IPITATION command.

EXAMPLES

See **PREC**IPITATION 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 **PRES**SURE 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 diffetent from the value at the node depending on the method of averaging (see the **PROP**ERTY 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

COMMAND VISCOSITY

PURPOSE To specify the viscosity and to select associated options.

MODE 1: Generic Functional Form for Viscosity

SYNTAX VISC {func[ξ]} {N_1, N_2, .., N_n | fname} [EFFE] [operation] [ALWA] [phase] [subrgn]

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.

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.

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 **REPL**ACE, **ADD, SUBT**RACT, **MULT**IPLY, **DIVI**DE, **ABS, ABSOLUTE**, **POSI**TIVE and **NEGA**TIVE. See Section 4.3 for further details.

ALWA By default, for **PORFLOW™** Software Tool the **VISC**OSITY 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 **ALWA**YS 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 **VISC**OSITY command is recommended as the preferred mode of input.

The effective viscosity may also be set by the **COND**UCTIVITY 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 **VISC**OSITY, **SET** and **COND**UCTIVITY commands may be specified in combination. In this case, the **COND**UCTIVITY 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, $\mathbf{K}_{ij}$, is computed as:

$$K_{ij} = K^{*}_{ij} \frac{\mu^{*}}{\mu}$$

Where K^{*}_{ij} is the reference value of hydraulic conductivity specified through the **COND**UCTIVITY or **HYDR**aulic commandS, and **μ** and **μ*** 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.

MODE 2: **Pre-Defined Viscosity Functions**

SYNTAX **VISC {SUTH | POWE|EXPO} [phase] [μ_0] [α] [β] [T_a]**

CONS The fluid viscosity is constant. This is the default option.

SUTH Sutherland equation for viscosity of gases is used:

$$\mu = \mu_0 \frac{\alpha + \beta}{T + \beta} \left[\frac{T}{\beta}\right]^{3/2}$$

For this relation, T must be in absolute units. If no numerical values are specified; then the default values are μ_0=1.827E-5, α=291, β=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:

$$\mu = \mu_0 \; 10^{\left(\frac{\alpha}{T + T_a - \beta}\right)}$$

The default values are μ_0=2.414E-5, α=247.8, β=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 μ_0=7.20912E-6, α=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.

μ_0 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 **VISC**OSITY 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 **POWE**R and **EXPO**NENTIAL options and equal to the value o**f** μ_0 for the **SUTH**ERLAND option.

EXAMPLES

VISCosity EXPOnential option
VISCosity from SUTHERLAND equation
VISCosity EXPOnential option: mu* = 0.544E-3, b = 1450 K for FIELD values

COMMAND **WALL**

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 **BOUN**DARY 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_{ROUG} 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 **INLE**T, **OPEN**, **OUTL**ET, **PERI**ODIC and **SYMM**ETRY 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 (**ADIA**BATIC 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; l walls 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 **BOUN**DARY, **INIT**IAL, **READ** or **SET** commands

ADIA The gradient of the specified variables at the wall is set to zero.

GRAD Same as **ADIA**BATIC; 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 **BOUN**DARY and **ADIA**BATIC 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=Z_{rough}] [TYPE=C_{rough}]**

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 **BOUN**DARY, **INIT**IAL, **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 **BOUN**DARY command.

ADIA The gradient of the specified temperature at the wall is set to zero.

ROUG See Mode 1 of command.

Z_{ROUGH} See Mode 1 of command.

TYPE See Mode 1 of command.

C_{ROUG} 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 **BOUN**DARY, **INIT**IAL, **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 {HOLE} {dir} [subrgn] {d_{hole}} [N_1, . N_n] [IJK | ELEM] [N_{vec1}, . N_{vecm}] [ε]**

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_{hole} The diameter of the hole to be "drilled" in the specified wall.

