SOFTWARE QUALIFICATION REPORT
For ANSWER Version 4.00
Fluid Dynamics, Heat and Mass Transport Computer Program

CSCI: 30075 V4.0
DI: 30075-2003, revision 00A
MI: 30075-M09-001

Prepared by: ______________________ Date: __________
David Carrington
Repository Subsurface Design

Reviewed by: ______________________ Date: __________
M. N. Haas, Lead Nuclear Engineer
Repository Subsurface Design

Concurred by: ______________________ Date: __________
R. A. Morgan, Manager
Engineering Assurance

Approved by: ______________________ Date: __________
D. G. McKenzie III, Manager
Repository Subsurface Design

Civilian Radioactive Waste Management System
Management and Operating Contractor
CONTENTS

1. INTRODUCTION (SUMMARY) ................................................................. 4

1.1 OVERALL NATURE AND PURPOSE OF SOFTWARE ................................. 4

1.2 DESCRIPTION OF SOFTWARE ............................................................... 4

1.2.1 Documentation .................................................................................. 4

1.2.2 Mathematical Models and Numerical Methods .................................... 5

1.3 FUNCTIONAL REQUIREMENTS ............................................................... 5

1.4 SOFTWARE VALIDATION ................................................................. 5

1.4.1 Tasks ................................................................................................. 5

1.4.2 Methods ............................................................................................. 5

1.4.3 Implementing Documents ................................................................. 5

1.4.4 Acceptance Criteria .......................................................................... 6

1.5 SOFTWARE DOCUMENTATION VERIFICATION................................. 6

1.5.1 Mathematical Models and Numerical Methods .................................... 6

1.5.2 User Information ............................................................................... 6

1.5.3 Results of Software Documentation Verification ............................... 8

1.6 ADDITIONAL SOFTWARE DOCUMENTATION .................................... 8

2. SOFTWARE INSTALLATION ................................................................. 8

2.1 INSTALLATION PROCEDURE ............................................................. 8

2.2 VERIFICATION OF INSTALLATION ..................................................... 8

2.3 RESULTS OF THE INSTALLATION TESTS ........................................... 9

2.4 FILE LISTING ....................................................................................... 9

3. SOFTWARE VALIDATION ........................................................................ 9

3.1 TEST CASES ....................................................................................... 10

3.1.1 Independent Test Cases ................................................................. 10

3.1.2 Supplementary Test Cases .............................................................. 12

3.1.3 Regression Testing .......................................................................... 13

3.1.4 Validation Results for Independent Test Cases ............................... 13

3.1.5 Validation Results for Supplementary Test Cases ............................ 14

3.2 SUMMARY AND EVALUATION OF VALIDATION RESULTS .................. 15
3.3 REFERENCE LIST .................................................................................................................. 15

3.4 LISTING OF COMPUTER INPUT AND OUTPUT FILES FOR TEST RUNS ............ 15
  3.4.1 Independent Test Cases .................................................................................................. 15
  3.4.2 Supplementary Test Cases .......................................................................................... 15

4. RECOMMENDATION .............................................................................................................. 16
  4.1 List of Validated Software Elements ................................................................................ 16
  4.2 Software Components Not Validated ............................................................................... 16
  4.3 Recommendation for Approval ......................................................................................... 16

5. REFERENCES ............................................................................................................................... 17

6. ATTACHMENTS ...................................................................................................................... 18
  ATTACHMENT I CRWMS/M&O Software Change Request (SCR) Form ......................... 1
  ATTACHMENT II Software Acquisition Correspondence ................................................. 1
    II.1 ADP Justification ............................................................................................................. 1
    II.2 Software Price Quote .................................................................................................. 2
    II.3 License for ANSWER CFD Software Tool ............................................................... 3
  ATTACHMENT II Installation Information/Notes ................................................................. 1
    III.1 Installation Procedure ............................................................................................... 1
    III.2 Code Compilation .................................................................................................... 1
    III.3 Code Execution ....................................................................................................... 1
    III.4 Listing of ANSWER files in the ‘/usr3/answer/answer-1’ Directory ...................... 2
    III.5 Approval of ANSWER Software Validation by D. Carrington ............................ 3
  ATTACHMENT IV TEST CASE 1 ............................................................................................ 1
    IV.1 ANALYTIC SOLUTION TEST CASE 1 ................................................................. 1
    IV.2 NUMERICAL SOLUTION TEST CASE 1 ............................................................... 4
  ATTACHMENT V TEST CASE 2 ............................................................................................ 1
    V.1 ANALYTIC SOLUTION TEST CASE 2 ................................................................. 1
    V.2 NUMERICAL SOLUTION TEST CASE 2 ............................................................... 5
  ATTACHMENT VI SUPPLEMENTARY TEST CASES ........................................................ 1
1. INTRODUCTION (SUMMARY)

This Software Qualification Report (SQR) documents the installation, verification, and validation of the ANSWER fluid dynamics, heat and mass transfer code (Ref.1). The installation was performed on a Silicon Graphics Indigo 2 workstation. This SQR is as per Quality Assurance Procedure QAP-SI-O (Ref. 2) and QAP-SI-3 (Ref. 3) for acquired software. This qualification validates the capabilities of the ANSWER code, including solution of benchmark problems that are indicative of the type of problems that are expected within the Monitored Geologic Repository (MGR) emplacement drifts.

1.1 OVERALL NATURE AND PURPOSE OF SOFTWARE

The ANSWER code solves fluid dynamic problems with or without energy and mass transfer in both two and three-dimensions in a discretized domain. The method employed is a variational method, specifically it is weighted residual formulation of the governing equations.

The ANSWER code’s weighted residual formulation produces a control-volume (conserving) discretization of the Navier-Stokes, Energy and Mass transport equations utilizing either structured or unstructured computational domains or grids. For the salient features, refer to Attachment II – Justification of Software Acquisition and to the vendor-supplied user manual (Ref. 1).

