

#### Department of Energy

Carlsbad Area Office
P. O. Box 3090
Carlsbad, New Mexico 88221

A-93-02 II-I-10

February 26, 1997

Ms. Ramona Trovato, Director US Environmental Protection Agency Office of Radiation Programs 401 M. Street SW Washington, DC 20460

Dear Ms. Trovato:

The Carlsbad Area Office (CAO) is pleased to submit this fifth and final group of responses to requests for supplemental information contained in the EPA letter of December 19, 1996 to Al Alm. We have submitted four previous groups (January 17 and 24, and February 7 and 14) as the material was developed in order to provide EPA with the requested information as early as possible. This final group completes our responses to your request. As in the earlier submittals, we have reproduced the issue verbatim from the December 19, 1996 letter and inserted the CAO response in each case.

We are confident that the EPA will find this supplemental information helpful in your review process. Should you have any questions regarding this information or require anything further, please contact me at (505) 234-7300.

Sincerely,

George E. Dials Manager

Enclosure

cc:

F. Marcinowski, EPA

EPA Comment Enclosure 1, Page 4 194.14(a)(2)

#### **Comment Text**

#### 194.14(a)(2)

Part 194 requires a description of the geology, geophysics, hydrogeology, hydrology, and geochemistry of the disposal system and its vicinity and how these conditions are expected to change and interact over time.

The CCA does not include updated information obtained from recent site investigation-related studies. The CCA states that "these recent studies... provide detailed information necessary to construct the conceptual models," but does not summarize what these studies entailed and how they impact the understanding of site characteristics relative to older data. The CCA implies, on page 2-9, Section 2.1, that these data are included in Chapter 6 and associated appendices.

The CCA should include more detailed information pertaining to the more recent studies so that an understanding of the site conditions and linkages of this information with the conceptual model development can be achieved. In addition, the CCA should provide a discussion of newly acquired site-specific information (i.e., information on Culebra and retardation studies presented at the 10/11/96 meeting between DOE and State of New Mexico representatives), and discuss how this information impacts site conceptual model development.

#### **DOE** Response

Detailed information pertaining to recent development on the conceptual model for transport in the Culebra that was presented at the October 11, 1996 meeting between DOE and State of New Mexico representatives is contained in SAND97-0194 Conceptual Model for Transport Processes in the Culebra Dolomite Member, Rustler Formation by R. M. Holt. This report is in review at Sandia National Laboratories and is not available for distribution at this time. Arrangements can be made through the records center for EPA representatives to see a high-quality, near-final draft of this report. A publication pre-print will be available for release in March. The concepts of Culebra transport contained in this report were used in development of the performance assessment parameter values. These concepts represent a significant increase in confidence regarding the predictability of Culebra transport processes and a significant decrease in associated uncertainties.

The SAND report by Holt focusses on the Culebra field tests and conceptual insight gained from them. It also contains a brief description of the intact-core column testing elution experimental technique; identification of the radioactive tracers used as non-sorbing and sorbing tracers; presentation of typical elution breakthrough curves for Na-22 and U-232; observation of the fact that, of the actinides, only Np and U have eluted (so Am, Pu, and Th have not). In addition, the report contains petrographic descriptions of the core columns and interpretations of the advective and diffusive porosity distributions in the cores.

EPA Comment Enclosure 1, page 5 194.22(a)(2)(iii)

#### **Comment Text**

#### Models and Computer Codes

Part 194 requires that the CCA include a description of conceptual models and scenario construction used to support the CCA. In addition, Part 194 states that documentation of all models and computer codes must be included.

There is a significant problem with the completeness of the CCA documentation that deals with the CCDF formalism and the codes that implement it. While the current versions of the formalism and codes may be doing exactly what is required of them, and while those intended activities may be what is needed for the PA, it is often difficult and sometimes impossible to determine what it is, exactly, that they are doing and to verify that this is all happening as intended. The documentation is, in places, too sparse to enable a reviewer to acquire a comprehensive understanding of the current form of the formalism and codes.

DOE needs to provide documentation for the CCDF formalism and for the codes that implement it. Specific examples are provided below.

#### **DOE Response**

Because the comment on 194.22(a)(2)(iii), enclosure 1, page 5 and 194.23(a)(3)(ii), enclosure 1, page 7, raise very similar points, the DOE has chosen to address them with a common response.

Because these two comments raise very similar points, the DOE has chosen to address them in a single response.

Many of the questions raised here are addressed in Appendix SA of the CCA, where the construction of CCDFs for cuttings and cavings releases, spallings releases, and direct brine releases are described. For example, Section SA.3, and Table SA-1 specifically, describe the construction of CCDFs for cuttings and cavings, including a description of the use of interpolation. Section SA.5, and Tables SA-2 and SA-3, contain similar information for spallings releases. Section SA.8, and Tables SA-4 and SA-5 provide the analogous information for direct brine releases.

Additional documentation of the construction of CCDFs has been provided to the EPA

EPA Comment Enclosure 2, Page 3 194.23(a)(3)(iv)

#### **Comment Text**

#### 194.23(a)(3)(iv)

Section 194.23(a)(3)(iv) requires documentation that the "...computer codes are free of coding errors and produce stable results."

One feature of the SECOFL2D computer code (SECO User's Manual) that was not tested was that the code implements the transition from a regional grid to a local grid.

The Department needs to devise a test of this key component and document the accuracy of the bilinear interpolation scheme for both boundaries and properties.

#### **DOE** Response

PRESECOFL2D, the pre-processor for SECOFL2D, is the code that implements the transition from regional properties to local properties for SECOFL2D. Documentation of the testing of PRESECOFL2D which documents the accuracy of the bilinear interpolation scheme for the properties is found in the QA records for PRESECOFL2D: PRESECOFL2D, Version 4.02ZO, Version Date 5/20/94, Requirements Document and Verification & Validation Plan contains the design of the test problem, and the results of the test are found in PRESECOFL2D, Version 4.02ZO, Version Date 5/20/94, Validation Document (both documents are attached).

SECOFL2D implements the transition from the solution on the regional grid to the local grid boundary. Documentation of the testing of SECOFL2D which documents the accuracy of the bilinear interpolateion scheme for the boundaries is found in the QA records for SECOFL2D: SECOFL2D, Version 3.01ZO, Version Date 8/9/93, Requirements Document and Verification & Validation Plan contains the design of the test problem, and the results of the test are found in SECOFL2D, Version 3.01ZO, Version Date 8/9/93, Validation Document (both documents were previously supplied to the EPA).

### WIPP PA

## REQUIREMENTS DOCUMENT AND VERIFICATION AND VALIDATION PLAN (RD/VVP)

for

PRESECOFL2D

Version 4.02ZO

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#### 1.0 INTRODUCTION

The purpose of this document is to identify the requirements of the PRESECOFL2D code and to describe the testing, including coverage analysis and regression testing, that will be performed. This code was qualified as Level A under QAP 19-1 Rev. F. The QA package for this code, referred to as the primitive baseline, is on file in the SWCF. The verification section of that package demonstrates that the functional requirement R.1 stated in this document is satisfied.

#### 1.1 Software Identifier

PRESECOFL2D Version 4.02ZO

WIPP PA Code Prefix: SF2D1

#### 1.2 Points of Contact

Code Sponsor: Rebecca L. Blaine Code Consultant: Rebecca L. Blaine

Ecodynamics Research Associates. Inc.

P. O. Box 9229

Albuquerque, New Mexico 87119

(505)843-7445

#### 1.3 Description

The purpose of PRESECOFL2D is to create all of the input files required to run the code SECOFL2D. Material properties and grid information are obtained from CAMDAT databases.

#### 2.0 REQUIREMENTS

#### 2.1 Functional Requirements

- R.1 Creates all input files needed to run SECOFL2D. These files are:
  - 1) An ASCII file containing run parameters
  - 2) A binary file containing regional material property information obtained from a CAMDAT database.
  - 3) A binary file containing local material property information.
- R.2 Interpolates material properties from the regional grid to the local grid.

#### 2.2 Performance Requirements

This code has no performance requirements.

#### 2.3 Attribute Requirements

This code has no attribute requirements.

#### 2.4 External Interface Requirements

- R.3 This code reads an ASCII input file containing run parameters.
- R.4 This code reads an input regional CAMDAT database with grid information material properties.
- R.5 This code reads an input local CAMDAT database with grid information.
- R.6 This code produces all of the input files necessary to run SECOFL2D.
- R.7 This code must be linked to the libraries CAMCON\_LIB, CAMDAT\_LIB and CAMSUPES\_LIB.

#### 2.5 Other Requirements

There are no other requirements for PRESECOFL2D that need verification.

#### 3.0 DESIGN OVERVIEW

#### 3.1 I/O Description

The following is a description of the input and output files associated with PRESECOFL2D. The first three output files are used as input to SECOFL2D. All file names shown here are for example only. The user chooses the appropriate file names for the particular calculation being done at PRESECOFL2D execution time.

#### Input Files:

presecofl.inp - ASCII input file containing run parameters.

secofl\_loc.cdb - Input local CAMDAT database containing local grid information.

secofi\_reg.cdb - Input regional CAMDAT database containing material property and grid information.

#### Output Files:

- secofl.inp ASCII output file created by PRESECOFL2D containing run directives and boundary condition information. Used as an input file by SECOFL2D.
- secofl\_reg.prp Binary output file created by PRESECOFL2D containing the grid material property information for the regional grid. Used as an input file by SECOFL2D.
- secofl\_loc.prp Binary output file created by PRESECOFL2D containing the grid and material property information for the local grid. Used as an input file by SECOFL2D.

presecofi.dbg - ASCII output debug/log file

#### 3.2 Context Diagram

The data flow design for PRESECOFL2D is presented using the context diagram in Figure 3.1.

FIGURE 3.1
Data Flow for PRESECOFL2D

secofi\_loc.cdb

presecofi.inp secofi\_reg.cdb

PRESECOFL2D

secofi.inp presecofi.dbg

secofi reg.prp secofi loc.prp

#### 3.3 Design Constraints

This code has already been developed and therefore has no design constraints.

#### 4.0 ADDITIONAL FUNCTIONALITY TO BE TESTED

There is no additional functionality to be tested.

#### 5.0 FUNCTIONALITY NOT TESTED

The following features will not be tested because they will not be used as part of the WIPP PA.

- 1) Input of well parameters standard and time dependent.
- 2) Input of lake, river, and precipitation factors.

#### 6.0 TESTING ENVIRONMENT

Hardware Platform:

DEC Alpha

Operating System:

OpenVMS Version 6.1.

Directory:

WP\$TESTROOT:[SF2D1]

#### 7.0 STATIC TESTING

Static testing will be performed using both the source code analyzer FLINT and the source code analyzer DECset-SCA. FLINT is used to detect non-ANSI standard FORTRAN coding. DECset-SCA is used to reveal any uncalled modules, to reveal any unreferenced variables, and the display the calling tree. Since PRESECOFL2D is a multimodule program, a single file should be created with all of the modules appended together. FLINT should be used on this file. The output from FLINT will be examined by the code sponsor and any findings will be resolved.

DECset-SCA will be invoked during the build process. The build process will be performed using the build script SF2D1\_BUILD.COM. This process will be described in more detail in the WIPP PA Implementation Document for PkESECOFL2D Version 4.02ZO. As a result of the build process, a debug executable capable of doing PCA (Performance Coverage Analysis) analysis will be created and the SCA code analyzer will create the following files:

SF2D1\_SCA\_MOD\_NOT\_REF.TXT SF2D1\_CALLTREE.TXT SCA\$EVENT.DAT

These files will be described in complete detail in the WIPP PA Validation Document for PRESECOFL2D Version 4.02ZO. A complete description of the process outlined below to convert the data in SCASEVENT.DAT to a readable format will also be contained in that document.

Following the build process, SCA will be invoked at the VMS \$ prompt and the following commands should be executed on the SCA\$EVENT.DAT file in the WP\$TESTROOT: [SF2D1.SCA] directory to convert data in the file to ASCII format:

SCA> set lib []
SCA> show module/all/output=sf2d1\_modules.out
SCA> exit

The SCA output will be examined by the code sponsor. Unreachable coding will either be changed so that it is reachable, or justified as not being relevant to the performance of the software as it relates to WIPP PA.

#### 8.0 COVERAGE TESTING

The coverage analysis for PRESECOFL2D will be performed using DECset PCA. This tool will be used to identify modules that are not exercised by the test set. A unique executable will be created for the purpose of coverage analysis during the build process. This executable will be generated by using the SCMS build script, SF2D1\_BUILD.COM. The creation of this executable will be described in more detail in the WIPP PA Implementation Document for PRESECOFL2D Version 4.02ZO.

The command file SF2D1\_TESTCASE\_PCA\_CUM.COM will be used to run the PRESECOFL2D test cases with PCA. The PCA output will be examined by the code sponsor and any unexercised modules must be justified.

#### 9.0 FUNCTIONAL TESTING

Verification of functional requirement R.1 has been done and is on record in the primitive baseline submitted to the SWCF. The following test case will be used for verifying requirement R.2, for coverage analysis, and for regression testing.

All files needed to test PRESECOFL2D can be fetched from the SCMS. The directory WP\$TESTROOT:[SF2D1.TESTCASES] on the DEC Alpha has been created and should be used for running the test case. To verify requirement R.2 and for regression testing, Test Case I (described below) is run using the command file SF2D1\_TEST\_NODBG\_RUN.COM. This file is shown in Figure 9.1.