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 circular hole. 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 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_1, . N_n]** 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}, . 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.**

ε 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 tol=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:

$$\Phi_{out} = \alpha\, \Phi_{computed} + \beta$$

STAC The output variable is scaled by coefficients **a** and b specified on a previous **STACK WRITE** command according to:

$$\Phi_{out} = a\, \Phi_{computed} + b$$

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:

$$\Phi_{out} = \Phi_{min} + (\Phi_{computed} - \Phi_{min}) / (\Phi_{max} - \Phi_{min})$$

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:

$$\Phi_{out} = \Phi_{computed} - \Phi_{N}$$

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 SELEcted 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 **WRIT {Φ} [option] [walltype] [SUMM] [SCALE|STAC|UNIT|ELEM] [N|α] [β] [subrgn] [dir] [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.

option	INTERPRETATION
INLE	Only the boundaries specified by the **INLE**T command are selected.
OUTL	Only the boundaries specified by the **OUTL**ET command are selected.
OPEN	Only the boundaries specified by the **OPEN** command are selected.
IO	All boundaries specified by INLET, **OUTL**ET or **OPEN** commands are selected.
BOUN	All external boundaries of the specified (or default) subregion are selected.
SYMM	Only the boundaries specified by the **SYMME**TRY command are selected.
WALL	Only the walls are selected.

walltype The type of wall to be selected for output if the **WALL** modifier is present.

walltype	INTERPRETATION
ALL	All walls are selected. This is the default option.
EXTE	Only the exterior walls of the computational domain are selected.
INTE	Only the walls located in the interior of the computational domain are selected.
BLOC	Only the walls of the blocks (**BLOC**K command) are selected.

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.

SCAL See Mode 1 Specification.

STAC See Mode 1 Specification.

UNIT See Mode 1 Specification.

ELEM See Mode 1 Specification.

N See Mode 1 Specification.

α See Mode 1 Specification.

β See Mode 1 Specification.

subrgn The subregion for computations. If no subregion is specified, the entire domain is selected.

dir 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.

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 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.PRB'
WRITe T and RHO only for EXTErior WALLs to the file 'WALL_EXT.PRB'
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.

method	INTERPRETATION
LINE	The values are computed by inverse linear distance interpolation from the computed values at nearest neighbors. This is the default option.
SQUA	The values are computed by inverse distance squared interpolation from the computed values at nearest neighbors.
AVER	The values are computed by arithmetic average of computed values at nearest neighbors.
NEAR	The value is set equal to that at the nearest neighbor.
X	Same as **LINE** except that the distance is set equal to the separation in the x-coordinate.
Y	Same as **LINE** except that distance is set equal to the separation in the y-coordinate.
Z	Same as **LINE** except that the distance is equal to the separation in the z-coordinate.

STAC The output variable is scaled by coefficients **a** and **b** specified on a previous **STAC**K **WRIT**E command according to:

$$\Phi_{out} = a\,\Phi_{computed} + b$$

The STAC modifier is effective only for **real** variables. It is ignored if no previous **STAC**K **WRIT**E command was specified.

subrgn The sub region for output. The sub region must have been previously specified by a **LOCA**TE **LIST COOR**DINATE 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 1st element.

HEAD By default only the numeric values for the selected variable(s) are written to the file without any header information. If the **HEAD**ER 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 **BLOC**K 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^{th} 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 **CONN**ECTIVITY 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'

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 **MATE**RIAL, **ROCK** or **SOIL** commands, together with **LOCATE** command, have replaced its function. These latter commands should be used..

EXAMPLES

See Mode 1 of the **MATE**rial command.

REFERENCES

F. Adenot and M. Buil, 1992. Modelling of the corrosion of the cement paste by deionized water. **Cement and Concrete Research 22, (2-3), p. 489**

B. Abramzon and W.A. Sirignano, 1989. Droplet Vaporization Model for Spray Combustion Calculations, **International Journal of Heat and mass Transfer, 32, pp. 1605-18.**

Bary, Benoît and Antoine Bregeon, 2003. Etude de la carbonatation des materiaux cimentaires en conditions saturees:: Modelisation simplifiee et simulations numeriques. **Réf. CEA, NT DPC/SCCME 03-230-A Novembre 2003.**