1.2 DESCRIPTION OF SOFTWARE

1.2.1 Documentation

The current version of the ANSWER code, designated as ANSWER version 4.00h, was obtained from the code’s developer, Analytical and Computational Research, Inc. located in Bel-Air California. As Per QAP-SI-0 (Ref. 2), this software is classified as “Acquired Software”. Attachment II provides the acquisition correspondence, including justification for acquiring this software.

The following identifiers have been obtained from the Software Configuration Secretary (SCS) relative to this software are:

- Software Name: ANSWER
- Software Change Request number: version 4.0
- CSCI Identifier: 30075 V4.0
- Medium Identifier: 30075-M09-001

Software documentation for the ANSWER code is available in the vendor-supplied user’s manual (Ref. 1). The user’s manual (Ref. 1) includes all the necessary information required for a basic understanding and ability to execute the code. The manual describes the theory and methods for solution of fluid momentum, heat and mass transport, and combustion.
1.2.2 Mathematical Models and Numerical Methods

The mathematical model is in a class of methods known as integral projection methods or weighted residual methods. ANSWER’s weight is essentially a step function, having a value of one in the integral’s domain and zero otherwise. This use of the step function for the weight results in a method known as subdomain method, control-volume method or as stated in the user’s manual (Ref. 1, page ), Nodal Point Integration method.

The numerical technique applied for the solution of the Navier-Stokes equations employs the continuity equation to create a velocity-pressure correction method similar to the standard SIMPLE algorithm used for incompressible flows (Ref 1, pages 33-34). In the ANSWER code, this is referred to as the DEFCON approach (Ref 1, page 34) which is more general than the SIMPLE algorithm as it also allows for the solution of compressible flows (Ref. 1, pages 33-34).

1.3 FUNCTIONAL REQUIREMENTS

For the analysis required concerning repository design, the primary use of the code will be to determine the fundamental behavior of fluid dynamic phenomenon and the associated heat and mass transport processes occurring within the emplacement drifts. The code will also support evaluation of these processes in the main drifts.

1.4 SOFTWARE VALIDATION

1.4.1 Tasks

The validation tasks include development and execution of validation test cases, documentation of validation records, and verification of the results in conformance with the acceptance criteria.

1.4.2 Methods

Validation of the ANSWER software uses the test cases developed independently of the software supplier/developer (referred to as independent test cases), and supplementary test case provided by the software supplier/developer. Developer supplied test cases are a part of the code package.

1.4.3 Implementing Documents

The documents used to implement code validation for the ANSWER code validation procedure are: References 1, 2, 3, 4, 5, 6, and 7, for the independent test cases. Reference 1, and the data file accompanying the software “Ansd.dat” and “Coswirl_RNG.dat for the supplementary test cases.
1.4.4 Acceptance Criteria

For the independent test cases, the results of the ANSWER code should be compared to those in References 4 and 6. The solution of the problems posed for the independent test cases are analytic, therefore a solution from ANSWER should be in general agreement with these solutions.

For the supplementary cases, results from the purchased and installed version of ANSWER should be verified against those supplied in the code package. These results should be in general agreement, allowing for different representations of zero and other real numbers in general.

1.5 SOFTWARE DOCUMENTATION VERIFICATION

Developer supplied user’s manual ‘ANS_4_R1.pdf’ which is in electronic format serves as the documentation for the ANSWER code.

1.5.1 Mathematical Models and Numerical Methods

The following items required by QAP-SI-0 (Ref. 2) on documentation of the mathematical models and numerical methods for ANSWER were checked and determined to be adequate:

a. Overall nature and purpose of the software is given in Reference 1 Chapter 1.0

b. Intended use and associated requirements are found in Reference 1, Chapter 1.0

c. Description and equations of mathematical models are given in Reference 1, Chapters 2.0 and 3.0

d. Identification of input and output parameters are found in Reference 1, Chapter 6.0 and 7.0

e. Experimental and observational basis of mathematical models is not applicable to this except in that, ANSWER is based on physical and mathematical theory. Numerous concepts from any model involve the determination of whether actual observations are represented by mathematical equations and numerical processes. In this sense, all of the processes have an experimental or observational basis. These observations provide foundation for the mathematical representation of the physical processes.

f. Mathematical formulations of numerical methods are given in Reference 1, Chapter 4.0

1.5.2 User Information

The following items required by QAP-SI-0 (Ref. 2) on documents of the user information for ANSWER were checked and determined to be adequate:
a. Description of software usage
   i. Input and output options specified in Reference 1, chapters 6.0 & 7.0
   ii. Data files, input and output data, defaults and file formats, Reference 1, chapters 6.0, 7.0, appendix B and in the 97 vendor supplied validation tests, ‘ANS.DAT’ and ‘Case8_RNG_coswirl.txt’.
   iii. Error and warning messages with corrective actions are specified during execution and are written to the user specified output file along with all the diagnostics.
   iv. Hardware and software environments include the need for the standard math libraries found with the Silicon Graphics computer operating system Irix 6.2 to be able execute ANSWER, that is, to run the “answer4.00h,” executable file. This executable file is residing on the computers hard disk. Other necessary supporting files which are needed to run “answer4.00h,” are the license files, “Acrinit.acr,” “Trwinit.acr,” “Trw_lcns,” and the data file “cphtdfld.acr.”

b. Sample (Validation) problems as supplied with the software and are in the data files ‘Ansd.dat’ and ‘Coswirl_RNGl.dat’. These validation problems include:
   33 conduction – diffusion problems
   16 advection – diffusion problems
   21 force convection problems
   2 natural convection problems
   14 validation problems – problems compared to analytical solutions
   6 problems with no known analytic solution - benchmarked solutions
   1 turbulent flow problem for the k-e RNG model

   c. Installation procedure is simply performed by copy files to the hard drive.