## FIGURE 9.1 SF2D1\_TEST\_NODBG\_RUN.COM - Command file for Running The Test Case

```
$ set noon
$!
$! This file runs all test cases for PRESECOFL2D using the NOOE8UG executable
$ !
$ TESTDIR_SYM == "wp$testroot:[sf2d1.testcases]"
$ PRESECOFL2D == "$ wp$prodroot:[sf2d.exe]presecof(2d.exe"
5!
$ define /proc testdir wpstestroot:[sf2d1.testcases]
5.1
$ show sym testdir_sym
$ IF F$MODE () .EGS. "BATCH" .AND. F$ENVIRONMENT ("DEPTH") .EQ. 0 THEN -
    SET DEFAULT !TESTDIR SYM!
$! Set up the first test case and run PRESECOFLIZO
$ WRITE SYSSOUTPUT "STARTING THE RUN FOR THE PRESECUFIED TEST CASE"
$
$ PRESECOFL2D SF2D1_REGION_TEST.CDB SF2D1_REGION_TEST.CDB -
    SF2D1_LOCAL_TEST.CD8 CANCEL SF2D1_PRESECOFL_TEST.INP SECOFL2D_TEST.INP -
    SF2D1_REGION_TEST.PRP_SF2D1_LOCAL_TEST.PRP_CANCEL_PRESECOFL_TEST.DBG
S
$ write sys$output "SUCCESSFUL COMPLETION OF TEST EXECUTION"
```

## INFORMATION ONLY

#### 9.1 Test Case 1 - Interpolation Test and Regression Test

#### 9.1.1 Test Objective

This test is run to test the interpolation of properties from the regional grid to the local grid. This test case satisfies requirement R.2. This test is also run for regression testing. The purpose of the regression test is to show that PRESECOFL2D produces identical results when writing the regional binary property file as were produced in the verification process documented in the primitive baseline. The entire verification process is not relevant to this regression test and so only the portion of the results in the primitive baseline that relate to writing the binary property file will be used. The regression test will show that data currently written to the regional binary property file is exactly the same as in the baseline verification process. PRESECOFL2D also writes an ASCII input file and a debug file. The ASCII input file was verified by visual inspection and by demonstrating that SECOFL2D read and used the input data correctly. The nature of this verification is not useful for regression testing and is not included here. The debug file does not contain information relevant to the verification process in the baseline and is not documented there.

#### 9.1.2 Test Procedure

The following is a list of all the files that are associated with this test case. All of the input files are input for PRESECOFL2D. The output files have designated in parenthesis which program has produced them. The testing tools have designated, in parenthesis, the test they are used for. Input files:

WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_REGION\_TEST.CDB WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_LOCAL\_TEST.CDB WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_PRESECOFL\_TEST.CDB

#### Output Files:

WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_REGION\_TEST.PRP (PRESECOFL2D)
WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_LOCAL\_TEST.PRP (PRESECOFL2D)
WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_REGION\_TEST.ASC (READ\_PRP)
WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_LOCAL\_TEST.ASC (READ\_PRP)
WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_TEST\_READ.OUT (TEST\_READ\_1)

#### Testing Tools:

WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_READ\_PRP.FOR (Interpolation) WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_TEST\_READ\_1.FOR (Regression)

Run the test case with the command file shown in Figure 9.1. The procedure to follow for regression testing is stated in Section 10 below. For the interpolation test, following the

execution of the command file, the program SF2D1\_READ\_PRP (compiled and linked from SF2D1\_READ\_PRP.FOR) should be executed twice, once using the regional data and once using the local data. This program converts the regional binary property file, SF2D1\_REGION\_TEST.PRP, to an ASCII file, SF2D1\_REGION\_TEST.ASC, and the local binary property file, SF2D1\_LOCAL\_TEST.PRP, to an ASCII file, SF2D1\_LOCAL\_TEST.ASC, so that they can be examined with an editor. All of the material properties used to run SECOFL2D are constants except for hydraulic conductivity. Therefore, checks of porosity (phi) and bulk compressibility (alpha) need only show that they have remained constant. A hand-calculation is done for hydraulic conductivity to show that the values have been correctly interpolated (using bilinear interpolation) from the regional grid to the local grid.

To verify that the porosity and bulk compressibility have remained constant, edit the file SF2D1\_REGION\_TEST.ASC. First, search for the string "alpha". Examination of this array shows that this is a constant value of 7.57E-01 for each element in the grid. (The value of bulk compressibility is 7.57E-10 on the database, but it has been scaled by 10<sup>9</sup> as required by SECOFL2D.) Next, search for the string "phi". Examination of this array shows that this is a constant value of 1.4542E-01 for each element in the grid. Now repeat this process with the file SF2D1\_LOCAL\_TEST.ASC. Searching for the string "alpha" shows that this array is a constant value of 7.57E-01, and searching for the string "phi" shows that this array is a constant of 1.4542E-01.

To verify the interpolation for the non-constant values of hydraulic conductivity, four points are checked by hand-calculation. The four element locations in the local grid are cells (12,15), (20,47), (35,25) and (40,40). First, the element locations relative to the regional grid are found. The element locations in meters are converted to locations (in meters) in regional domain. The x and y offsets of the local grid from the origin of the regional grid are 12826.1 and 10665.8 respectively. The angle of rotation is 38° counter clockwise. The coordinates (in meters) of the cell centers of the elements in the local grid are:

Element 1 (12,15): 1437.5, 1812.5 Element 2 (20,47): 2437.5, 5812.5 Element 3 (35,25): 4312.5, 3062.5 Element 4 (40,40): 4937.5, 4937.5

The regional coordinates are calculated by:

Element 1:  $12826.1 + 1437.5\cos 38^{\circ} - 1812.5\sin 38^{\circ} = 12842.97903$  $10665.8 + 1812.5\cos 38^{\circ} + 1437.5\sin 38^{\circ} = 12979.08286$ 

Element 2:  $12826.1 + 2437.5\cos 38^{\circ} - 5812.5\sin 38^{\circ} = 11168.34389$  $10665.8 + 5812.5\cos 38^{\circ} + 2437.5\sin 38^{\circ} = 16746.78735$ 

Element 3:  $12826.1 + 4312.5\cos 38^{\circ} - 3062.5\sin 38^{\circ} = 14338.93311$  $10665.8 + 3062.5\cos 38^{\circ} + 4312.5\sin 38^{\circ} = 15734.12305$ 

```
Element 4: 12826.1 + 4937.5cos38° - 4937.5sin38° = 13677.07456
10665.8 + 4937.5cos38° + 4937.5sin38° = 17596.43163
```

Next, the cell centers of the adjacent cells are used (the properties reside at the cell center) to calculate the proportional distances used in bilinear interpolation.

Element 1 proportions from coordinates of regional cells (32,10) and (33,11):

$$xp = (12842.97903 - 12625.0)/(12850.0 - 12625.0) = 0.9687956889$$

$$vp = (12979.08286 - 12750.0)/(13125.0 - 12750.0) = 0.6108876267$$

Element 2 proportions from coordinates of regional cells (24,34) and (25,35):

$$xp = (11168.34389 - 11075.0)/(11225.0 - 11075.0) = 0.6222926$$

$$yp = (16746.78735 - 16725.0)/(16950.0 - 16725.0) = 0.0968326666$$

Element 3 proportions from coordinates of regional cells (39.26) and (40.27):

$$xp = (14338.93311 - 14150.0)/(14450.0 - 14150.0) = 0.6297770333$$

$$yp = (15734.12305 - 15600.0)/(15800.0 - 15600.0) = 0.67061525$$

Element 4 proportions from coordinates of regional cells (37,38) and (38,39):

$$xp = (13677.07456 - 13675.0)/(13887.5 - 13675.0) = 0.009762635294$$

$$y_p = (17596.43163 - 17475.0)/(17630.0 - 17475.0) = 0.783429871$$

Then, the bilinear interpolation is done.

#### Element 1:

$$a1 = 498.5 + 0.9687956889(1498.0 - 498.5) = 1466.811291$$

$$a2 = 670.3 \pm 0.9687956889(707.4 \pm 670.3) = 706.2423201$$

$$a = 1466.811291 + 0.6108876267(706.2423201 - 1466.811291) = 1002.189117$$

#### Element 2:

$$a1 = 182.5 + 0.6222926(267.1 - 182.5) = 235.145954$$

$$a2 = 109.1 + 0.6222926(119.8 - 109.1) = 115.7585308$$

$$a = 235.145954 + 0.0968326666(115.7585308 - 235.145954) = 223.5853515$$

#### Element 3:

$$a1 = 495.8 + 0.6297770333(960.2 - 495.8) = 788.2684543$$

$$a2 = 816.1 + 0.6297770333(1041.0 - 816.1) = 957.7368548$$

$$a = 788.2684543 + 0.67061525(957.7368548 - 788.2684543) = 901.9165481$$

#### Element 4:

$$a1 = 159.6 + 0.009762635294(277.6 - 159.6) = 160.751991$$

$$a2 = 117.4 + 0.009762635294(28.47 - 117.4) = 116.5318088$$

$$a = 160.751991 + 0.783429871(116.5318088 - 160.751991) = 126.1085794$$

## FIGURE 9.1-1 SF2D1\_PRESECOFL\_TEST.INP - ASCII Input File for Running Test Case 1

```
*RUN TYPE
    SET AGER, TYPE=DEE, AGER_ID=1.001
    SET_GREG, TYPE=def, GREG_ID=1.302
    SET_GLOC, TYPE=DEF, GLOC_ID=1.025, X_REL=12826.1, Y_REL=10665.8, THETA=38.0
    FLOW, both=transient, LOC_BOUND=yes
*constant
     screen io=BRIEF
TINITIAL_CONDITIONS
      CAMDAT, HEAD=HEADat, TYPE=ATTA
      RESET
*ATTR
HYCND_Y=HYCND_X
*REG_TIME
      SED, NUM STEP=10, START=0.0, FINISH=10000.
      AUTO, OPTION=DEL_TIME
*LOCAL_TIME
      SEQ, NUM_STEP=10, START=0.0, FIN1SH=10000.
      AUTO, OPTION=DEL_TIME
*BOUNDARY
      REG, BOUNDARY=LOWER, TYPE=HEAD, END=25000., Clim_frac=0.
REG, BOUNDARY=UPPER, TYPE=HEAD, END=10000., Clim_frac=1.
      Reg, BOUNDARY=UPPER, TYPE=HEAD, END=17300., Clim_frac=0.
      REG, BOUNDARY=UPPER, TYPE=GRAD, END=25000., clim_frac=0. REG, BOUNDARY=RIGHT, TYPE=HEAD, END=27240., clim_frac=0. REG, BOUNDARY=RIGHT, TYPE=GRAD, END=30000., clim_frac=0.
      REG, BOUNDARY=LEFT, TYPE=HEAD, END=4000., clim_frac=0.
      REG, BOUNDARY=LEFT, TYPE=GRAD, END≈18595., clim_frac=0.
REG, BOUNDARY=LEFT, TYPE=⊬EAD, END≈30030., clim_frac=1.
      LOCAL, BOUNDARY=LOWER, TYPE=HEAD, END=5750.
      LOCAL, BOUNDARY=UPPER, TYPE=HEAD, END=5750.
      LOCAL, BOUNDARY=RIGHT, TYPE=GRAD, END=6625.
LOCAL, BOUNDARY=LEFT, TYPE=HEAD, END=6625.
*REG_CLIMATE
      LAKE, AMP=0.0, CYCLES=1.0, START=0.0, FINISH=25000., RATIO=2.0
      RECHARGE, AMP=0, CYCLES=1., START=0.0, FINISH=10000.
      HEAD, AMP=amplitud, CYCLES=cycles, head_fac=climtidx
                  START=0.0, FINISH=40000.
*END
```

(Page 1 of 4)

SF2D1\_READ\_PRP - Program Used to Convert the Binary Property File to ASCII

```
PROCRAM READ PRP
      Reads binary property file (FORO20.DAT) written by SET_GREG2 and
С
      translates it into an ASCII output file.
С
      Prompts user for the input file name (i.e. FORO20.DAT) and the
C
      user's choice of output file names.
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IMPLICIT NONE ************ REMOVED
      dimension IMPARR(0:100,0:100), IMPVEC(0:100)
      INTEGER I, J, 100M1, 100M2, ISECO2, IL, JL, 10FIL_GREG REAL RDUM1, RDUM2, RDUM3 ******** superceded
      CHARACTER#40 INFILE
      DATA ISECO2/10/
      DATA IDFIL_GREG/20/
(000000000000
C...BEGIN PROCEDURES...
0000000000000
      WRITE(6,*) 'Enter the name of the input file:'
      READ(5,'(A)') INFILE
      OPEN(UNIT=ISECO2, FILE=INFILE, STATUS='OLD', READONLY,
            FORM="UNFORMATTED")
      WRITE(6,*) 'Enter the name of the output file:'
       READ(5, '(A)') INFILE
      OPEN (UNIT=10FIL_GREG, FILE=INFILE, STATUS='NEW')
   10 CONTINUE
         WRITE (IDFIL GREG, 9520)
 9520
         FORMAT (' OUTPUT from program SET_GREG2/SET_GLOC2.',/
     $
                 ' Numeric FORMATS are',/
                 ' 3(216, 1PE13.5)',/
' 3(216, 110, 3x)',/
      $
                 1 3( 16, 1PE13.5)1,/
                 ' $ET_GREG2 run with ilgR,jlGR, GREG_ID,',
      $
                                     ' ilgr,jlgr, AgfR_ID = ')
         READ(ISECO2) IL, JL, RDUM1, IDUM1, IDUM2, RDUM2
         WRITE (IDFIL_GREG,953) il, jl, RDUM1, il, jl, RDUM2
   953
         FORMAT (3(216, 1PE13.5))
         READ(ISECO2) ROUN1, ROUM2, ROUM3
         WRITE (IDFIL GREG, 956) ROUM1, ROUM2, ROUM3
        FDRMAT (' x1_rel, y1_rel, thet1_rel =',/,1P3E13.5)
 c 1-D arrays
         FORMAT (3(16, 1PE13.5))
 ¢
         Read x-coordinates
          READ(ISECO2) (TMPVEC(I),1=0,IL+1)
          WRITE (IDFIL_GREG, 9540)
  9540
        FORMAT (' (i,x(i), i=0, ilGR+1) ')
          WRITE (IDFIL_GREG, 955)
```