J. Bear, 1972. *Dynamics of Fluids in Porous Media*. American Elsevier, **New York, New York.**

J.D. Bittener, and J.B. Howard, 1978. Role of Aromatics in Soot Formation, **Alternate Hydrocarbon Fuels: Combustion and Chemical Kinetics, Ed. C.T. Bowman and J. Birkeland, Academic Press, New York.**

N.E. Bixler, 1985. NORIA-A Finite Element Computer Program for Analyzing Water, Vapor, Air, and Energy Transport in Porous Media, **Report No. SAND84-2057, UC-70, Sandia National Laboratories, Albuquerque, New Mexico 87185.**

K.N.C. Bray, P.A. Libby and J.B. Moss, 1985. *Unified Modeling Approach for Premixed Turbulent Combustion - Part I: General Formulation, **Combustion and Flame, 61, pp. 87-102.***

R.H. Brooks and A.T. Corey, 1966. Properties of porous media affecting fluid flow. **J. Irrig. Drain. Div., Am. Soc. Civil Eng. 92 (IR2), pp. 61-88.**

N.T. Burdine, 1953. Relative permeability calculations from pore-size distribution data. **Petr. Tans., Am. Inst. Mining Metall. Eng., 198, pp. 71-77.**

S. Candel, D. Veynante, F. Lacas, E. Maistret, N. Darabiha and T. Poinsot, 1990. Flamelet Descriptions of Turbulent Combustion. **Invited Lecture, 9th International Heat Transfer Conf., Aug. 19-24, 1990, Jerusalem, Israel.**

K.Y. Chien, 1982. Predictions of Channel and Boundary-Layer Flows with a Low-Reynolds-Number Turbulence Model, **AIAA, 20, 1, p 33-38.**

A.J. Chorin, 1967. A Numerical Method for Solving Incompressible Viscous Flow Problems, **J. *Computational Physics, Vol. 2, pp. 12-26.***

T.J. Craft, N.Z. Ince and B.E. Launder, 1996. Recent developments in second-moment closure for buoyancy-affected flows. **Dynamics ofAtmospheres and Oceans, 23, p.99-114.**

J. DeRis, 1979. Fire Radiation - **A Review, Seventeenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA.**

R. Edelman, J. Boccio and G. Weilerstein, 1973. The Role of Mixing and Kinetics in Combustion Generator NO_x, **AIChE Sym. on Control of NO_x Emissions in Direct Combustion Power Sources.**

D.K. Edwards and A. Balakrishnan, 1973. Thermal Radiation by Combustion Gases, **Int. J. Heat Mass Transfer, 16, pp. 25-40.**

R.A. Freeze and J.A. Cherry, 1979. *Groundwater*, **Prentice-Hall, Englewood Cliffs, New Jersey.**

A.G. Gaydon and H.G. Wolfhard, 1979. Flames, **Fourth Edition, Chapman and Hall Ltd., London.**

William R. Goodin, D. Ian Austin and A. K. Runchal, 1980. A Model Verification and Prediction Study of SO_2/SO_4 Concentrations in the San Francisco Bay area. **Proc. Second Joint Conf. on Applications of Air Pollution Meteorology, AMC/APCA, New Orleans, LA, March 24-27, pp. 328-333.**

W. R. Goodin, A. K. Runchal and G.Y. Lou, 1982. The Random-Walk Advection and Dispersion Model (RADM). **AIChE, Environmental Progress, 1(3), p. 178-181.**

S. Gordon and B.J. McBride, 1971. Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations, **NASA SP-273.**

H.C. Hamaker, 1947. Radiation and Heat Conduction in Light-Scattering Material, **Phillips Research Report, Volume 2, pp. 55-67.**

A. Harten, 1983. High Resolution Schemes for Hyperbolic Conservation Laws. **Journal of Computational Physics, Vol. 49, pp. 357-393.**

A. Harten, 1984. On a Class of High Resolution Total-Variation-Stable Finite-Difference Schemes, **SIAM J. Num. Anal., Vol. 21, pp. 1-23.**

D.J. Hautman, F.L. Dryer, K.P. Schug and I. Glassman, 1981. A Multiple-Step Overall Kinetic Mechanism for the Oxidation of Hydrocarbons, **Comb. Sci. Tech., 25, pp. 219-235.**

B.S. Haynes and H.G. Wagner, 1981. Progress in Energy and Combustion Science, 7, 229 pp.