   d. Requirements and design information
      i. Performance requirements and design constraints: Reference 1, Chapters 1.0
         ii. Interface with external data, hardware, or other software. The code utilizes external an external data file, “cphtfld.acr,” for combustion and chemical reaction solutions. The code has the ability to use outside user-specified tables, solver algorithm libraries, etc. This information is contained throughout the manual (Ref. 1).
         iii. Aspects of software and hardware operation are found in Reference 1, Section 1.0. One aspect of the codes usage that is unique to this platform is that the input file must be named as “input.” The output file always has the name “output.” The “output” file contains the diagnostic analysis of the input’s execution. The “input” file specifies a name for all the history and other diagnostic files or, “archive files,” the user might require including

---

1 Solutions Applicable to the intended use of this code are provided in the reference section of this document.
files for graphical visualization. These archive files can either be viewed by ACRPLOT, a separate graphics package purchased from ACRI Inc., or be converted to a TECPLOT format by the “acrplototecplot.f” code supplied on the diskette supplied by ACRI Inc with the ANSWER code.

iv. Functional requirements of the software are found in Reference 1, chapter 1.

v. Description of software structure is found in Reference 1, chapter 1.

1.5.3 Results of Software Documentation Verification

Based on the review of the ANSWER user manual ‘ANS_4_R1.pdf’ on the CDROM, it is judged that the requirements of QAP-SI-0 for the software documentation are fully met. It should be noted, software of this complexity and versatility is going to require a great deal on understanding about physics, numerical modeling, and the language structure required to implement the desired calculations. The user manual supplies the language constructs, the physical processes available, functional relationships, definable functions, and examples.

1.6 ADDITIONAL SOFTWARE DOCUMENTATION

Additional documentation for the ANSWER code is the rich text format file ‘ASOUR.rtf’, which describes the use of a new source, ‘MODE 8: Flux Transfer Between Adjacent Elements’ that is incorporated in ‘answer4.00h’ executable and validated in Test Case 2. The ‘ASOUR.rtf’ file is included on the software CDROM

2. SOFTWARE INSTALLATION

2.1 INSTALLATION PROCEDURE

The UNIX version of the ANSWER code was acquired for ACRI Inc. by ‘ftp’ a digital file transfer process and was then placed on a single CDROM. The code was installed by D. Carrington of the Repository Subsurface Design Group on a Silicon Graphics Indigo 2 workstation operating with an IRIX 6.2 operating system. The installation was performed by copying all the files from the CDROM to the workstation’s hard drive with the use of operating system’s utilities.

2.2 VERIFICATION OF INSTALLATION

Verification of the installation of ANSWER was performed by comparing files between the installation disk and the target drive and by whether the code would perform calculations on the developer-supplied data.
2.3 RESULTS OF THE INSTALLATION TESTS

All the files copied in the installation process reside in /usr3/answer/answer-1 on the workstation known as “vortex.ymp.gov”. The application of the above test method (section 2.2) verifies that the ANSWER code and its accompany files transfer properly and that the code was in operational order.

2.4 FILE LISTING

A listing of all the files including the executable file and supporting data files in the /usr3/answer/answer-1 directory is given in Section II of Attachment III. The directory contains the main executable file named “answer4.00h.” This SQR qualifies the “answer4.00h” file created September 23, 1998 at 4:11 PM. The “answer4.00h” file size is 1,270,616 bytes. No other executables are contained in the CFD code package, which require qualification.

In the code package there are two other executables, ‘ans2tecplot.exe’ and ‘Arcplot.exe’. Both executables are related to graphics processing and therefore are not subject to the requirements of QAP-SI-0 REV 4 (Ref. 2, page 1).

The file ‘ans2tecplot.exe’ is a computer code for transforming data written in the ‘*.arc’ format created by ANSWER to a format which is used by Tecplot Version 7.0². The file ‘ans2tecplot.exe’ was created for use on Windows95/NT platforms from the file ‘ans2tecplot.for’.

The file ‘Arcplot.exe’ is a computer code for reading data in the ‘*.arc’ format created by ANSWER and generates a graphical display of the ‘*.arc’ data.

All the files for the ANSWER code will be placed under the control of the Software Configuration Secretary (SCS) to provide security protection to these files. The media containing the files will be part of the baseline submittal package, and will be turned over to the SCS.

3. SOFTWARE VALIDATION

There are 2 independent test cases and 93 developer supplied supplementary test cases used for the software qualification. These test cases verify and validate the computational fluid dynamics, heat and mass transport processes expected to be of significant importance to its use.

The software validation was performed by D. Carrington. D. Carrington is acting independently of the developer to execute the validation and verification process. It should be noted though, that software of this complexity and flexibility does require specific training from the developer, and prolonged training in the field of momentum, heat and mass transport with specific emphasis on model development

² Tecplot is an industry standard graphics display computer code
3.1 TEST CASES

3.1.1 Independent Test Cases

This validation includes two test cases developed independently of the software developer. These cases are representative to the mass transport problems expected MGR excavations.

3.1.1.1 Test Case 1: Deposition of Particles with an Aerodynamic Diameter of 0.03 Microns

This case is a mass transport and deposition problem with particles having an aerodynamic diameter of three hundredths of a micron in a tube at laminar flow. Figure 1 illustrates the grid or computational domain with the appropriate boundary conditions.

![Figure 1: Grid with Boundary conditions for Test Case 1: Particulate with an Aerodynamic Diameter of One Micron in a Tube at Laminar Flow.](image)

Boundary Conditions (see Attachment IV for specific values for diffusivity and inlet velocity)

**inlet**
- $U \text{ in meters per second } V = 0$
- $C$ is a continuous source $1 \mu g / m^3$

**outflow**
- Pressure $= 0$
- $\frac{\partial U}{\partial x} \cdot \frac{\partial V}{\partial r} = 0$

**tube wall**
- $U$ and $V = 0$
- $C = 0$s
3.1.1.2 Test Case 2: Deposition of Particles with an Aerodynamic Diameter of Ten Microns

This case is a mass transport and deposition problem with particles having an aerodynamic diameter 10 microns in a square tube at laminar flow. Figure 2 illustrates the grid or computational domain with the appropriate boundary conditions.