`\$ (i, TMPVEC(I), l=0,il+1)

## INFORMATION ONLY

#### **FIGURE 9.1-2**

(Page 2 of 4)

SF2D1\_READ\_PRP - Program Used to Convert the Binary Property File to ASCII

```
Read y-coordinates
       READ(ISECO2) (TMPVEC(1),1=0,JL+1)
       WRITE (IDFIL_GREG, 9541)
      FORMA* (' (j, y(j), j=0, jtgr+1) ')
       WATTE (IDFIL_GREG, 955)
    $ (j, TMPVEC(J), J=0, j(+1)
       Read delta x's
       READ(ISECO2) (TMPVEC(1), (=D,1L+1)
       WRITE (1DFIL_GREG,9542)
9542 FORMAT (' (i, adx(i), i=0, ilGR+1) ')
       WRITE (IDFIL_GREG,955)
    $ (i, TMPVEC(I), I=0,i(+1)
       Read delta y's
       READ(ISECO2) (TMPVEC(I), I=0, JL+1)
       WRITE (IDFIL_GREG,9543)
       FORMAT (' (j, ady(j), j=0, jlGr+1) ')
WRITE (1DFIL GREG,955)

    $ (j, TMPVEC(J), J=0, jl+1)

c 2-D arrays
       Read x relative offsets
       READ(1SECO2) ((TMPARR(I,J), I=D,IL+1), J=0,JL+1)
       WRITE (IDFIL_GREG,9529)
       FORMAT (' ((i,j,x_relRA(i,j), i=0, ilGR+1), j=0, jlGR+1) ')
       WRITE (IDFIL_GREG,953)
    $ ((i,j,TMPARR(1,J), I=0,i1+1), J=0,jl+1)
        Read y relative offsets
       READ(1SECD2) ((TMPARR(1,J), L=0, LL+1), J=0, JL+1)
       WRITE (IDFIL GREG, 9528)
      FORMAT (' ((i,j,y_re\RA(i,j), i=0, ilGR+1), j=0, jlGR+1) ')
       WRITE (IDFIL GREG, 953)
    $ ((i,j,TMPARR(1,J), !=0,i!+1), J=0,j!+1)
        Read x hydraulic conductivies
       READ(1SECO2) ((TMPARR(1,J),I=0,IL+1),J=0,JL+1)
       WRITE (IDFIL_GREG,9531).
9531
       FORMAT (' ((i,j,aKx(i,j), i=0, i(GR+1), j=0, j(GR+1) ')
       WRITE (IDFIL_GREG,953)
    $ ((i,j,TMPARR(1,J), l=0,i(+1), J=0,j(+1)
        Read y hydraulic conductivies
        READ(ISECO2) ((TMPARR(1,J),[=0,1L+1),J=0,JL+1)
        ⊌RITE (IDFIL_GREG,9532)
9532 FORMAT (' ((ī,j,aKy(i,j), i=0, i(GR+1), j=0, j(GR+1) ')
WRITE (IDFIL_GREG,953)
     $ ((i,j,TMPARR((L,J), I=0,il+1), J=0,jl+1)
        Read fluid compressibility
        READ(ISECO2) ((TMPARR([,J), [=0, [L+1), J=0, JL+1)
        WRITE (IDFIL GREG, 8532)
 8532
       FORMAT (' ((i,j,alpha (i,j), i=0, ilGR+1), j=0, jlGR+1) ')
        WRITE (1DFIL GREG,953)
     $ ((i,j,TMPARR(I,J), I=0,i(+1), J=0,j(+1)
        Read porosity
```

(Page 3 of 4)

SF2D1 READ\_PRP - Program Used to Convert the Binary Property File to ASCII

```
READ(ISECG2) ((TMPARR(1,J), I=0, IL+1), J=0, JL+1)
        WRITE (IDFIL_GREG,8533)
       FORMAT (' ((\hat{i},\hat{j},\hat{p}h\hat{i} (\hat{i},\hat{j}), \hat{i}=0, \hat{i}(\hat{i}GR+1), \hat{j}=0, \hat{j}(\hat{i}GR+1) ')
        WRITE (IDFIL_GREG, 953)
     $ ((i,j,TMPARR(1,J), 1=0,il+1), J=0,ji+1)
        Read specific storage
        READ(ISECO2) ((TMPARR(1,J),I=0,1L+1),J=0,JL+1)
        WRITE (IDF1L_GREG, 9533)
       FORMAT (' ((i,j,spec_stor(i,j), i=0, ilgR+1), j=0, jlgR+1) ')
 9533
        WRITE (IDFIL_GREG, 953)
     $ ((i,j,TMPARR(|,J), 1=0,il+1), J=0,jl+1)
        Read aquifer storitivity
        READ(ISECO2) ((TMPARR(1,J),I=0,IL+1),J=0,JL+1)
        WRITE (IDFIL_GREG, 9534)
 9534 FORMAT (' ((i,j,aq_stor(i,j), i=0, ilgR+1), j=0, jlgR+1) ')
        WRITE (IDFIL_GREG, 953)
     $ ((i,j,TMPARR(1,J), I=0,i(+1), J=0,j(+1)
        Read aguifer thickness
         READ(ISECO2) ((TMPARR(I,J), I=0, IL+1), J=0, JL+1)
        WRITE (IDFIL GREG, 9535)
 9535 FORMAT (' ((\overline{i},j),aq_thick(i,j),i=0,ilGR+1),j=0,jlGR+1)')
         WRITE (IDFIL_GREG, 953)
      $ ((i,j,TMPARR(I,J), I=0,il+1), J=0,jl+1)
         Read aquifer bottom
         READ(ISECO2) ((TMPARR(\{1,J\}), I=0, Ii+1), J=0, Jl+1)
         WRITE (IDFIL GREG, 9635)
         FORMAT (' ((i,j,aq_bot(i,j), i=0, ilGR+1), j=0, jlGR+1) ')
         WRITE (IDFIL_GREG, 953)
      $ ((i,j,TMPARR(I,J), I=0,il+1), d=0,jl+1)
         Read well/river recharge term
         READ(ISECO2) ((TMPARR(1,J),1=0,1L+1),J=0,JU+1)
         WRITE (IDFIL_GREG, 9536)
  9536 FORMAT (' ((i, j,c10_rch(i, j), i=0, ilGR+1), j=0, jlGR+1) ')
         WRITE (IDFIL_GREG,953)
      $ ((i,j,TMPARR(I,J), I=0,il+1), J=0,jl+1)
 С
         Read river conductivity
         READ([SECO2) ((TMPARR(1,J),I=0,IL+1),J=0,JL+1)
         WRITE (IDFIL_GREG, 9537)
         FORMAT (' ((\overline{i},j,riv\_con(i,j), i=0, ilgR+1), j=0, jlgR+1) ')
         WRITE (IDFIL_GREG, 953)
      s = ((i,j,TMPARR(I,J), I=0,il+1), J=0,jl+1)
          Read river head
 C
          READ(ISECOZ) ((TMPARR(1,J), I=0, IL+1), J=0, JU+1)
          WRITE (1DFIL_GREG,9637)
         FORMAT (' ((\(\bar{i},j,riv_head(i,j), i=0, ilgR+1), j=0, j(GR+1) ')
  9637
          WRITE (IDFIL_GREG, 953)
      s ((i,j,TMPARR(I,J), I=0,i(+1), J=0,j(+1)
          Read river bottom
 С
          READ(ISECO2) ((TMPARR(1,J),I=0,IL+1),J=0,JL+1)
          WRITE (|DFIL_GREG,9737)
          FORMAT (' ((i,j,riv_bot(i,j), i=0, i(GR+1), j=0, j(GR+1) ')
  9737
```

(Page 4 of 4)

#### SF2D1\_READ\_PRP - Program Used to Convert the Binary Property File to ASCII

(Page 1 of 3)

SF2D1\_TEST\_READ\_1 - Program Used Read Selected Data from the Binary Property File

```
PROGRAM TEST READ 1
C....6-9-94 ELLEN'S. DOMBROSKI
C.....THIS PROGRAM WAS WRITTEN FOR THE SINGLE PURPOSE OF
C....VERIFYING BINARY OUTPUT FROM SECOFL2D.
C.... SPECIFIED RANGES OF SPECIFIED ARRAYS ARE PRINTED TO THE
C.....OUTPUT FILE FOR VERIFICATION BY INSPECTION.
      Reads binary property file (FORO20.DAT) written by SET_GREG2 and
      translates it into an ASCII output file.
      Prompts user for the input file name (i.e. FORO20.DAT) and the
C
      user's choice of output file names.
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      dimension TMPARR(0:100,0:100)
      CHARACTER*50 INFILE, OUTFILE
      OATA ISECO2/10/
      DATA IDFIL_GREG/20/
[000000000000000
C... SEGIN PROCEDURES...
[000000000000
      SCE = 1.D-9
       WRITE(6,*) 'Enter the name of the input file:'
       READ(5, '(A)') INFILE
       OPEN(UNIT=1SECO2, FILE=INFILE, STATUS='OLD', READONLY,
           FORM='UNFORMATTED')
       WRITE(6,*) 'Enter the name of the output file:'
       READ(5,'(A)') OUTFILE
       OPEN(UNIT=IDFIL_GREG, FILE=OUTFILE, STATUS='NEW')
       WRITE (IDFIL_GREG, 9520) INFILE
  9520 FORMAT (' ASCI! OUTPUT FROM FILE ',A/
      $ ' THIS FILE CONTAINS SPECIFIC RANGES THAT WILL BE USED',
      $ ' FOR VERIFICATION. 6-9-94.')
 C 953 FORMAT (3(216, 1PE13.5))
   953 FORMAT (216, 1PE15.5)
 C.....READ(ISECO2) IL, JL, RDUM1, IDUM1, 10UM2, RDUM2
       READ(ISECO2) 11, JL
 C....READ(ISECO2) ROUH1, ROUM2, RDUM3
       READ([SECG2] ROUM1, RDUM2, ROUM3
 C....1-D arrays
 p.....Read x-coordinates
        READ(1SECO2)
  C.....Read y-coordinates
        READ(ISECO2)
  C....Read delta x's
        READ([SECO2)
  C....Read delta y's
        READ(ISECO2)
  C.....2-D arrays
  C....Read x relative offsets
```

(Page 2 of 3)

SF2D1\_TEST\_READ\_1 - Program Used Read Selected Data from the Binary Property File

```
READ(!SECO2)
C....Read y relative offsets
      READ(ISECO2)
C....READ AND ECHO THESE FOR TEST. 6-9-94
C.....Read x hydraulic conductivies
      READ(ISECO2) ((TMPARR(1,J),1=0,IL+1),J=0,JL+1)
      WRITE (IDFIL_GREG, 100)
  100 FORMAT'(' ((\overline{i},j,aKx(i,j), i= 1,10), j= 1, 1)')
      WRITE (IDFIL_GREG,953)
     \$((i,j,TMPARR(1,J)*SCF, l=1,10), J=1,1)
      WRITE (IDFIL_GREG, 102)
  102 FORMAT (' ((i,j,aKx(i,j), i=21, 30), j=28,28)')
      WRITE (IDFIL_GREG, 953)
     $((i,j,TMPARR(1,J)*SCF, !=21,30), J=28,28)
C....
      WRITE (IDFIL_GREG, 104)
  104 FORMAT (' ((\overline{i},j,aKx(i,j), i=41, 50), j=57,57)')
      WRITE (IDFIL_GREG, 953)
     $((i,j,TMPARR(1,J)*SCF, [=41,50), J=57,57)
C....READ AND ECHO THESE FOR TEST. 6-9-94
C....Read y hydraulic conductivies
      READ(ISECO2) ((THPARR(I,J),I=0,IL+1),J=0,JL+1)
      WRITE (IDFIL_GREG, 110)
  110 FORMAT (' ((\bar{i}, j, aKy(i, j), i = 1, 10), j = 1, 1)')
      WRITE (IDFIL_GREG, 953)
     s((i,j,TMPARR(I,J)*SCF, !=1,10), J=1,1)
c....
       WRITE (IDFIL_GREG, 112)
  112 FORMAT (^{1} ((\overline{i}, j, aKy(i, j), i=21, 30), j=28, 28))
       WRITE (IDFIL_GREG,953)
     $((i,j,TMPARR(I,J)*SCF, I=21,30), J=28,28)
       WRITE (IDFIL GREG, 114)
   114 FORMAT (' ((i,j,aKy(i,j), i=41, 50), j=57,57)')
       WRITE (IDFIL_GREG, 953)
      ((i,j,TMPARR(I,J)*SCF, I=41,50), J=57,57)
 C..... READ AND ECHO THESE FOR TEST. 6-9-94
C....Read fluid compressibility
       READ(1SECO2) ((TMPARR(1,J),1=0,1L+1),J=0,JL+1)
       WRITE (IDFIL_GREG, 120)
   120 FORMAT (' ((\overline{i}, j, alpha(i, j), i = 1, 10), j = 1, 1)')
       WRITE (IDFIL_GREG,953)
      ((i,j,TMPARR(i,j)*SCF, i=1,10), J=1,1)
       WRITE (IDFIL_GREG, 122)
   122 FORMAT (' ((\overline{i}, j, alpha(i, j), i=21, 30), j=28,28)')
       WRITE (IDFIL_GREG,953)
       $((i,j,TMPARR(I,J)*SCF, 1=21,30), J=28,28)
       WRITE (IDFIL_GREG, 124):
   124 FORMAT (' ((\overline{i}, j, alpha(i, j), i=41, 50), j=57,57)')
        WRITE (IDFIL_GREG, 953)
```