K.H. Homann, 1967. Carbon Formation in Premixed Flames, **Combustion and Flame, 11, pp. 265-287.**

H. Iacovides, B.E. Launder, and Y. Li, 1996. Application of a reflection-free DSM to turbulent flow and heat transfer in a square-sectioned U-bend. **Experimental Thermal and Fluid Science, 13, 4, p 419-429.**

W.P. Jones and J. H. Whitelaw, 1982. Calculation Methods for Reacting Turbulent Flows: A Review. **Combustion and Flame, 48, p 1-26.**

K.C. Karki, 1986. A Calculation Procedure for Viscous Flows at All Speeds in Complex Geometries, **Ph.D. Dissertation, Univ. of Minnesota.**

W.O. Kemper and J. C. van Schaik, 1966. Diffusion of Salts in Clay-Water Systems. ***Soil Sc. Am. Proc.* 30:534-540.**

B.E. Lander and B.I. Sharma, 1974. Application of the Energy Dissipation Model of Turbulence to the calculation of Flow Near a Spinning Disc. **Letters in Heat and Mass Transfer, 1, 2, p 131-138.**

B.E. Launder, G.J. Reece and W. Rodi, 1975. Progress in the development of a Reynolds Stress Turbulence Closure. **Journal of Fluid Mechanics, 68,3, p. 537-566.**

B.E. Launder and D.B. Spalding, 1972. Lectures in Mathematical Models of Turbulence, **Academic Press.**

B. Leckner, 1972. Spectral and Total Emissivity of Water Vapor and Carbon Dioxide, **Combustion and Flame, 19, pp. 33-48.**

S. Lee, H-J. Kim and A.K. Runchal, 2003., Large Eddy Simulation of Unsteady Flows in Turbomachinery, 2003, **submitted to the J. Power and Energy.**

S. Lee and W.C. Meecham, 1996. Computation of Noise from Homogeneous Turbulence and a Free Jet, **International Journal Acoustics and Vibration, 1996, 1, pp. 35-47.**

B.P. Leonard, 1979. A Stable and Accurate Convective Modeling Procedure based on Quadratic Upstream Interpolatio, **Comp. Methods Appl. Mech. Eng., 19,59-98.**

B.F. Magnussen, B.H. Hjertager, J.G. Olson and D. Bhaduri, 1978. Effects of Turbulent Structure and Local Concentrations on Soot Formation and Combustion in C_2H_2 Diffusion Flames, **Seventeenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA.**

M. Mainguy, C. Tognazzi, J.-M. Torrenti and F. Adenot, (2000). Modelling of leaching in pure cement paste and mortar. **Cement and Concrete Research 30, (1), p. 83**

F.R. Menter, 1996. A Comparison of Some Recent Eddy-Viscosity Turbulence Models. **J. Fluids Eng., ASME, 118, p 514-519.**

A.T. Modak, 1979. Radiation from Products of Combustion, **Fire Research, 1, pp. 339-361.**

H.C. Mongia and R.S. Reynolds, 1978. Combustor Design Criteria Validation, Volume III - User's Manual, **Report # USARTL-TR-78-55C, U.S. Army Res. and Tech. Lab., Fort Eustis, VA.**

Y. Mualem, 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. **Water Resources Res. 12, 3, pp. 513-522.**

J. Nagle and R.F. Strickland-Constable, 1962. Oxidation of Carbon Between 1000-2000 °C, **Proc. Fifth Conf. on Carbon, Volume I, Pergamon Press, New York.**

J. Nikuradse, 1937. Laws of flow in rough pipes, **NACA Tech. Mem.1292.**

H.B. Palmer and C.F. Culliss, 1965. The Formation of Carbon from Bases, Chemistry and Physics of Carbon, **Volume I, Ed. P.L. Walker, Marcell Dekker, New York.**

S.K. Park and K.W. Miller, 1988. Random Number Generators: Good Ones Are Hard To Find. **Communications of the ACM, October 1988, pp. 1192-1201**.