**Boundary Conditions (see Attachment V for specific values for diffusivity, settling velocity or 10 micron particle and inlet velocity)**

**inlet**

- \( U \) in meters per second
- \( V = W = 0 \)
- \( C \) is a continuous source 1 µg/m³

**Walls**

- \( U, V & W = 0 \)
- \( \text{source} \mid_{x=0} = -v_s \) (settling velocity of species \( C \))
- \( \frac{\partial C}{\partial y} \mid_{\text{wall}} \) and \( \frac{\partial C}{\partial z} \mid_{\text{wall}} = 0 = 0 \)

**outflow**

- Pressure = 0
- \( \frac{\partial U}{\partial x}, \frac{\partial V}{\partial y}, \frac{\partial W}{\partial z} = 0 \)

Figure 2) Grid with Boundary Conditions for Test Case 2: Particulate with an Aerodynamic Diameter of Ten Microns in a Tube at Laminar Flow.
3.1.1.3 Input and Output files

The two independent test cases were run directly using ASCII input files. The ASCII input files for the independent test cases are named as follows:

- Independent Test Case 1: tubepen2d.dat
- Independent Test Case 2: tubepen10.dat

Four output files from executing the code are named as follows:

- Independent Test Case 1: tubepen2d.out & tubepen2d.arc
- Independent Test Case 2: tubepen10.out & tubepen10.arc

The file having an *.out extension list the input deck as read by the code, diagnostics for the domain and each variable and the iteration information. The file having an *.arc extension is the graphic file which can be viewed by ARCPLOT.

Results form the execution of these test cases are presented in Attachment IV for Test Case 1 and Attachment V for Test Case 2. The results of these test cases are compared to analytical solutions in their respective attachments. These results are discussed in section 3.1.4.

Execution of these independent cases is performed in the by typing the executable file name followed by the desired data input file which is then followed by the desired output file name, that is,

- answer4.00h tubepen2d.dat tubepen2d.out
- answer4.00h tubepen10.dat tubepen10.out

3.1.2 Supplementary Test Cases

The supplementary test cases selected are the problems provided by the code developer. These cases demonstrate the major capabilities of the software and represent many of the problems encountered in the analysis of fluid flows with and without heat transfer. These example problems are referred to in this report as “Supplementary test cases.” A more detailed description of these test cases is provided in the input deck ‘Ansd.dat’ and ‘Coswirl_RNG.dat’ supplied by the developer. For specific information, it is requested that the developer be contacted.

The ANSWER Supplementary test cases include:
- 33 conduction – diffusion problems
- 16 advection – diffusion problems
- 21 force convection problems
- 2 natural convection problems
- 14 validation problems – problems compared to analytical solutions
- 6 problems with no known analytic solution - benchmarked solutions
- 1 problem specifically for the k-e RNG turbulent model
These sample problems validate the following models in ANSWER:
1) Diffusion transport equations
2) General transport equations by diffusion, and by advection and diffusion
3) Momentum transport in compressible and incompressible regimes. The incompressible flows include both validations for laminar and turbulent flow.
4) Forced convective transport
5) Natural convective transport

These problems are validated on various domains where analytical solutions exist and some are set up as benchmark solutions. Benchmark problems are those having no known analytic solution but have been compared to solutions from other computer codes.

Results from the execution these supplementary test cases are presented in Attachment VI. These results are discussed in section 3.1.5. The input files for the performance of validation and verification on the workstation are:
   1) Ansd.dat
   2) Coswirl_RNG.dat

The output files from the performance of validation and verification from the SGI platform are:
   1) ANSD_SGI.out
   2) Coswirl_RNG_SGI.out

The output files from the developers platform used for comparison to the validation and verification files from the SGI platform (mentioned above) are:
   1) ANSD_developer.out
   2) Coswirl_RNG_developer.out

These supplemental test cases are included in Attachment VI in compressed ‘zip’ file form.

3.1.3 Regression Testing

Regression testing only applies to software with an existing baseline. The ANSWER code is a new baseline; therefore, no regression testing is required.

3.1.4 Validation Results for Independent Test Cases

The results for the two independent test cases are given in section 3.1 and compared with corresponding results as determined from the Reference 4 and Reference 6 (page 111). The analytic models are from References 4 and 6 as listed in section 6.
3.1.4.1 Test Case 1: Deposition of Particles with an Aerodynamic Diameter of 0.03 Micron

As is seen in Attachment IV, the comparison of the amount of mass being transfer to the wall plus the amount leaving the domain to the amount of mass entering the domain

These input and output files are compared to analytical solution. The analytic model used for comparison to Test Case 1 is boundary equations as determined from Reference 4. The analytic model is shown in their respective Attachment IV. Software used to evaluate the analytic model was MathCad 7 Professional, an industry standard object oriented mathematics tool. No special macros were developed for MathCad (Ref. 7). The software MathCad 7 Professional is not subject to the Quality Assurance Requirements and Description or QARD (Ref. 8) since MathCad is an industry-standard mathematics tool and because no special macros were developed (Ref. 2, page 1).

Calculation of the outflow bulk concentration is made for this case using the output data and the computer software Excel (Ref. 10). The software Excel 4.0 is not subject to the Quality Assurance Requirements and Description or QARD (Ref. 8) since Excel is an industry-standard mathematics tool and because no special macros were developed (Ref. 2, page 1).

3.1.4.2 Test Case 2: Deposition of Particles with an Aerodynamic Diameter of 10 Micron

These input and output files are compared to analytical solution. The analytic model used for comparison to Test Case 2 is from Reference 6 (page 111). The analytic model is shown in Attachment V. Software used to evaluate the analytic model was MathCad 7 Professional, an industry standard object oriented mathematics tool. No special macros were developed for MathCad (Ref. 7). The software MathCad 7 Professional is not subject to the Quality Assurance Requirements and Description or QARD (Ref. 8) since MathCad is an industry-standard mathematics tool and because no special macros were developed (Ref. 2, page 1).