(Page 3 of 3)

SF2D1\_TEST\_READ\_1 - Program Used Read Selected Data from the Binary Property File

```
\$((i,j,THPARR(1,\hat{J})*SCF, 1=41,50), J=57,57)
C....READ AND ECHO THESE FOR TEST. 6-9-94
C.....Read porosity
      READ(ISECO2) ((THPARR(I,J), I=0, IL+1), J=0, JL+1)
      WRITE (IDFIL_GREG, 130)
  130 FORMAT (' ((\overline{i}, j, phi(i, j), i = 1, 10), j = 1, 1))
      WRITE (IDF[L_GREG, 953)
     ((i,j,TMPARR(L,J), I=1,10), J=1,1)
      WRITE (IDFIL_GREG, 132)
  132 FCRMAT (' ((\overline{i}, j, phi(i, j), i=21, 30), j=28,28)')
      WRITE (IDFIL_GREG, 953)
      $((i,j,TMPARR(1,J), L=21,30), J=28,28)
      WRITE (IDFIL_GREG, 134)
   134 FORMAT (' ((\overline{i}, j, phi(i, j), i=41, 50), j=57,57)')
      WRITE (IDFIL_GREG, 953)
      $((i,j,TMPARR(1,J), I=41,50), J=57,57)
C....,Read specific storage
      READ(ISECOZ)
C.....Read aquifer storitivity
       READ(ISECO2)
C.....Read aquifer thickness
       READ(ISECO2)
C....Read aquifer bottom
       READ(ISECOZ)
C....Read well/river recharge term
       READ(ISECO2)
     .. Read river conductivity
       READ([SECO2)
     ..Read river head
       READ(ISECO2)
.C....Read river bottom
       READ(.ISECO2)
C....Read constant head
 C
       READ(ISECO2)
c....
       STOP 'TEST_READ_1: NORMAL COMPLETION'
       END
```

#### 9.1.4 Acceptance Criteria

The acceptance criteria for the regression tesing is stated in Section 10 below.

For requirement R.2: The values for porosity and bulk compressibility remain constant. The values for hydraulic conductivity from LOCAL\_TEST.ASC (interpolated from the regional grid) will agree with the hand-calculation to 6 decimal places.

	From file	LOCAL_TEST.ASC		From hand-calculation
Element 1	(12,15)	1.00219E+03	,	1002.19
Element 2	(20,47)	2.23585E+02	•	233.585
Element 3	(35.25)	9.01917E+02		901.917
Element 4	(40.40)	1.26109E+02	•	126.109

#### 10.0 INSTALLATION AND REGRESSION TESTING

Test Case 1 is suitable for installation and regression testing. For regression testing against the primitive baseline on file in the SWCF, after the command file to run this test case is executed. run the program SF2D1\_TEST\_READ\_1 (compiled and linked from SF2D1\_TEST\_READ\_1.FOR). The FORTRAN file is shown in Figure 9.1-3. The user will be prompted for input and output file names. The input file is SF2D1\_REGION\_TEST.PRP. The output file name is SF2D1\_TEST\_READ.OUT. This program was previously used to produce the output on pages 4-6 of the verification section of the primitive baseline using the regional property file created during that verification process. Copies of these pages are included as Appendix B. This program should produce the identical results to the previous results in the primitive baseline when run during this testing exercise. The results from the current execution in the ASCII file SF2D1\_TEST\_READ.OUT can be printed.

#### 11.0 REFERENCES

- 1) WIPP-PA Qualification Guide for Pre-existing Software, Version 2.0, dated 8/24/95.
- 2) WIPP-PA Implementation Document for PRESECOFL2D Version 4.02ZO, WPO# 23296
- 3) WIPP-PA Validation Document for PRESECOFL2D Version 4.02ZO WPO# 23319
- 4) Rechard, R.P., ed. 1992, User's Manual for CAMCON: Compliance Assessment Methodology Controller Version 3.0. SAND 90-1983, Albuquerque, NM: Sandia National Laboratories.
- 5) WIPP-PA User's Manual for PRESECOFL2D Version 4.02ZO, WPO# 23297

## 12.0 APPENDICES

### APPENDIX A - REVIEW COMMENTS

See attached

#### WASTE ISOLATION PILOT PLANT

## Requirements Document Reviewer's Form

Sandia PLA National Laboratories

Form Number: 458 Effective: 7/31/95

	Frocedure. Tys	Revision:		<del></del> -	Page _		of	1_
WPO Number: 23	318	Software Classification	n:	5 NL	- 54	ノ 		
Reviewer Instructions:							<del></del> -	
Check "Yes for each item	reviewed and found	cacantable						
Check "No" for each item	which requires forth	acceptable.						
Check "N/A" for items wh								
Check "N/R" for items not				•				
For multiple reviewers, ea	ch reviewer chall co.	re are mulitiple reviewers	s).			•	,	
Pnor to sign-off of the RD, "N/A" may be checked, or nonconformance.	all "No" items shall be f a memo from the DN	e appropriately addressed M shall be attached to the		ode spo aining th	nsor so t ne reason	hat "Y for th	es" or e	-
This form snall be included	d as part of the base	lline RD.				•		
Functionality     Are the functions that to	he software is to perf	form adequately identified	d? ∑ Ye	s [	No 📋	N/A		N/R
Performance     Are the time-related iss recovery time, or respo	sues of software oper onse time identified?	ations such as speed,	☐ Ye	s 🗍	No 🔀	N/A		WR
Design Constraints     Are elements that will r	estrict design options	s identified?	Ye:	5	No 🔀	N/A		N/R
Attributes     Are non-time related iss     acceptance criteria, acc	sues of software oper cess criteria, and mai	ration such as portability intainablility identified?	Yes	3 <u> </u>	No ∑	N/A		N/R
5. External Interfaces Are required interaction identified?	s with people, hardw	are, and other software	∑ Yes		No 🗍	N/A		WR
6. Completeness Are the requirements co	omplete?		X Yes		No [	N/A		ONLY
7. Verifiability Can meeting the require	ements be verified?		X Yes		No 🗌	N/A		ATTON
8. Consistency Are the requirements co	onsistent with each ot	her?	∑ Yes		No [	N/A		FORM
Technical Feasibility     Are the requirements technical	chnically feasible?	e e e e e e e e e e e e e e e e e e e	X Yes		Vo 📋	N/A		N/R
C. David Updes	raff C.	Dand Uhde	mall	,			<del></del> -	
Reviewer Name (printed)	Signal	ture	The		— ——— Date	<u> </u>	<u>4 7</u>	2_
		······································			Date	•		

#### WASTE ISOLATION PILOT PLANT

Sandia F National Laboratories

## Verification and Validation Plan Reviewer's Form

Form Number: 460

		Procedure:	19-1	Revision:				Pag	e <u>1_</u>	of.	
٧	WPO Number:	23318		Software Classifica	ation;		SNL	- <i>S</i> 4			
R	Reviewer Instruction	is:		<u></u>							<b></b>
С	heck "Yes for each item	reviewed and found acc	eptable.								
C	heck "No" for each item	which requires further we	ork.								,
С	Check "N/A" for items whit	ch are not applicable.						•			
C.	heck "N/R" for items not	reviewed (anily if there ar	re muitiple	reviewers)							
		ch reviewer shall complet									
Pi	rior to sign-off of the VVP	. al "Vo" items shall be a	Annonaria	ly addressed by the code . te reason for the nonconfo	sponso mance	or so thai	t"Yes" o	r "N/A" m	ay be chi	ecked, o	ra
TI	his form shall be included	das part of the baseine	VVP.			•					
1,	criteria to ensure thi	tify sufficient test case e final software end-p RD? <i>(Check "N/A" if</i>	product sa	atisifies the	$\boxtimes$	Yes		No [	NVA		N/R
2.	<ul> <li>performs all intende problems encompas</li> </ul>	emonstrate that the c ed functions and produ ssing the range of per 's Manual? (See Sect	luces valid	d results for	$\boxtimes$	Yes		No [	_ N/A	·	N/R
3.	demonstrate require	ol ed for operational cor ed performance over t trolled function or pro	the range	ests of		Yes		No [	⊠ N/A		N∕R
4.	unintended function:	ons now that the code doe that either by itself or degrade the intended	r in combi	ination with		Yes		4o [S	Ŋ/A		N∕R
5.	<ul> <li>hand calculations;</li> <li>calculations using</li> <li>empirical data and data</li> <li>correlation and/or results from other</li> </ul>	sults compared to on-	problems nfirmed p or similar o	ublished		Yes	_ r	io [	□ N/A		Z JEORMATION ONLY
6.	Pear Review If peer review will be in the VVP?	e required to validate	the softw	are, is it identified		<del>Yes -</del>		io 🖒	₹ N/A		NFOR INFOR
7.	Installation and Re Are test cases which testing identified from	egression Testing h are suitable for insta m the set of verification	allation te	sting and regression alidation test cases?	$\boxtimes$	Yes	N	io [	] N/A		N/R
<u>_</u>	. David Up	degraff	0	Sand Up	10g2	4/	<u> </u>		110		75
Rev	viewer's Name (printed)	<del>-</del>	Signatu	ıre ,		// -			D-4-		

#### WASTE ISOLATION PILOT

Sandia PLANT lational caboratories

## Review Comment (Software)

Form Number: 299

(.aboratories	Procedure:	QAP 19-1_	Revision:			Page1 of2
File Code: SWCF-	A	1.1.6.9				PA :SFT
Keywords: (Used for PRESE(0)	unique identific	was #(s) ation) S F ⊴	201			Alpha Code
·	,					
SECTION I						· · · · · · · · · · · · · · · · · · ·
1. Software Name:  PRESECOFL20		Version ID:			Version Da	te: 5/20/94
2. Type of Comment:	(check one)	∑ Requ	ired	☐ Su	ggested	Епог
Software.Type: <i>(ch</i>	леск спе)	Comr	nercial	∑ De	veloped	System
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#### PRIMITIVE BASELINE DOCUMENTS APPENDIX B -

The following pages are from the verification section primitive baseline documentation currently stored in SWCF as a part of the prior QA efforts. The results of the current test will be compared to these numbers with the numbers matching exactly.