S.V. Patankar and D.B Spalding, 1972. A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-Dimensional Parabolic Flows, **Int.J.Heat Mass Transfer, 15, p. 1787.**

R.H. Perry and C.H. Chilton, 1973. Chemical Engineers' Handbook, 5th Edition, **McGraw Hill, New York.**

S.B. Pope and S.M. Correa, 1986. Joint PDF Calculations of non-Equilibrium Turbulent Diffusion Flame, **Paper # 53, 21st Sym. (International) on Combustion, Munich, August 3-8.**

W.E. Ranz and W.R. Marshall, 1952. Evaporation from Drops, **Chemical Engineering Progress, 48, pp. 141-46 and pp. 173-180.**

C. Richet, C. Gallé, P. Le Bescop, H. Peycelon, S. Béjaoui, I. Tovena, I. Pointeau, V. L'Hostis and P. Lovera, (2004). Synthèse des connaissances sur le comportement à long terme des bétons. Applications aux colis cimentés. **CEA-R-6050.**

P. J. Roache, 1972. ***Computational Fluid Dynamics,*** **Hermosa Publishers, Albuquerque, New Mexico.**

A.K. Runchal, 1972. Convergence and Accuracy of Three Finite Difference Schemes for a Two-Dimensional Conduction and Convection Problem, **Int. J. Num. Meth. Eng., 4, pp. 541-550.**

A.K. Runchal, 1977. Comparative Criteria for Finite Difference Formulations for Problems of Fluid Flow, **Int. J. Num. Methods in Eng., 11, pp. 1667-1679.**

A.K. Runchal, 1980. A Random Walk Atmospheric Dispersion Model for Complex Terrain and Meteorological Conditions. **2nd AMS/APCA Joint Conf. on Applications of Air Pollution Meteorology, New Orleans, LA, March 24-27, p. 430-437.**

A.K. Runchal, 1987a. Theory and Application of the PORFLOW Model for Analysis of Coupled Fluid Flow, Heat and Radionuclide Transport in Porous Media, in **Coupled Processes Associated with Nuclear Waste Repositories, pp. 495-516, Academic Press, 1987, Ed. C-F. Tsang.**

A.K. Runchal, 1987b. CONDIF: A Modified Central-Difference Scheme for Convective Flows, **Int'l J. Num. Methods in Engg., 24. 1593-1608.**

A.E. Scheidegger, 1961. General Theory of Dispersion in Porous Media, **J. Geophys. Res., 66, pp. 3273-3278.**

A. Sarkar and R.M.C. So, 1997. A Critical Evaluation of Near-Wall Two-Equation Models Against Direct Numerical Simulation Data, Int. J. Heat & Fluid Flow.

T.H. Shih, J. Zhu, W. Liou, K.-H. Chen, N.-S. Liu and J.L. Lumley, 1997. Modeling of Turbulence Swirling Flows. **NASA Tech. Memo. 113112, ICOMP-97-08, CMOTT-97-03.**

R.G. Siddall, 1972. Flux Methods for the Analysis if Radiant Heat Transfer, **Fourth Symp. on Flames and Industry, British Flame Research Committee and the Institute of Fuel, Imperial College, London, September.**

J. Smagorinsky, 1963. General Circulation Experiments with the Primitive Equations, Part I: the Basic Experiment, **Monthly Weather Rev., 91, pp. 99-164.**

D.B. Spalding, 1971. Mixing and Chemical Reaction in Steady Confined Turbulent Flames, **Thirteenth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA.**

D.B. Spalding, 1972. A Novel Finite-Difference Formulation for Differential Expressions Involving Both First and Second Derivatives, **Int. J Num, Methods Eng., 4, p. 551-559**