3.1.5 Validation Results for Supplementary Test Cases

The output files for the developer-supplied sample problems run on the SGI platform ‘vortex.ymp.gov’ are named as follows:
1) ANSD_SGI.out
2) Coswirl_RNG_SGI.out

The output files produced on the developer’s platform are named as follows:
1) ANSD_developer.out
2) Coswirl_RNG_developer.out

A comparison of these output files produced on the SGI platform ‘vortex.ymp.gov’ with those produced on the developer’s platform reveals no significant difference. The performance of the computer code on the SGI platform versus the developers platform shows only differences in how zeros are being represented on the machines. This comparison was made with the use of the
3.2 SUMMARY AND EVALUATION OF VALIDATION RESULTS

The results of the ANSWER code meet the specified software validation acceptance criteria for both independent and supplementary test cases. The code is qualified for the range of applicability in accordance with the user’s manual. The results for the test case validate the code, and verify that convective-diffusion analysis in conjunction with the solution of the Navier-Stokes equations governing fluid flow are functioning correctly. Verification of the “k-w” turbulence model needs to be performed before its use. At this time, such a model is not necessary as the “k-e RNG” turbulence equation validated in the developers sample problems will suffice. There may come a time that such a model needs validation.

3.3 REFERENCE LIST

The specific documents relevant to this software qualification are References 1, and 4 as listed in section 5.0.

3.4 LISTING OF COMPUTER INPUT AND OUTPUT FILES FOR TEST RUNS

3.4.1 Independent Test Cases

The input and output files are “tubepen2d.dat” and “tubepen2d.out” for the first test case. The second test case input and output files are “tubepen10.dat” and “tubepen10.out.” All these files reside in the “/usr3/answer/vvdata” directory on the computer known as “vortex.ymp.gov.” The input and output files are listed in Attachment IV for Test Case 1 and Attachment V for Test Case 2.

3.4.2 Supplementary Test Cases

The input and output files are ‘Ansd.dat’ and ‘Coswirl_RNG.dat’ for the input data set and ‘ANSD_developer.out’ and ‘Coswirl_RNG_developer.out’ for the developer supplied sample/verification problems. All these files reside in the “/usr3/answer/vvdata” directory on the computer known as “vortex.ymp.gov.” The input and output files are listed in Attachment VI.
4. RECOMMENDATION

4.1 List of Validated Software Elements

This qualification document pertains to the ANSWER software elements listed in Section II.4 of Attachment III for the UNIX platform using IRIX 6.3 operating system. The qualified executable file ‘answer4.00h’ created on September 23, 1998 at 4:11 PM with the file size of 1,056,596 bytes. The validation applies to the solution of problems with the following models:

1) Diffusion transport equations
2) General transport equations by diffusion, and by advection and diffusion
3) Momentum transport in compressible and incompressible regimes. The incompressible flows include both validations for laminar and turbulent flow.
   Presently the turbulence models ‘k-e’, ‘k-e RNG,’ and the ‘k-e cubic” turbulence models are validated in the developer’s problem set.
4) Forced convective transport
5) Natural convective transport.

4.2 Software Components Not Validated

Verification of the ‘k-w’ turbulence model needs to be performed before its use. Presently such a model is not necessary as the ‘k-e RNG’ turbulence model is validated in the developer’s problem set. Until such time when the establishment of a baseline for the ‘k-w’ model occurs, the model should not be used.

4.3 Recommendation for Approval

In summary, the developer-supplied user’s manual ‘ANS_4_R1.pdf’ which is in electronic format provides sufficient information required for using the code. The user should have expertise in computational methods for the solution of heat, mass and momentum transport and have at least a master’s degree in engineering or computational mathematics. The test cases were executed and found to meet the specified criteria. The only problems encountered during the qualification activities were those relating to complexity of developing the appropriate problems. Such a code takes a good deal of practice to become proficient. Thus, ANSWER was shown to satisfy the QAP-SI-0 (Ref. 2) and QAP-SI-3 (Ref. 3) requirements as a fully qualified code on the Silicon Graphics workstation known as “vortex.ymp.gov.” It is therefore recommended that the ANSWER code be approved for use in work that is quality affecting.
5. REFERENCES

Bel Air, California: Analytic & Computational Research, Inc. TIC. 242406

Las Vegas, Nevada: Author. MOL.19980205.0304.

Las Vegas, Nevada: Author. MOL.19980205.0331.

& Sons, Inc. TIC. 241140

Particles*. New York, New York: John Wiley & Sons, Inc. TIC. 241149

MacMillian Co. TIC. 241094

Standard*. Cambridge, Massachusetts: Mathsoft, Inc. TIC. 242289

8. DOE OCRWM 1998. *Quality Assurance Requirements and Description for the Civilian 
Radioactive Waste Management Program*. DOE/RW-0333P REV 8. Las Vegas, Nevada: 
Author. MOL.19980601.0022


10. Microsoft Excel for Windows (version 4.0) documentation kit : vol. 1 : User's guide 1; vol. 2 
User's guide 2 ; vol. 3; Functional reference; vol. 4 Q+E Microsoft Excel user's guide; vol.5 
Switching to Excel from Lotus 1-2-3; vol.6 Tools quick reference. TIC. 9857
6. ATTACHMENTS

Attachment I: CRWMS/M&O Software Change Request (SCR) Form
Attachment II: Software Acquisition Correspondence
Attachment III: Installation Information/Notes
Attachment IV: Test Case 1
Attachment V: Test Case 2
Attachment VI: Supplementary Test Cases
ATTACHMENT I  CRWMS/M&O Software Change Request (SCR) Form
ATTACHMENT II  Software Acquisition Correspondence

II.1  ADP Justification
II.2 Software Price Quote
II.3 License for ANSWER CFD Software Tool
III.1 Installation Procedure

Installation of the Answer code on a SGI Indigo II workstation is straightforward. The following procedure is performed:

1) Log into the workstation from a Unix system, preferably the workstation’s monitor and keyboard and change directories by typing ‘cd /usr3/answer/answer-1’ to get to the directory where the files are to be transferred. (This could be any directory depending on the machine and preferences.)