### (Page Lof 3)

Pages 4-6 of the Verification Section of the Primitive Baseline

Page 4 of 16

```
ASCII DUTPUT FROM FILE nfs1:: [camcon.presecofl2d.test]regdat_test.inp
THIS FILE- CONTAINS SPECIFIC RANGES THAT WILL BE USED FOR VERIFICATION. 6-9-94.
((i, j, akx (i, j), i=1, 10), j=1, 1)
             1.89500E-04
         1
             2.04700E-04
             3,45600E-05
  3
              2.67800E-05
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              1.87400E-05
              2.04300E-05
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              1,68900E-05
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              7.59600E-06
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 ((i,j,aKx (i,j), i=21, 30), j=28,28)
              1.50900E-07
  21
         28
         28
              1.320008-07
  22
              1.42400E-07
         28
  23
              1.63900E-07
         28
  24
              4.32500E-07
  25
         28
              1.86500E-06
         28
  26
         28
              1.87000E-06
  27
               1.15800E-06
  28
         28
               1.30800E-06
  29
         28
              1.49000E-06
  30
         28
 ((i,j,akx (i, j), i=41, 50), j=57, 57)
              4.20400E-10
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         57
         57
              1.85600E-10
   42
              2.02000E-10
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         57
               2.59200E-10
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               1.62500E-10
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                2.043COE-05
                2.96700E-05
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    21
                1.32000E-07
           28
    22
                 1.42400E-07
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Page 5 of 15

## FigureB-1 (Page 2 of 3) Pages 4-6 of the Verification Section of the Primitive Baseline

1,63900E-07 4.32500E-07 25 28 25 28 1,86500E-06 27 1.870005-06 28 1.15800E-06 28 28 28 1.30800E-06 29 1.49000E-06 30 28 (i , jaky (i, j), i=4 1, 5 0) , j=57, 5 7) 41 57 4.20400E-10 42 57 1.85600E - 10 2.02000E-10 43 57 44 .57 2.59200E-10 57 2.66900E-10 45 46 57 1.62500E-10 57 2.15800E-10 47 48 57 2.51900E-10 49 57 1,78000E-10 50 57 2.5090CE-10 alpha (I, j), i=1,10), j=1, 1) 1 7,57000E-10 <(i,j 7.57000E-10 2 3 7.57000E-10 7.57000E-10 5 7.57000E-10 7.57000E-10 6 7 7.57000E-10 7.17000E-10 8 1 9 7.57000E-10 1 7.57000E-10 10 1 alpha (i, j), i=21, 30), j=28, 28) 21 7.57000E-10 28 7,57000E-10 22 28 7.57000E-10 23 28 7.57000E-10 28 25 7.57000E-10 28 7.57000E-10 26 28 27 28 7.57000E-10 7.57000E-10 23 28 29 28 7.57000E-10 7,57000E-10 30 28 alpha (i, j) , i=41, 50), j=57, 57) (i, j, 7.57000E-10 57 <u>4</u>1 42 57 7.57000E-10 43 57 7.57000E-10 44 57 7.57000E-10 45 .57 7.57000E-10 46 57 7.57000E-10 47 57 7.57000E-10 48 57 7.57000E-10 49 57 7.570C0E-10 50 57 7.57000E-10 j, phi (i, j) , i=1, 10), j=1, 1) 1 - 1.45420E-0L 1.45420E-01-2 3 1.45420E-01 1.45420E-01 1.45420E-01

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Page 6 of 6

## FigureB-1 (Page 3 of 3) Pages 4-6 of the Verification Section of the Primitive Baseline

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### APPENDIX B - PRIMITIVE BASELINE DOCUMENTS

The following pages are from the verification section primitive baseline documentation currently stored in SWCF as a part of the prior QA efforts. The results of the current test will be compared to these numbers with the numbers matching exactly.

Figure B-1
(Page 1 of 3)
Pages 4-6 of the Verification Section of the Primitive Baseline

ASCII OUTPUT FROM FILE nfs1:: [camcon.presecofl2d.test]regdat\_test.inp THIS FILE. CONTAINS SPECIFIC RANGES THAT WILL BE USED FOR VERIFICATION. 6-9-94. ((i, j, aKx (i, j), i=1, 10), j=1, 1)1.89500E-04 2.04700E-04 3.45600E-05 3 2.67800E-05 5 2.38800E-05 1.87400E+05 2.04300E-05 8 2.96700E-05 9 1.68900E-05 10 7.596006-06 ((i,j,aKx (i,j), i=21, 30), j=28,28) 1.50900E-07 21 28 1.32000E-07 22 28 1.424Q0E-07 23 28 1.63900E-07 24 28 4.32500E-07 25 28 28. 1.86500E-06 26 1.87000E-06 27 28 28 28 1.15800E-06 28 1.30800E-06 29 30 28 1.49000E-06 ((i,j,aKx (i, j), i=41, 50), j=57, 57) 41 57 4.20400E-10 1.85600E-10 42 57 43 57 2.02000E-10 44 57 2.59200E-10 2.66900E-10 45 57 46 57 1.62500E-10 47 57 2.1580CE-10 48 57 2.51900E-11 49 1.78000E-10 57· 57 2.50900E-09 50 j), i=1, 10), j=1, 1) ((i,j,aKy(i, 1.89500E-04 2.04700E-04 2 3 3.45600-=-05 2.67800F--05 2.38800E-05 5 1.87400E-05 2,04300E-05 8 2.96700E-05 1.68900E-05 7.59600E-06 10 ((i,j,aky (i,j)i=21,30),j=28,28)1.50900E-07 21 28 22 1.32000E-07 23 1.42400E-07

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### Figure B-1 (Page 2 of 3)

### Pages 4-6 of the Verification Section of the Primitive Baseline

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### **Figure B-1** (Page 3 of 3)

### Pages 4-6 of the Verification Section of the Primitive Baseline

1.45420E-01 1.45420E-01 9 1.45420E-01 1.45420E-01 10 (i, j) , i=21, 30), j=28, 28) 1.45420E-01 21 22 23 28 1.454202-01 1.45420E-01 28 24 25 28 1,45420E-0L 1,45420E-01 28 26 27 28 29 30 28 1.45420E-01 1,45420E-01 28 28 28 1.45420E-01 1.45420E-01 23 1.45420E-01 ((i, j, phi (i, j) , i=41, 50), j=57,57) 41 57 1.45420E-01 42 57 1.45420E-01 57 1.45420E-01 43 1.45420E-01 44 45 46 47 57 57 57 57 1.45420E-01 1.454206-01 1.45420E-01 57 57 48 -1.45420E-01 49 1.45420E-01 1.45420E-01

### WIPP PA

### VALIDATION DOCUMENT

for

### PRESECOFL2D

Version 4.02ZO

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### 1.0 INTRODUCTION

The purpose of this document is to summarize the results of the testing activities prescribed in the RD/VVP and to provide evaluations based on those results. The PRESECOFL2D code has previously undergone a QA process complete with a review and is currently qualified as Level A under QAP-1 Rev. F. Both static testing and coverage testing was carried out in the same manner as with all other codes, but the functional testing consisted primarily of regression testing.

#### 1.1 Software Identifier

PRESECOFL2D version 4.02ZO

(WIPP PA Code Prefix: SF2D1)

### 1.2 Points of Contact

Code Sponsor: Rebecca L. Blaine

Code Consultant: Rebecca L. Blaine

Ecodynamics Research Associates, Inc.

P.O. Box 9229

Albuquerque, NM, 87119

(505) 843-7445

### 2.0 TESTING ENVIRONMENT

Testing for PRESECOFL2D was performed in the following computer environment:

Hardware platform:

DEC Alpha

Operating System:

OpenVMS version 6.1

Directory:

WPSTESTROOT:[SF2D1]

#### 3.0 TEST TOOLS

The testing tools which were used as part of the software validation are described in Table 3-1.

Table 3-1
Software Testing Tools

Tool Name	Usage
FORTRAN-Lint (FLINT)	Source Code Analyzer used to identify non ANSI standard coding.
DECset SCA	Source Code analyzer used to identify uncalled modules, to identify unreferenced variables, and to display the calling tree.
DECset PCA	Performance Coverage Analyzer, used to identify any unexercised modules
DEC FORTRAN Compiler version EV6.2-508-274	Compiler, used to create the executables and identify compilation errors and warnings.

#### 4.0 STATIC TESTING

For PRESECOFL2D, static analysis was performed using both the source code analyzer FLINT and the source code analyzer DECset-SCA. FLINT was used to detect non-ANSI standard FORTRAN coding. DECset-SCA was used to reveal any uncalled modules, to reveal any unreferenced variables, and to display the calling tree.

The DECset SCA analysis was performed on directory WP\$TESTROOT: [SF2D1.BUILD] during the generation of the PCA executable. The FLINT analysis was carried out in the WP\$TESTROOT:[SF2D1.SRC] directory.

### 4.1 Flint Analysis: Procedure And Results

PROCEDURE: Since PRESECOFL2D is a multimodule program. FLINT was used on a file created by appending all the modules together in alphabetical order. The file resulting from running FLINT, SF2D1\_FLINT.OUT, is shown in Figure 4.1-1.

RESULTS: As a result of running FLINT, two types of issues were noted. First, it was noted that several variables were defined but not referenced. This was as expected by the code sponsor.

Second, it was noted that some lines in the code were over the ANSI standard 72 columns in length. It was found to be a result of padding with blanks and is of no concern with the platform and compiler with which the WIPP PA will be performed.

### Figure 4.1-1 (Page 1 of 5)

### FLINT Output for Code Modules

#### Comments by Judy Rollstin.

This file, SE2D1\_FLINT.OUT, is the curput files resulting from using FLINT to analyze a single file created by appending all modules in the PRESECOFL2D computer code. In this way, each module was checked for adherence to ANSI standard FORTRAN.

```
Sefault options: WARMINGS /USAGE SUPPRESS=107,076,08,164 TREE GYREF.
Sammand options: GUTPTT=sfid1_filmt.out
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    -Sabroutine IELTAS
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SKATAN WARNING #531: line léngot (exceeds )[lecolimbe)
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        Subtoutine GETEND
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SFOCAL FOR GETANT Line 488 SI SFOOL_SECOPTING DITESTATES AND STATES OF STATES AND SECOND OF SECOND S
 Suproutine GETLIS
                                                                                                                                                                                          Line 595.
                                                                                                             File SEID1 FOR
SPOCE FOR GETETS line 640 63 (SPOCE_LOGIC.INC,2);
SYNTAX WARNING #5314 line length exceeds 72 columns
        Subroutine GETRTS
                                                                                                                   File SF2D1 FOR
                                                                                                                                                                                                   Line 73a
 SF2D1 FOR GETRTS 11me 782 51 SF2D1_SECO2R INC/2) -
 SYNTAX WARNING #531- line length exceeds 72 columns.
 sfoot For GETROS Line 783.63 (sfoot_logic.inc, 2)?
 SYNTAX WARMING #531- line length exceeds 70 columns.
        Subroutine GETAUN
                                                                                                                       File SF2D1.FOR
                                                                                                                                                                                                   Sine 877
  SF2D1 FOR: GETRYN, line 975.63 (SF2D1_Logid, INC, 2)}
```

### Figure 4.1-1 (Page 2 of 5)

SYNTAN WARNING #531- Line length exceeds	, Tî selumns.	
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Pragram FREADORDAD		ing Ing
Saczustor Passectros Line (404.55 Est. Styrtak WARNING 4531-Line Length exceed		
Suproutine PRECIS	rile sr2Di.Fok	Line 2488
SPICE FOR PROCES LINE 2639 %3 (SFIELLC STATAM WARNING 4531- line length exceed	GTC INC 22: s 72 columns.	
Subroutine Passoo	File SFEDU FOR	Utae 3 Ne
SF2D1 FOR PRSECO line 3343 63 (SF2D1_60 SYNTAK WARNING #531- line length exceed Subroutine PRSCRC	GEC INC 3)= is 72 columns.	
Subroutine PRSCRO	File SF101 FOR	1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.1.
SECTION POR PROCESSION 1531-1110-163 (SF2D1_60 SYNTAX WARNING #531-1110-160gth exceeds	ogis, INC,3): is 72 celumns	
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### Figure 4.1-1 (Page 3 of 5)

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Subroucine ROSSCO	File Gradi FCR	line 5011	
BF121 F0P BDSECO line 5095 63 (S SYNTAX WARNING #531- line length	F301_LOGIC ING(2): exceeds 73 columns		
Subroutine RDSQLV	File SF2D1 FOR	::::::::::::::::::::::::::::::::::::::	
SF2D1.FOR:RDSOLV Line 5584.5% s	FSD1_secola.inc.2		
SYNTAX WARNING #531- line length	exceeds 72 columns.		
Qubroupine REWELL	FELE SRICC FOR	-ine 5740	
SF2D1 FOR ROWBLL line 5792.51 (S SYNTAX WARNING #531- line length	SF1D1_SECOIR INC (1)		
SF2D1 FOR RDWELL line 5793.63 (S SYNTAX WARNING *531- line length	SF2D1_LÖĞIÖ.INC,EY		
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### Figure 4.1-1 (Page 4 of 5)

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a Britane Warfinia (#531.a June Dengah Broekasa) 12 pagumas. Pron Pron Wengala buna (1925.a)   SF131   SECC18 1110:10	
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STORE WARNING #531 - Line Length expends [Longland   1975] FOR WARNING #531 - Line Taling For Line 1887.  Secretarine WREST   Line 1737 has SF2D1_LogIC. INC. 2   Line 1887.  SPORT FOR WREST   Line 7737 has SF2D1_LogIC. INC. 2   SYNTAX WARNING #531 - line Length exceeds T1 columns.	
STORE WARNING #531 - Line Length expends [Longland   1975] FOR WARNING #531 - Line Taling For Line 1887.  Secretarine WREST   Line 1737 has SF2D1_LogIC. INC. 2   Line 1887.  SPORT FOR WREST   Line 7737 has SF2D1_LogIC. INC. 2   SYNTAX WARNING #531 - line Length exceeds T1 columns.	
SERVING FSS: Line Length expends Cloquents  SERVING FOR WRISS: Line Length expends Cloquents  Suproutine WRISS: Line 7737/53 SF2D1_Logic.INC; 2:: SYNTAX WARNING #531- line Length exceeds Cloquents  Subroutine WRISS: Fine Length exceeds Cloquents  Subroutine WRISS: Fine Length exceeds Cloquents  File SF2D1 FOR Line 7816	
SYNTAX WARNING #531 - Line Teach exceeds 1 columns  Subroutine WRTSIR ine 1737 63 SF2D1_LOGIC.INC:2:  SYNTAX WARNING #531 - Line length exceeds 71 columns  File SF2D1 FOR: WRTSIR line 7838 51 (SF2D1_EGGIC.INC:2):  Sibroutine WRTSIR line 7838,51 (SF2D1_SECOIR.INC:2):  SYNTAX WARNING #531 - line length exceeds 72 columns  Sibroutine WRTSIR line 7838,51 (SF2D1_SECOIR.INC:2):  SYNTAX WARNING #531 - line length exceeds 72 columns  SF2D1 FOR: WRTSIR line 7838,51 (SF2D1_SECOIR.INC:2):	
STORY WARRING #531 Line length expends [1 cq. 4515]  STORY FOR WETS I Take story of second se	

### Figure 4.1-1 (Page 5 of 5)

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Page 12

### 4.2 SCA Analysis: Procedure and Results

PROCEDURE: DECset-SCA was invoked during the build process. The build process was performed using the build script SF2D1\_BUILD.COM developed by Mike Williamson. The build script is shown in Figure 4.2-1. The build script is self-contained and is executed in the directory containing the needed input files with the command.

### @SF2D1\_BUILD

During the build process, the input file SF2D1 MMS is required and is fetched from SCMS. That input file is shown in Figure 4.2-2.

As a result of the build process, a debug executable capable of doing PCA analysis was created and the SCA code analyzer created the three output files. These files are listed in Table 4-1 along with a brief description of each file and a reference to where a listing of each file can be found in this document.

Table 4-1
Files Created by the SCA Code Analyzer

Output File	Description Figure
SF2D1_SCA_MOD_NOT_REF.	A listing of the modules in the code that are   Figure 4.2-3 not referenced
SPIDI_CALLTREE.TXT	A listing of the calling tree for the code Figure 4.2-4
SCASEVENT DAT	A binary file containing information about the SCA process.

Following the build process. SCA was invoked at the VMS \$ prompt and the following commands were executed on the SCA\$EVENT DAT file in the WP\$TESTROOT: [\$F2D1.SCA] directory:

SCA> set lib []
SCA> show module/all/output=sf2d1\_modules.out
SCA> exit

This procedure converts information in a binary file to an ASCII format file. The resulting ASCII file, SF2D1\_MODULES.OUT, is a listing of the modules referenced during the SCA, including such information as the date each module was compiles, the language in which each module is written, etc. associated with each dile used. This listing is shown in Figure 4.2-5.

RESULTS: The SCA procedure revealed the only module not being called is the main program itself, as to be expected.

### Figure 4.2-1 (Page 1 of 9)

### SF2D1 BUILD.COM Build Script

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sane_veulty e fouerosy i This sames the user's desting
Retunerprop notice cyposisting _st08__uilled.log
                    Pecame and the result of the r
II FLUARATE
II GELGUE VILU 198
           Does the build for SFCII prefix (PREBECUFILE) dolects. This file will be modified or enamoed later for full prodiction builds. Based on input parameters the build is link in ACA, build from latest and reatest or a MS is as and build all trom sources.
                                                                                                                                                                                                                                                                                                                                  INFORMATION ONLY
              Para≒4teta/
           Parameters

Fig. - Type of busis. "T" = test. "S" = Brod. D = Seve.opers local

Fig. - Type of busis. "T" = test. "S" = Brod. D = Seve.opers local

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Fig. - SROM_SOURCES while letault is "S", any otheries not fixed_fourpes.

Fig. - Build for PCA Walle PCA expected

Fig. - Build and load SCA, and run SCA tests. Value STA expected

Fig. - Build debug wersion. Expected valued DBG, NCOBS
              Mike Willemses - Claital Equipment Corporation.
         greation Tate: 3-Aug-1995
GSCE prestele:
                        SOSUB start_mai
                       GCSUB do_cultid
GCSUB load_aca
                    Gorê Ferminadê
EXIV
 SIENO OF MAINLINE
 St Subroutines, most of the situal work is done in the subroutines.
ತಕ್ಕಬ್ಬಾ<u>ಗಿದೆದಲ್ಲಿ</u>
$1 Write the mis macro file to contain bequested options:
St This file needs to be written dynamically as the options san
 st. dhange based on parameters passed for this command procedure:
              CPEN/wgite mms_tile wp_bdi/d:wp_gen_macros mms
 3! Specify the CMS flag, specifically any class requirement.
                                                WRITE mms_file : cmsflags = /occlude=none/generation=''p2'
                                    WRITE mms_file "omsflags = /osclude=none"
```