S.K. Srivatsa, 1983. Computation of Soot and NO_x Emissions from Gas Turbine Combustors, **NASA CR-167930, NASA, Cleveland, OH.**

J.C. Street and A. Thomas, 1955. Carbon Formation in Pre-Mixed Flames, **Fuel, 34, pp. 4-36.**

C. Tognazzi, 1998. Couplage fissuration-dégradation chimique dans les matériaux cimentaires caractérisation et modélisation. **Thèse de Ph D, INSA Toulouse.**

J.M. Torrenti, O. Didry, J.P. Ollivier and F. Plas, 1999. La dégradation des bétons, couplage fissuration-dégradation chimique. **HERMES Sciences Publications, Paris.**

R. van Genuchten, 1978. Calculating the unsaturated hydraulic conductivity with a new closed-form analytical model, **Report 78-WR-08, Water Resources Program, Department of Civil Engineering, Princeton University, Princeton, NJ 08540.**

R.S. Varga, 1962. ***Matrix Iterative Analysis*****, Prentice-Hall, Englewood Cliffs, New Jersey.**

N.B. Vargaftik, 1975. ***Tables of Thermophysical Properties of Liquids and Gases,*** **2nd Ed., John Wiley & Sons, New York, NY.**

J.A. Wheeler, 1973. Simulation of heat transfer fom a warm pipeline buried in permafrost, **Paper 27b, 74th National Meeting, American Institute of Chemical Engineers, New Orleans, Louisiana, 11-15 March.**

D.C. Wilcox, 1993. Comparison of Two-Equation Turbulence Models for Boundary Layers with Pressure Gradient. **AIAA, 31, 8, p 1414-1421.**

Z. Yang and T.H. Shih, 1993. A New Time Scale Based k-e Model for Near Wall Turbulence, **AIAA, 31, 7, p 1191-1198.**

(This page left intentionally blank.)

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 the 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:

$$C_M = \sum_{n=1}^{n+N} q_n[(\delta V_n \cap \delta V_M)/\delta V_M]/\delta V_M \quad , \qquad \text{(C.2.1)}$$

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
δV_n is the volume of the n^{th} particle
δV_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 α_n^M is the fractional contribution of the n^{th} particle to the M^{th} element, the above formula can be written as:

$$C_M = \frac{1}{\delta V_M} \sum_{n=1}^{n=N} \alpha_n^M q_n$$

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::

$$\alpha_n^M = \frac{1/d_n^2}{\sum_k 1/d_k^2}$$

Here the subscript k denotes the immediate neighborhood that consists of the elment in which the particle is located and its immediate neighbors. For a hex grid there will be 4 neighnbors in 2D and 6 in 3D; therefore the total mass of the particle will be distributed over 5 elments 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:

$\alpha_n^M = 1$ if particle in M ; $\alpha_n^M = 0$ otherwise

C.2.3 Species Concentration from Particle density

With the assumption that each particle has a volume based upon the 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:

$$R_n = \frac{1}{2}\left(\frac{q_n}{\rho}\right)^{1/3} \quad ; \quad R_M = \frac{1}{2}\delta V_M^{1/3} \quad ; \quad d_n = \sqrt{\sum_{i=1}^{i=3}(x_{Mi} - x_{ni})^2}$$

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:

$$\alpha_n^M = \frac{R_M + R_n - d_n}{R_M + R_n} \quad \text{if} \quad d_n < R_M + R_n \; ; \quad \alpha_n^M = 0 \quad \text{otherwise}$$

C.2.4 Species Concentration from Radius of Influence

The expressions used are:

$$R_M = \frac{1}{2}\delta V_M^{1/3} \quad ; \quad d_n = \sqrt{\sum_{i=1}^{i=3}(x_{Mi} - x_{ni})^2}$$

$$\alpha_n^M = 1 \quad \text{if} \quad d_n \le R_M \quad ; \quad \alpha_n^M = \frac{R_M^2}{R_n^2} \quad \text{if} \quad R_M < d_n < \beta R_M \quad ; \quad \alpha_n^M = 0 \quad \text{if} \quad d_n \ge \beta R_M$$