2) If a directory ‘/usr3/answer/answer-1’ is not already present, make that directory by typing ‘mkdir /usr3/answer3/answer-1’.

3) Insert CDROM in to the drive on SGI Indigo II workstation

4) Once this is accomplished, double click on the ‘CD-ROM’ icon on the screen. Under the Desk icon, open the remote directory by selecting remote directory. Search the remote directory until you find ‘/usr3/answer/answer-1’ directory. Select okay to open directory ‘/usr3/answer/answer-1’. A window for this directory will appear.

5) Highlight the icons which are listing the files on the CD-ROM with the right mouse button. Holding the mouse button down drag and drop the icons of the selected files onto the now open directory window, ‘/usr3/answer’.

This completes the installation of the ANSWER cfd code.

III.2 Code Compilation

The code is in an executable form from the developer – no compilation is necessary.

III.3 Code Execution

The code is executed by typing the name of the executable file ‘answer4.00h’ and pressing the ‘return’ or ‘enter’ key. The input file is determined by the user, and is the output file. Many code diagnostics are available in the output file. Also specified in input file are files for special history and graphic display.
III.4 Listing of ANSWER files in the ‘/usr3/answer/answer-1’ Directory

- drwxr-xr-x 2 dave user 4096 Jan 21 11:32 .
- drwxrwxrwx 8 dave sys 4096 Nov 23 10:28 ..
- -rwxrwxrwx 1 dave user 51178 Oct 8 15:47 ACRINIT.ACR
- -rwxr-xr-x 1 dave user 1272278 Oct 8 16:33 ANS_4_R1.pdf
- -rw-r--r-- 1 dave user 222104 Dec 2 12:58 B05.ARC
- -rw-r--r-- 1 dave user 4832 Oct 23 11:49 Coswirl_RNG.dat
- -rwxrwxrwx 1 dave user 34254 Oct 8 15:47 P501.GRD
- -rwxrwxrwx 1 dave user 304891 Oct 8 15:47 P502.GRD
- -rwxrwxrwx 1 dave user 21504 Oct 8 15:47 P504.GRD
- -rwxrwxrwx 1 dave user 35 Oct 8 15:47 PARAM.ACR
- -rwxrwxrwx 1 dave user 1752 Jan 20 15:19 TRW_LCNS
- -rw-r--r-- 1 dave user 144896 Oct 22 14:39 ans2tecplot.exe
- -rw-r--r-- 1 dave user 21426 Oct 22 14:39 ans2tecplot.for
- -rwxrwxrwx 1 dave user 122077 Oct 8 15:47 ansd.dat
- -rw-r--r-- 1 dave user 2464508 Oct 8 16:38 ansd.out
- -rw-r-xr-x 1 dave user 1180920 Oct 28 13:43 answer4.00h
- -rwxrwxrwx 1 dave user 64 Oct 8 15:47 compile-sgi.sh
- -rwxrwxrwx 1 dave user 3449 Oct 8 15:47 cphtdfilt.acr
- -rw-r--r-- 1 dave user 1736730 Oct 22 14:53 tubepen10.arc
- -rwxr-xr-x 1 dave user 1483 Oct 23 11:38 tubepen10.dat
- -rw-r--r-- 1 dave user 606931 Oct 22 14:53 tubepen10.out
- -rw-r--r-- 1 dave user 2393519 Jan 20 18:19 tubepen2d.arc
- -rw-r--r-- 1 dave user 2056 Jan 21 11:32 tubepen2d.dat
- -rw-r--r-- 1 dave user 761693 Jan 20 18:19 tubepen2d.out
- -rw-r--r-- 1 dave user 1137637 Jan 21 08:04 tubepen2d.plt
III.5 Approval of ANSWER Software Validation by D. Carrington
ATTACHMENT IV TEST CASE 1

IV.1 ANALYTIC SOLUTION TEST CASE 1

Determination of Particulate Deposition By Diffusion in a Round Tube for Particles with a 0.03 µm Aerodynamic Diameter at 20 ºC and at 1 atmosphere

1.1 Physical Data and Required Constants

1.1.1 Density of Air

\[ \rho_{\text{air}} = 1.205 \text{ kg/m}^3 \]  
(Reference 4, page 603)

1.1.2 Viscosity of Air

\[ \mu_{\text{air}} = 1.81 \times 10^{-5} \text{ kg/m sec} \]  
(Reference 4, page 603)

1.1.3 Kinematic Viscosity of Air

\[ \nu_{\text{air}} = \frac{\mu_{\text{air}}}{\rho_{\text{air}}} \text{ m}^2 / \text{sec} \]  
(Reference 9, page xxxi)

\[ \nu_{\text{air}} = 1.5020746887967 \times 10^{-5} \text{ m}^2 / \text{sec} \]

1.1.4 Diffusivity for 0.3 micron Particle

\[ D_{\text{jcm}} = 6.23 \times 10^{-5} \text{ cm}^2/\text{sec} \]  
(Reference 5, backcover)

\[ D_{\text{jmeter}} = D_{\text{jcm}} \left( \frac{1}{100} \right) = 6.23 \times 10^{-9} \text{ m}^2/\text{sec} \]

1.1.5 Schmidt number for 0.03 micron Particle

\[ Sc_j = \frac{\mu_{\text{air}}}{(D_{\text{jmeter}} \cdot \rho_{\text{air}})} \]  
(Reference 9, pages xxvi and xxix)

\[ Sc_j = 2.411034813477 \times 10^3 \]
1.1.6 Drift Diameter

\[ D_{\text{drift}} = 0.01 \]

1.1.7 Drift Inlet Area

\[ \text{Area}_{\text{drift}} = \left(\frac{D_{\text{drift}}}{2}\right)^2 \cdot \pi \cdot m^2 \]