### \* Figure 4.2-1 (Page 2 of 9)

### SF2D1 BUILD.COM Build Script

```
ENLIF
 Des the compute and link blags that will be used by the final despitable to the note most must be sombile class and not same as what ever the node owner was libraries.

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WRITE TESTINI "ilasias e videcetas en Company
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           75 E4V - 413 ( " 904"
               - Waste mms_Close "Axe name s Pressortion sestually Axe" ( %) w
- it recention "Libsorsuc" ( yes) "" THEN FREASSISN LibsdetWs
ENSSE
       and the water of the water the contract of the
          laenerai_ii/ig
                   waine has fale "awe name energicostic la sae indibar eve
                ir di egg. "PCA"
                  WRITE mms_file "exe_name = FRESECCTLID_local_dbg exe"
IS RETRUNK("LIBEDEBUG") NES "" THEN DEKSELGN LEBEDDUG
           ENDIF
        ENDIT
        CLOSS mms_file
$ CHECK_PARAMS:
$! Verify reasonable pagamater settings, prompt where indicated
       _mode = fsmode()
$ 5
or uppercase any impusyparama, they are expected to be blank or uppercase
        TP pl .nee. "" THEN pl = "fsedit " | 'pl ", "upcase"
```

### Figure 4.2-1 (Page 3 of 9)

### SF2D1 BUILD.COM Build Script

```
17 p2 nes "" THEN p2 = (Semit "" p2"", "spcase"
17 p2 nes "" Then p2 = Stedit "" p3", "upcase"
TT "4 nes "" Then p2 = Scent "" p4 " "spcase"
17 % nes "" Then p2 = Scent "" p2" "" "spcase"
17 % nes "" Then p2 = "Sect "" p2", "upcase"
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    ENDIF
Hedr IMS Class Taran
If pl. ens ""
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          IT of hegs "P" ward inode thest "BATCH"
          DE Wertenbrig ob rowse of Water grotten volunteer
Tawar Safar Marianda hoosaa maa rake
             7 01 Me33. *2"
               bulla_solraes = FSEDIT: "'\bulla_sources'", "urcase"
EF bulla_soutces (.egs. "Y" THEN p3 = "S"
     ENDIF
     If n3 legs: "S" and I'm legs: "D"
          WRITE SysSoutput "Development builds are not allowed to be from soutces?" p3 = "N"
     ENDIF
If this is a production busid, then PCA cam not be used as it requires a debug compile and link, and prod is by defination not debug.
     IF pl eqs. *P*
           IF p4 .nes. ""
           THEN-
             Write syssourput "Can not have a production build for SCA"
           ENDIF
```

### Figure 4.2-1 (Page 4 of 9)

### SF2D1\_BUILD.COM Build Script

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54 ₹
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                The Need a symbol for the MMS/SSL indicating 37% sondiction:
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busid_Sar_sad = RABOWT:"Undulld_Sar_sad " / Muchase"
In marcd_sar_sad - eds: "V" THEN of Brisch
        SNCJE kominist
         13 15 PATS - "SQA"
             mme_sta_file: = " sca=sca@llbrard"
             mme_sca_tlag = " nosca"
         END 17
. Pracuosian is .waya modesia.
             dbg_x;ias = 1 opc nodebug*
| abg_cclas = 1 nodecus noppanecas:*
         그를 하다 (출생동 제공구학자)
공원主왕
                                          The grant planted large all value described
             po e "lee"
dbg_geleg e t noopt debud"
gbg_fleg e "wdebug" tracepabe!
         IP charges. *P*
THEN
                                           ! Test and Sevelopmens can be debug.
              dbg_[1]ag :== ""
              TF po legs " . and mode nes "BATCH"
                INQUIRE/hopung dbg_flag "Suild debug ( Y or N ) [Y] : *
dbg_flag = fSedit ("''dbg_flag"", "upcase")
              ENDIF
              IF dbg_Ilag .eqs. "N" or. p6 .eqs. "NODEG"
              THEN
                 pe = "Nobed"
                dbg__clai_= "Yopt/nodebug;notraceback"
dbg__clai_= "Yopt/nodebug;notraceback"
              ELSE
                 p6 = "DBG"
                 dbg_silag = "/noopt/debug"
dbg_silag = "/debug/traceback"
              ENDIF.
 S
         ENDIF
```

Seguina and

# Figure 4.2-1 (Page 5 of 9) SF2D1 BUILD.COM Build Script

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                                       ENDIF
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THEN
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czarneuncjay wella welcytla wella opt
czausni
   spc_BUILD:
   S: Di chis is a CMS class dependent build we need to fetch the CAMCON :: Libraries from the correct class. This code should be replaced with the Libraries references in the MMS file when the CAMCON libraries are.
     s! in CMS.
                                          IF p3 .eqs. ...
                                           THEN
                                                                gen_52ag :== **
                                           ELSE
                                                                  gen_flag :== "/gen=''pl/"
                        Fetch the CAMCON libraries that are needed.
                                           THEN-
                                                           _SET def wp_olb
                                                                     CMS fet orchude none 'gen flag camcon lic.olb
       5
                                                         CMS fet/coclude=none | gen_flag camdat_lib.olb
```

# Figure 4.2-1 (Page 6 of 9) SF2D1 BUILD,COM Build Script

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The state of the provides of the provides of the control of the state of the control of the cont
```

```
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Location (== ESERVITORDED: "ESFAULT")

Tron_sources (== ""

mail_swich (== ")

general_offic (== ")

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cefine noicg cmsilin (== SFIDI_L_LD), c_wp

float

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fron_sources = "/skip_intermediate"

substance

fron_sources = "/fron_sources"

Substance

fron_sources = "/fron_sources"

substance

fron_sources = "/fron_sources"

substance

subs
```

# Figure 4.2-1 (Page 7 of 9) SF2D1 BUILD.COM Build Script

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748);
             Fille Clas. coccoccade with bland on paler Sicasc
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        Nef_rot = iSenvisonment "åetault"
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SEFTNE:polog >>>>>>>>>>
             OBRINE not og volgie
              g det_loc upsprodsoct (6700.015), westestroot (87001.025
            e nogau public thare are mms files than must be present
En present "wollnisidetaunt ittles mms to Has ""
             . Ms ferce op mostderates rules mas .
ENDES
              IF fasegran "SFCDL.mms" ...eqs..."."
                CMS PERCH SF2D1 thms
             .IF/Essearch: *PRESECOFLGZLDB c.b*% egs. **
                 copy wb_ole:?RESECOFULDLIB.ole def_cott...
                   isbyote PRESECCTLEDLIB.ofb
                ENDIF
              ENDIF
         ENTIF
్రా
$!
$\ Send the user hail lif a error occurs.
$\ mail_list == f6ger)pi( "", "username").
SI MMS san generate some warnings that we don't need to stop for, disable error
- $1, handling so that we don't stop for trivial
```

# Figure 4.2-1 (Page 8 of 9) SF2D1 BUILD.COM Build Script

```
SET INJOH
               RETURN
          f The user-sequessed a 20% build and load then shedw for a 20%.
Downty rease is if it does not exist. Load modules, and is some
        BUA (esta)
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                                   wegs " THEN som cheate lib scall brack
                                                                                                                                                                                                                                                        INFORMATION ONLY
                            SCO
                           secolibrary scallibrar/
                            load revision wrists. and
                          find symbol=variable and occurrence=primary
                             AND NOT EXPAND, sympol=variable and occurrence=seference1, output=wp_criticlesFCS1_oca_Far_not_ref.tx0 find called_by end=PRESECOFUID; depth=alle youtput=wp_build.SRIDI_calltree.tx3
     don/t do the rest until the proper headers are in the code. report incernals / tax=txt /output_wp_bulld_offici.
                                     EKIT .
                   RETURN
 <del>2. 2.1244. M. Co</del>ntrol of the second of the
 il A (MS mail message is sent out it the build fails
by Progride busic setts/for the message.
                mail_suppers == 'build for '
mailsibe == 'wp_build.mail_bulld.mag'

OPEN/Write mail_file 'mailsile

Write mail_file '''Estlyb', ' Beginning ''subsystem' bulld bype ''Siv'
                   RETURN
STERMINATE
 St Check for error status, if the mail flag is set send the message
S: Then cleanup and exit.
 5! Try to notify the user if there where any build issues.
                    DEASSIGN /proc syssoutput | Closes the build log for this file.
                    SET noverliv
         If there was no previously flagged error on problem, search the log flies
S! for any facal, error, or warning messages.
                    IF mail_switch ne. 1
                               Search wp_build:SF2D1_build.log.wp_build:SF2D1_mms.log
"-f-","-e-","-w-"/mateor
                               IF SSTATUS .eq. 1
                                WRITE mail_file "The cyild for SFID1 returned an error of warning
                                WRITE mail_file "Please examine in the build directory:
```

# Figure 4.2-1 (Page 9 of 9) SF2D1 BUILD.COM Build Script

# Figure 4.2-2 (Page 1 of 6) SF2D1.MMS Input File for Build Script

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       LIERARYMODULES = 4
     | Wp_slb:852D1_WRTS2b.
| Wp_slb:852D1_WRTS2R.
        wo_clb:SF2D1_WRTSEC,
        Wp_clb:SF2D1_WRTWEL
        LIBRARIES = wp_olb:presecofildlib.olb(%(LIBRARYMODULES))
       ! dependencies
        wp_clt:camsupes_lib.olb/lib.
                        sysSlibrary:vaxcrtl.olb/lib.
                        wp_build:wp_id.opt/options
          wp_ole:sf2Bi_ADDMEM.cbj ...wp_srd:sf3D1_ADDMEM.for,
```

### Figure 4.2-2 (Page 2 of 6)

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WE_SCIRETON_FILEUN, ind

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wt_spoweF221_DadE1.whc.
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 WELFLEY NEFF CLIFFEND NO.
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WT_STO:SFOOR_SBOOR_The
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Wp_sto:SF2D1_F3LEUN.ind,
Wp_sto:SF2D4_INDEX.ind, -
Wp_sto:SF2D1_LOGIC ind, -
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 wp_are erablisacettine.
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                                 fortran &(eflags) wp_are:SF2D1_deTRUN for
 wp_clb;SF2B1_GETSLV.obj : wp_sre;SF2D1_GETSLV.for;
                                 #p_sto:SF2Dl_FILEUN.inc.
#p_sto:SF2Dl_SEGO23.inc,
#p_sro:SF2Dl_SECO2R.inc
#p_sro:SF2Dl_SECO2R.inc
foreran & cclags | wp_sro:SF3Dl_GETSLV.for
 wp_clb:SF2D1_ININAM.cbj ::
  wo old SF201 INISEC. co: : wo src: SF2D1 INISEC. for,
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### Figure 4.2-2 (Page 3 of 6)

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wp_srd.sfCDi_CoAT.com,

wp_srd.sfCDi_CoAT.com,

forcusar.com, sflags: wp_srd.sfCDi_PRESECORLCO.com)
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wp_src:SF2D1_ARRAY.inc.
 wr_olb:SF2D1_PRSECO.bbj
                                           wp_src:SF2D1_FILEUN.inc.
wp_src:SF2D1_gEOPAR.inc.
                                           wp_src.SF2D1_LOCAT.inc,
wp_src.SF2D1_LOCFAR.inc,
wp_src.SF2D1_LOGIC.inc,
               wo_src:SP2D1_REGPAR.ind
fordran/s/ofjags; wg_arc:SP2D1_PRSECO.for
 wp_sib sfib1_2RscRC.obj : wp_src.sFib1_PRSCRC.fcc.
                                            wp_src SF2D1_ALTNAM inc.
                                            wp_src:sF2D1_ARRAY.ins;
wp_src:sF2D1_F1LEUX.ins;
wp_src:sF2D1_LOGIC.inc
               fortran $ (2514gs) wp_src(SF2D1_PRSCRC for
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### Figure 4.2-2 (Page 4 of 6)

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 rezalb sachizachtiv es
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  Ap_sib:SF2D1_RDSSCC.op; 
                                                                                                      wp_src:SF2D1_RDSECO.for/
                                                                                                       wp_src:SF2D1_ARRAY.inc.
                                                                                                       wp_src/SFCD1_FILEUN,inc,
                                  wp_src(SF2D1_FFRDAT)inc.
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  wp_clb:SF3D1_R3WELL cbj wp_src:SF2D1_RDWELL for: -
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### Figure 4.2-2 (Page 5 of 6)

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forchan & stillger wp_sr3, df3D1_1f5f7f0cRD.fist
    wp_prik_dreci_sendHe.bus / wp_src/uPJei_sendHe.ibs
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         AD albhafial_WATMlR.obj :
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wp_src.sf2Di_FIUSUN.inc,

wp_src.sf2Di_LoGIC.ing/

wp_src.sf2Di_SEGOLD.inc,
        wp_oit:sfibi_WRTSil.ob; :
                                                         wp_stc sF2D1_sECO2R/inc
Tortian %(cflags) wp_stc:SF2D1_WRTS2I for
         wp_olb:sf2D1_WRTs2R.bbj : wp_sfe:sf2D1_wRTs2R.for,
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forthan S'cflags) wp_src.SF2D1_WRTS2R.for
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# Figure 4.2-2 (Page 6 of 6) SF2D1.MMS Input File for Build Script

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# INFORMATION ONLY

### Figure 4.2-3 SCA Output File of Modules Not Referenced

PRESECCELLS propedure PRESECTELLS

SUBROUTINE or PROGRAM declaration

### Figure 4.2-4 (Page 1 of 3) SCA Call Tree Output

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           ESECTELS procedure of SECTEN routine

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MILITATIONS INC.

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                ACRAMICATION CONTRACTOR

CAPAGE COURTINE

CASTUP CENTURE

RECORD COURTINE

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MAN CARCELON See above
MAKE CORCECT See above
QAABORT COLLINE See above
DELASCRICTURE
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                               DESTANCE TOUCHER
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MEMADISTOLE FOR THE
                                                             MDSTAT routine
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INTSEC routine
PRAGER routine calls
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                                                DBISTER robtine
                                                DBIVAR routine
                                                QAABORT routine (See above)
                                 QAABOFT rautine (See above)
                                 SCANSI routine calls
                                  PRRDFLDS routine
GSTBND Boutine bails
                                                               FERDFUDS routine (See above)
                                                               QAABORT routine (See above)
                                                 GETLTS routine calls
                                                               FFRDFLDS routine
                                                                                                                                                             See above)
                                                                QAABORT routine see above
                                                 GETRTS routine calls
                                                 FFRDFLDS routine - See above
                                                    QAABORT routife (See above:
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# Figure 4.2-4 (Page 2 of 3) SCA Call Tree Output

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                                      FFRDFLDS toutline', (See above)
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# INFORMATION ONLY

# Figure 4.2-4 (Page 3 of 3) SCA Call Tree Output

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DBLB function | See above

Figure 4.2.5
SCA Output File of All Modules Included in Static Analysis

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## 5.0 COVERAGE ANALYSIS

The coverage analysis for PRESECOFL2D was performed using DECset PCA. A unique executable, called WP\$TESTROOT:[SF2D1.EXE]PRESECOFL2D\_TEST\_PCA.EXE was created for the purpose of coverage analysis. This executable was generated by using the SCMS build script, SF2D1\_BUILD.COM. The build script is shown in Figure 4.2-1. The coverage analysis was performed in the directory WP\$TESTROOT:[SF2D1.PCA].

The command file SF2D1\_TESTCASE\_PCA\_CUM.COM, shown in Figure 5-1, was used to run the PRESECOFL2D test case with PCA. The PCA output for the test case has been included and can be located by referring to Table 5-1. A log of the process was created and can be found in Figure 5-2.

Table 5-1
Location of Coverage Analysis Output Files

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	Cumulative PCA Coverage Analysis Test Cases	2

The code sponsor was asked to review the output files from the coverage analysis and to write a summary of that review. The code sponsor's comments can be found in Figure 5-5. Nothing unexpected was revealed during the PCA process.

# Figure 5-1 (Page 1 of 2) Script Used to Run Test Case for PCA Analysis

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# Figure 5-1 (Page 2 of 2) Script Used to Run Test Case for PCA Analysis

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# INFORMATION ONLY

# Figure 5-2

## (Page 1 of 2)

# PCA Log of Coverage Analysis

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# Figure 5-2 (Page 2 of 2) PCA Log of Coverage Analysis

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Figure 5:3
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# Figure 5-4 (Page 4 of 7) Cumulative PCA Coverage for Test Case

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# Figure'5-4 (Page 6 of 7) Cumulative PCA Coverage for Test Case

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# Figure 5-4 (Page 7 of 7) Cumulative PCA Coverage for Test Case

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No filters are defined

PROGRAM\_ADDRESS BY ROUTINE

# Figure 5-5 Code Sponsor's Response to Coverage Analysis

Most of the modules that show up in the performance coverage analysis as not being called are modules in the CAMCON libraries that the code is linked to. The following is a list of the non-CAMCON modules in PRESECOFL2D that are not called. The reason why each routine is not called is that feature is not used by the WIPP PA unless otherwise stated. The remaining uncalled modules are CAMCON modules

GETSLV - Prelimary set up of solving parameters. This routine is not called because the default settings are used by the WIPP PA.

FIND\_IJA - Finds the location of a cell in the regional computational grid relative to the problem defining grid. For WIPP PA, these two grids are identical so routine is not called.

INTF - Interoplates the properties from the problem defining grid to the regional computational grid. For WIPP PA, these two grids are identical so this routine is not called.

PRSORC - Used for time dependent wells.

QAABORT - Used for error handling. If no errors occur, this routine will not be called.

QABATCH - Used only if code is run in CAMCON batch mode.

RDAQFR - Used to define precipitation, rivers, lakes and constant head cells. These are not used in WIPP PA.

RDSOLV - Used to set up solving parameters. The defaults are used for WIPP PA.

RDWELL - Sets up wells. Wells are not used in WIPP PA.

SETGHR - Used if databases are predefined with all properties.

WRTWEL - Writes well informtion to SECOFL2D input file. Wells are not used in WIPP PA.

# INFORMATION ONLY

# 6.0 FUNCTIONAL TESTING

A list of requirements for POSTSECOTP2D can be found in Figure 6-1. PRESECOFL2D has already undergone QA and is qualified as level A under QAP 19-1 Rev F. Therefore, the test case consisted of running the current code for the purpose of coverage analysis and regression testing.

The test case was run in the directory WP\$TESTROOT:[SF2D1.TESTCASES], and all files associated with the functional testing are located in this directory. To run the test case a script was used, and that script can be seen in Figure 6-2.

An evaluation of the test case can be found in Sections 6.1

# Figure 6-1 Requirements of PRESECOFL2D

# Functional Requirements:

- R.1 Creates all input files needed to run SECOFL2D. These files are:
  - 1) An ASCII file containing run parameters
  - 2) A binary file containing regional material property information obtained from a CAMDAT database.
  - 3) A binary file containing local material property information.
- R.2 Interpolates material properties from the regional grid to the local grid.

# Performance Requirements:

This code has no performance requirements.

# Attribute Requirements:

This code has no attribute requirements.

# External Interface Requirements:

- R.3 This code reads an ASCII input file containing run parameters.
- R.4 This code reads an input regional CAMDAT database with grid information and material properties
- R.5 This code reads an input local CAMDAT database with grid information..
- R.6 This code produces all of the input files necessary to run SECOFL2D.

# Additional Requirements:

There are no additional requirements for PRESECOFL2D that need verification.

# Figure 6-2 Script Used for Running Test Case for Functional Analysis

```
Comparison

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# 6.1 Test Case #1: Regression Testing And Coverage Test Case

## 6.1.1 Test Objective

This test case was run to do the following:

- 1) test the interpolation of properties from the regional grid to the local boundary,
- 2) regression test the current code in the CMS so that it gets the same results obtained when the code was previously QA'd to the A level, and
- 3) assure modular coverage.

The issue of modular coverage has been addressed in both the use of DECset SCA and in the PCA Analysis.

## 6.1.2 Test Procedure

PART 1: (To test the interpolation of properties from the regional grid to the local boundary)

The pre-processor is executed followed by the execution of the program READ\_PRP.FOR. This program converts the regional binary property file, REGION\_TEST.PRP, to an ASCII file, REGION\_TEST.ASC, and the local binary property file, LOCAL\_TEST.PRP, to an ASCII file, LOCAL\_TEST.ASC, so that they can be examined with an editor. All of the material properties used to run SECOFL2D are constants except for hydraulic conductivity. Therefore, checks of porosity (phi) and bulk compressibility (alpha) need only show that they have remained constant. A hand-calculation is done for hydraulic conductivity to show that the values have been correctly interpolated (using bilinear interpolation) from the regional grid to the local grid.

To verify that the porosity and bulk compressibility have remained constant, edit the file REGION\_TEST.ASC. First, search for the string "alpha". Examination of this array shows that this is a constant value of 7.57E-01 for each element in the grid. (The value of bulk compressibility is 7.57E-10 on the database, but it has been scaled by 10° as required by SECOFL2D.) Next, search for the string "phi". Examination of this array shows that this is a constant value of 1.4542E-01 for each element in the grid. Now repeat this process with the file LOCAL\_TEST.ASC. Searching for the string "alpha" shows that this array is a constant value of 7.57E-01, and searching for the string "phi" shows that this array is a constant of 1.4542E-01. The above mentioned searches were done and the constant values were verified. The first two rows of each 47x54 array are shown for completeness. Figure 6.1-1 gives a listing of the testing tool READ\_PRP.FOR used to convert the CDB files to ASCII files. The first two rows of the "alpha" array can be seen in Figure 6.1-2 and the first two rows of the "phi" array can be seen in Figure 6.1-3. The data in both figures was extracted from the LOCAL\_TEST.ASC.

Four points are checked by hand-calculation for the hydraulic conductivity. The four element locations in the local grid are (12,15), (20,47), (35,25) and (40,40). First, the cell locations relative to the regional grid are found. The cell locations in meters are converted to locations (in

meters) in the regional domain. The x and y offsets of the local grid from the origin of the regional grid are 12826.1 and 10665.8 respectively. The angle of rotation is 38° counterclockwise. The coordinates (in meters) of the cell centers in the local grid are:

```
Element 1 (12,15): 1437.5, 1812.5

Element 2 (20,47): 2437.5, 5812.5

Element 3 (35,25): 4312.5, 3062.5

Element 4 (40,40): 4937.5, 4937.5
```

The regional coordinates are calculated by:

```
Element 1: 12826.1 + 1437.5\cos 38^{\circ} - 1812.5\sin 38^{\circ} = 12842.97903

10665.8 + 1812.5\cos 38^{\circ} + 1437.5\sin 38^{\circ} = 12979.08286

Element 2: 12826.1 + 2437.5\cos 38^{\circ} - 5812.5\sin 38^{\circ} = 11168.34389

10665.8 + 5812.5\cos 38^{\circ} + 2437.5\sin 38^{\circ} = 16746.78735

Element 3: 12826.1 + 4312.5\cos 38^{\circ} - 3062.5\sin 38^{\circ} = 14338.93311

10665.8 + 3062.5\cos 38^{\circ} + 4312.5\sin 38^{\circ} = 15734.12305

Element 4: 12826.1 + 4937.5\cos 38^{\circ} - 4937.5\sin 38^{\circ} = 13677.07456

10665.8 + 4937.5\cos 38^{\circ} + 4937.5\sin 38^{\circ} = 17596.43163
```

Next, the cell centers of the adjacent cells are used (the properties reside at the cell center) to calculate the proportional distances used in bilinear interpolation.

```
Element 1 proportions from coordinates of regional cells (32.10) and (33.11):  xp = (12842.97903 - 12625.0)/(12850.0 - 12625.0) = 0.9687956889   yp = (12979.08286 - 12750.0)/(13125.0 - 12750.0) = 0.6108876267  Element 2 proportions from coordinates of regional cells (24,34) and (25.35):  xp = (11168.34389 - 11075.0)/(11225.0 - 11075.0) = 0.6222926   yp = (16746.78735 - 16725.0)/(16950.0 - 16725.0) = 0.0968326666  Element 3 proportions from coordinates of regional cells (39,26) and (40,27):  xp = (14338.93311 - 14150.0)/(14450.0 - 14150.0) = 0.6297770333   yp = (15734.12305 - 15600.0)/(15800.0 - 15600.0) = 0.67061525  Element 4 proportions from coordinates of regional cells (37,38) and (38.39):  xp = (13677.07456 - 13675.0)/(13887.5 - 13675.0) = 0.009762635294   yp = (17596.43163 - 17475.0)/(17630.0 - 17475.0) = 0.783429871
```

Then, the bilinear interpolation is done.

```
Element 1:
```

```
a1 = 498.5 + 0.9687956889(1498.0 - 498.5) = 1466.811291

a2 = 670.3 + 0.9687956889(707.4 - 670.3) = 706.2423201

a = 1466.811291 + 0.6108876267(706.2423201 - 1466.811291) = 1002.189117
```

## Element 2:

- a1 = 182.5 + 0.6222926(267.1 182.5) = 235.145954
- a2 = 109.1 + 0.6222926(119.8 109.1) = 115.7585308
- a = 235.145954 + 0.0968326666(115.7585308 235.145954) = 223.5853515

### Element 3:

- a1 = 495.8 + 0.6297770333(960.2 495.8) = 788.2684543
- a2 = 816.1 + 0.6297770333(1041.0 816.1) = 957.7368548
- a = 788.2684543 + 0.67061525(957.7368548 788.2684543) = 901.9165481

## Element 4:

- a1 = 159.6 + 0.009762635294(277.6 159.6) = 160.751991
- a2 = 117.4 + 0.009762635294(28.47 117.4) = 116.5318088
- a = 160.751991 + 0.783429871(116.5318088 160.751991) = 126.1085794

# Acceptance Criteria:

The values for porosity and bulk compressibility remained constant. The values for hydraulic conductivity from LOCAL\_TEST.ASC (interpolated from the regional grid) will agree with the hand-calculation to 6 decimal places.

|           | From file LO | From hand-calculation |         |
|-----------|--------------|-----------------------|---------|
| Element 1 | (12,15)      | 1.00219E+03           | 1002.19 |
| Element 2 | (20,47)      | 2.23585E+02           | 233.585 |
| Element 3 | (35,25)      | 9.01917E+02           | 901.917 |
| Element 4 | (40,40)      | 1.26109E+02           | 126.109 |

Figure 6.1-4 shows rows 15, 25, 40, and 47 of the 47x54 array AKX in the LOCAL\_TEST.ASC file created. Visual inspection verifies that the results are in agreement with the hand calculations performed.