1.2 Flow Characteristics

1.2.1 Average Velocity in Drift

\[ U_{\text{avg}} := 3.2 \text{ meter/sec} \]

1.2.2 Determination of Flow Regime

\[ D_{h} := D_{\text{drift}} \quad \text{(Reference 4, page 102)} \]

\[ \text{Re} := \frac{D_{h} \cdot U_{\text{avg}}}{v_{\text{air}}} \quad \text{(Reference 4, page xxiv)} \]

\[ \text{Re} = 2.13 \cdot 10^3 \quad \text{Laminar Flow Regime} \]

1.3 Bulk Concentration at the Tube’s Outlet

Equation 3.70 in Reference 4, page 115 states

\[ T_{o} - T_{m}(x) = (T_{o} - T_{1}) \exp \left[ \frac{-\alpha \cdot \text{Nu} \cdot (x - x_{1})}{r_{o}^2 \cdot U} \right] \]

where

- \( T_{o} \) = Temperature at the wall
- \( T_{m}(x) \) = the bulk temperature as a function of distance

(Reference 4, page 109 combined with page 115)
Making appropriate analogy to heat transfer, we have the following variables in mass transfer corresponding to variables in heat transfer.

\[ T \equiv C \quad \text{Temperature to Concentration} \quad \text{(Reference 4, page 481)} \]
\[ \alpha \equiv D_{\text{meters}} \quad \text{Thermal diffusivity to Mass diffusivity} \quad \text{(Reference 4, page 481)} \]
\[ \text{Nu} \equiv \quad \text{Nusselt number to the Sherwood} \quad \text{(Reference 4, page 482)} \]

and letting

\[ r := \frac{D_{\text{drift}}}{2} \quad \text{Radius of the tube} \]

\[ C_1 := 1.0 \quad \text{Entrance Concentration} \]

And using the average Sherwood number (Sh) over the developing boundary layer

\[ \text{Sh} := 10. \quad \text{(Reference 4, page 488 and figure 3.14 on page 124)} \]
Then the bulk (mean) concentration is given as a function of Length after making the substitutions as just described

$$C_{m}(\text{Length}) := \exp\left(-D \text{ jmeter} \cdot \text{Sh} \cdot \frac{\text{Length}}{r^2 \cdot U_{avg}}\right)$$

(Reference 4, page 115)

The average Sherwood number (Sh) for this developing mass transfer boundary layer in this relatively short tube is about 10.0 (see reference 4, figure 3.14 on page 124 and page 488). This 30.5-meter length of tube is short for deposition from diffusion of a fine particulate since the mass diffusion boundary isn’t fully developed until the length is well beyond 1000 meters (Reference 4, Page 488).

The bulk concentration at the outlet, that is, at 30.5 meters downstream from the inlet, calculated from this boundary layer equation is

$$C_{m}(\text{Length}) = 0.981$$

IV.2 NUMERICAL SOLUTION TEST CASE 1

The analysis of this case is consists of evaluating the bulk concentration at the outflow and determining how well it fits the analytical solution.

The calculations to determine a bulk concentration for this Test Case is found in the file ‘bulkC_sm2dss.xls,’ which is an Excel (Ref. 10) spreadsheet. This file is found on the attached DISK 3 having the name ‘Independent Test Cases.’ All the files for Test Case 2 are in the compressed file ‘Test_Case1.zip.’ Included in the *.zip file are the following input, output, graphical display, and analysis files, ‘tubepen2d.dat,’ ‘tubepen2d.out,’ and ‘tubepen2d.plt,’ and ‘bulkC_sm2dss.xls,’ respectively.

The calculation for bulk concentration at the outflow, as seen in the spreadsheet calculation is 0.98, which represents a penetration of 98 percent since the bulk concentration at the inflow is 1.00. The analytic model calculation in this section (above) has a penetration of 98.1 percent. The analytic model and the numerical model agree therefore, this test case verifies mass diffusion processes for the ANSWER code for particulate with high Schmidt numbers. The solution to the problem also verifies that the allocation command for scalar variables is being preformed correctly by the code.
V.1 ANALYTIC SOLUTION TEST CASE 2

Determination of Particulate Deposition by Gravitation Settling in a Square Tube for 10.0 µm Aerodynamic Diameter Particles in Suspended in Air at 20 °C and 1 atmosphere

1.1 Physical Data and Required Constants at 1 atm

1.1.1 Settling Velocity for the particle

\[ v_{sUO} = 3.05 \times 10^{-1} \text{ cm/sec} \]  

(Reference 5, backcover)

\[ v_{sUO} = \frac{v_{sUO}}{100} \text{ conversion to m/sec} \]

\[ v_{sUO} = 3.05 \times 10^{-3} \text{ m/sec} \]

1.1.2 Density of Air

\[ \rho_{\text{air}} = 1.205 \text{ kg/m}^3 \]  

(Reference 4, page 603)

1.1.3 Viscosity of Air

\[ \mu_{\text{air}} = 1.81 \times 10^{-5} \text{ kg/m sec} \]  

(Reference 4, page 603)

1.1.4 Kinematic Viscosity of Air

\[ \nu_{\text{air}} = \frac{\mu_{\text{air}}}{\rho_{\text{air}}} \text{ m}^2/\text{sec} \]  

(Reference 9, page xxxi)

\[ \nu_{\text{air}} = 1.50207469 \times 10^{-5} \]
1.1.5 Diffusivity for 10 micron Particles

\[ D_j : = 2.40 \times 10^{-8} \text{ cm}^2/\text{sec} \quad \text{(Reference 5, backcover)} \]

\[ D_j := D_j \frac{1}{100^2} \quad \text{converting to m}^2/\text{sec} \]

\[ D_j = 2.4 \times 10^{-12} \text{ m}^2/\text{sec} \]

1.1.6 Schmidt number for 10 micron Particles

\[ Sc_j := \frac{\mu_{\text{air}}}{\left(D_j \rho_{\text{air}}\right)} \quad \text{given by (Reference 9, pages xxvi and xxix)} \]

\[ Sc_j = 6.25864454 \times 10^6 \]

1.1.7 Square Tube Inlet Area

\[ \text{Area}_{\text{tube}} := \left(\text{Tube height}\right)^2 \text{ meters} \]

1.1.8 Wetted Perimeter

\[ \text{wetted_perimeter} := 4 \times \text{Tube height} \text{ meters} \]

1.1.9 Hydraulic Diameter

\[ D_{\text{hydraulic}} := 4 \frac{\text{Area}_{\text{tube}}}{\text{wetted_perimeter}} \text{ meters (Reference 4, page 102)} \]

1.1.10 Specifying Velocity in the Tube

\[ U_{\text{avg}} := 0.01 \text{ m/sec} \]
1.2. Calculating Volumetric Flow Rate

\[ Q_{\text{flow}} := \text{Area}_{\text{tube}} \cdot U_{\text{avg}} \quad \text{m}^3 / \text{sec} \quad (\text{Reference 9, page 46}) \]

\[ Q_{\text{flow}} = 0.04 \quad \text{m}^3 / \text{sec} \]

1.3. Calculation Laminar Flow Regime

\[ \text{Re} := \frac{D_{\text{hydraulic}} \cdot U_{\text{avg}}}{\nu_{\text{air}}} \quad \text{(Reference 4, page xxiv)} \]

\[ \text{Re} = 1.3314917 \times 10^3 \]

1.4. Analytic solution of the Loss Fraction from Settling

Mass quantity in the suspended

\[ C_{\text{inUO}} := 1. \quad \text{grams / m}^3 \]

L := 0, 1... 13. \quad \text{Calculate over a section of the tube from 0 to 1.25 meters}

\[ \psi_{\text{loss}}(L) := \frac{\alpha_{\text{sUO}} \cdot L}{2 \cdot \text{Tube height} \cdot U_{\text{avg}}} \quad (\text{Reference 6, page 111}) \]

<table>
<thead>
<tr>
<th>L</th>
<th>( \psi_{\text{loss}}(L) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.07625</td>
</tr>
<tr>
<td>0.15</td>
<td>0.1525</td>
</tr>
<tr>
<td>0.3</td>
<td>0.22875</td>
</tr>
<tr>
<td>0.45</td>
<td>0.305</td>
</tr>
<tr>
<td>0.6</td>
<td>0.38125</td>
</tr>
<tr>
<td>0.53</td>
<td>0.4575</td>
</tr>
<tr>
<td>0.61</td>
<td>0.53375</td>
</tr>
<tr>
<td>0.76</td>
<td>0.61</td>
</tr>
<tr>
<td>0.83</td>
<td>0.68625</td>
</tr>
<tr>
<td>0.91</td>
<td>0.7625</td>
</tr>
<tr>
<td>0.99</td>
<td>0.83875</td>
</tr>
<tr>
<td>0.1</td>
<td>0.91</td>
</tr>
<tr>
<td>0.99</td>
<td>0.99125</td>
</tr>
</tbody>
</table>
1.5 Calculation of Penetration Percent

\[ C_{\text{penUO}_2}(L) = C_{\text{inUO}} \left( 1 - \psi_{\text{loss}}(L) \right) \]

<table>
<thead>
<tr>
<th>( C_{\text{penUO}_2}(L) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
</tr>
<tr>
<td>0.92375</td>
</tr>
<tr>
<td>0.8475</td>
</tr>
<tr>
<td>0.77125</td>
</tr>
<tr>
<td>0.695</td>
</tr>
<tr>
<td>0.61875</td>
</tr>
<tr>
<td>0.5425</td>
</tr>
<tr>
<td>0.46625</td>
</tr>
<tr>
<td>0.39</td>
</tr>
<tr>
<td>0.31375</td>
</tr>
<tr>
<td>0.2375</td>
</tr>
<tr>
<td>0.16125</td>
</tr>
<tr>
<td>0.085</td>
</tr>
<tr>
<td>8.75 \times 10^{-3}</td>
</tr>
</tbody>
</table>
V.2 NUMERICAL SOLUTION TEST CASE 2

Determining the validity of this case is done by visual inspection of the graphical representation of the output from Test Case 2 and comparing it to the charted solution presented above in this attachment. The location of the slice represented graphical is a vertical cross-section at the axial centerline as shown in Figure 3 below.

The data input and output files for Test Case 2 are: ‘tubepen10.dat,’ ‘tubepen10.out,’ and the graphical file ‘tubepen10.plt’ and are stored on the attached DISK 3 name “Independent Test Cases.” These files are in a compressed file, ‘Test_Case2.zip.’

Figure 3) Concentration (g/m$^3$) of 10 micron particulate as a function of distance

The simulation as shown in Figure 3 clearly indicates that settling is occurring. Although the penetration is moving beyond the 13 meters predicted analytically the answer is correct. The discrepancy is from the very slight diffusion of the particulate in the airstream and entrance effects of developing flow in a duct. Neither of these effects is considered in the analytic model.
V.1 Listing of Ansd.dat and Coswirl_RNG.dat Input Files and Output File Run on Machine Known as vortex.ymp.gov from Developer Supplied Supplementary Test Cases These files are listed on DISK 1 as ANSDOUTUE.zip.

V.2 Listing of Ansd.dat and Coswirl_RNG.dat Output Files from Developer Supplied Supplementary Test Cases as Executed by the Developer on a Different Platform These files are listed on DISK 2 as ANSDOUTSE.zip.

V.3 Listing of COMPARE.DAT, a comparison of the output file from the Developer Supplied Supplementary Test Cases as executed by the developer Verses the output file of the Developer Supplied Supplementary Test Cases run on machine known as vortex.ymp.gov. These files are listed on DISK 2 as ANSDCOMPARE.zip.