PART 2: (To show that the regression test of the current code in the CMS in fact gets the same results obtained when the code was previously QA'd to the A level)

Test Case 1 is suitable for installation and regression testing. For regression testing against the primitive baseline on file in the SWCF, this test case uses a utility program, TEST\_READ\_1. This program was used to produce the output on pages 4-6 of the verification section of the primitive baseline. Copies of these pages are included as Appendix B. This program should produce the identical results to the results in the primitive baseline when run during this testing exercise.

The input file for TEST\_READ\_1.FOR is the SF2D1\_REGION\_TEST.PRP output file. A listing of TEST\_READ\_1.FOR is shown in Figure 6.1-5, and the results from the current execution are in the file TEST\_READ.OUT as shown in Figure 6.1-6. This Program should

produce the identical results to the results in the primitive baseline when run during this testing exercise. The input file for this test case is shown in Figure 6.1-7.

## 6.1.3 Input/Output Files

Since only a single run of the PRESECOFL2D was made to perform the functional analysis, the command file and the input files used is the same for both parts of the analysis. They are:

Command File:

SF2D1\_TEST\_NODBG\_RUN.COM

Input Files:

WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_REGION\_TEST.CDB WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_LOCAL\_TEST.CDB WP\$TESTROOT:[SF2D1.TESTCASES]SF2D1\_PRESECOFL\_TEST.INP

A listing of the input file SF2D1\_PRESECOFL\_TEST.INP is shown in Figure 6.1-7.

The input files SF2D1\_REGION\_TEST.CSB and SF2D1\_LOCAL\_TEST.CDB have not been included in this documents because they are not only in binary format but are also very large. The size of ASCII file of the contents would be prohibitive and would lend little information related to the testing. Both files will be submitted and retained in SCMS.

Each part of the functional analysis required the use of different output files which were then examined using short utility codes written for that purpose with resulting output files from that process. These files will be described for each part of the test case.

## PART 1:

Output Files:

WP\$TESTROOT:[SF2D1\_REGION\_TEST.PRP]
WP\$TESTROOT:[SF2D1\_LOCAL\_TEST.PRP]

Testing Tool:

WP\$TESTROOT:[SF2D1\_READ\_PRP.FOR]

Output Files from Testing Tool:

WP\$TESTROOT:[SF2D1.TESTCASES]REGION\_TEST.ASC WP\$TESTROOT:[SF2D.TESTCASES]LOCAL\_TEST.ASC

## PART 2:

Output Files:

WP\$TESTROOT:[SF2D1\_REGION\_TEST.PRP

Testing Tools: WP\$TESTROOT:[SF2D.TESTCASES]TEST\_READ\_LFOR

Output: Files from Testing Tools: WP\$TESTROOT:[SF2D.TESTCASES]TEST\_READ.OUT

## 6.1.4 Evaluation

## PART 1:

The acceptance for this part of the functional analysis was that once the alpha and phi values input were in fact constant, the output for four points on the local grid boundaries would have AKX values consistent with the conductivity values derived with hand calculations. This was in fact the case and the acceptance criteria has been met.

## PART 2:

The acceptance for the regression testing of the current code required that the output from the current test case could be examined and the results would show no differences from the output file as noted in the primitive baseline. This was found to be the case and the acceptance criteria has therefore been met. However, only one file of the four generated by PRESECOFL2D was checked.

# Figure 6.1-1 (Page 1 of 4) Listing of READ PRP.FOR

```
PROGRAM READ PER
          Geads binary property (i)e FSRC20.DAMP Written by CST_GRESC and 
Cranshates to inco at BECTT payons file.
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          user s'illest of hutput file hamest
          IMPUICIT BOMBLE PRECISION ARBUCHING
           IMPLICIT NONE : *** * * * * * * * * * * BENGVED
          dimension TMPARR(0:100,0:100), TMPVEC(0:100)
INTEGER I 3: IDUMI: IBUMI: ISECCL IL. JL. IDFI
REAL RDUMI: RDUMI: RDUM3: ******* superceded
CHARACTER*40 INFILE
DATA ISECC2/10
DATA IDFILLIREG(2)
2. SEGIN PROCESURES
          WRITE(6,*) !Ender the name of the input file:
PRAD(5,"NAI": INFILE
OPEN UNITHISECOL, FILE-INFILE, STATUS="OLD" READONLY,
PERMATTED":
          WRITE(6, 1) Server the name of the output file; , , READ(5, '(A)) INFILE ORBNIUNITGIOTIL_GREG, FIRE INFILE, STATUS; 'NEW')
      10 COMPINUE
              WEITENGIOFIL AREG. 95201
FIRMAT : SUTFUT from program SET_IREGI SET_ICCC.
' Numeric FORMATS are
                                 2,254, 19513,5°, 1
3,276, 1280, 3xin%
3,35, 19513,5);;
    SET_GREGI run with ligh, ligh, greg_ID.

SET_GREGI run with ligh, ligh, greg_ID.

Nilgh, jigh, aoer_ID + //
READ(ISECC2) TL, JL, RDUM1, IDUM1, IDUM2, RDUM2

WRITE (IDFIL_GREG.953) i1, j1, RDUM1, i1, j1, RDUM2

953 FORMAT (3(216, 19E13.5))

READ(ISECC2) RDUM1, RDUM2, RDUM3

WRITE (IDEIL GREG.956) RDUM1, RDUM3
               WRITE (IDFIL_GREG.956) ROUM1, ROUM2, ROUM3
    956 FORMAT (' x1_rel, y1_rel, chet1_rel = ',/,123E13.5)
 c 1-D arrays
    955 FORMAT (3(16) 19513.5))
                Read x-coordinates -
 READ [ISECOS] TRMSVECTI., I=0, IL+1)
               WRITE (IDFIL GREG, 9540)
              FORMAT [ (1, x(1), 1=0, 11GR+1) WRITE (IDFIL_GREG, 955) (1, TMPVEC(1), 1=0,11-1)
                Read y-coordinates
  READ(ISECO2) (TMPVEC(I), I=0, JL+1)
```

# Figure 6.1-1 (Page 2 of 4) Listing of READ\_PRP.FOR

```
WRITE COFIL GRES (EAL)
RORMAN IN JAPAN ASS
WRITE SERIL JPSN ASS
TMPVEL IN JESS
          3541
   Rest dict of the rest of the r
        7540
   Read delia V.S.
ABAD JUBITA TMP/BDI / ISIN IL-
MRITTE IBETU JREG TEAU
RORMAT JAGY TAIL
WRITE IDEXILARED ASS
S-2-2 artayaw, A
  Factor versive consists of the control of the contr
  Read X Dydrail 2 condecinees

DEAT TEROOC TWENTY TO THE TERM THE TERM TO THE T
  Read, / mydrawlic conduct: les
READ.ISECCOY : TMRASE L.G. TEG., LL-1 .JeO.JL-1
IOFZ-LGREG,9533
  Read fluid compressibility
READ(ISECOL) ((TMPARR.I.J), I=0.IL-1).J=0;JL+1)
WRITE (IDFIL_3REG,8532)
  FORMAT ((1)) alpha (1,j) (1=0, 113R-1), f=>/ 310R-1) ()
WRITE (LDF=6_3REG, 961)
(1,j) TMPARE (1,j) (1=0,11+1), J=0,51-1)
               3532
                        Read, gorosity

READ(ISSCOI) ((TMPARRIL, J), 1=0, DL-1), J=0, JL-1

WRITE (IDFID_DREG, 8833)

9833 FORMAT ((, t.1, j, phi -1, j) (1=0, 119R+1), j=0 (13R+1)

WRITE (IDFID_BREG, 853,

5 (1, j, TMPARRIL, J), Z=0, X1-1, J=0, j1+1;
```

# Figure 6.1-1 (Page 3 of 4) Listing of READ PRP.FOR

```
Pead apecific scorage
       READ ISPOSIN (TMPARE I.E. 120.12-1.03-0.01-1.
WRITE IDPILISHED (633
FRAMATE IDFILISHED (633)
WRITE IDRIG (RET.):53
LECTOR (120.1-1)
        Read aquitèr cotcom
         READ TEEEOS. ATMEARR 1.3. TEO. 11-1 JEO. 55-1
WRITE (IDELL JREG. 2505
Read well cliver recharge term
READ, ISECOL TMPART INDICATES, TUPIT, Jep., JUPI
WRITE, JUPIC, JREG JESS 
SE FORMAT I STANDISTION (J.), LeD., LIGHT, Sec. SIJR-1.
WRITE STANDISTION (J.), LeD., LIGHT, Sec. SIJR-1.
Read States Conductions
Read States Conduction (J.)
READ, JESCOL TOMPARE IN JACKS (J.), LeD., LL-1, Jep., Light (J.), TMPARRY (J.), LeO., Light (J.), Jeo., Size(J.)
S. ((i.), TMPARRY (J.), Jeo., Light), Jeo., Size(J.)
3536
9537
          Read river head {
READ(ISECSE) ((TMPARR(I,J), I=0, ID+1),J=0,JD+1)
          WRITE (IDFIL_GREG, 9637)
         9637
    s (1,5,TMPARRILES), D=0,11+1), J=0,11+1)
          Read river bottom
          READ(ISECO2) ((TMPARR(I,J),I=0,IL+1),J=0,JL+1)
          WRITE LIDFIL GREG, 9737 k
      FORMAT ('((i,j,riv_bot(i,j), i=0, ligR+1), j=0, ligR+1)
WRITS (IDFIL_GREG.953)
S ((i,j,TMPARR(I,J), I=0,11-1), J=0,11-1)
          Read constant head
          READ(ISECO2) ((TMPARR(1,J), I=0, IL+1), J=0, JL+1)
          WRITE (IDFIL_GREG, 9538)
        WRITE (IDFIL_GREG, 953)
```

# NEORMATION ONLY

# Figure 6.1-1 (Page 4 of 4) Listing of READ\_PRP.FOR

7.57000E-01

# isting of Sample of Phi Values from LOCAL\_TEST ASC

|                   | * X                                              |                                       | 61.5                                     |                |            | 100              | 4 C C                 |                            | 7                 |                      | j<br>1 - 1 .  | n j            | ,;;      |                |              | 1 《新<br>2 使数    | )<br>57    | T da  |                  | ر<br>و ر         |                  |
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|                   |                                                  |                                       | es es s                                  | 26.6           | ) at       | ***              | 111                   | ( ) ( )                    |                   |                      | 3,937<br>2015 |                |          | ) ( )<br>  ( ) |              | 3               |            | 16    | 7                | 50 kg            | ្រា              |
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|                   |                                                  |                                       |                                          |                | 3.1.       | 100              | 5                     |                            |                   | 57                   | Arra Jina     | V 10.          | 1.5      |                | 9            | 275             |            |       |                  |                  | , -              |
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| ານ<br>ໂ           |                                                  |                                       |                                          | 77479<br>78474 |            |                  |                       |                            |                   |                      | 1400<br>1400  |                |          |                |              |                 |            |       |                  | da iri<br>Linear |                  |
|                   | t. 63                                            |                                       |                                          |                |            | \$ 100 m         |                       |                            |                   |                      | 2             |                | 1000     |                |              |                 |            |       | i i              |                  |                  |
| É.                | 1. 121<br>11. 11. 11. 11. 11. 11. 11. 11. 11. 11 |                                       | is a virte                               | , , , .        | T ( ) :    | 1977 S           | r o                   | ci in                      | (O -              | r Frir               | . ci          | n (n)          |          | r ( ;          |              | e.              | 7). c      | 1 (0  | ന '<br>ന         | -1 -1<br>-1 -1   | C-               |
| <b>3</b>          |                                                  |                                       |                                          | in the second  |            |                  |                       |                            |                   |                      | 50 F          |                |          |                |              |                 |            |       |                  |                  | Ý.               |
| <b>e</b> .        |                                                  |                                       |                                          |                |            |                  | 3/1                   |                            |                   |                      |               |                |          | 66.<br>1. 3    |              |                 | iv.        | 400   |                  | 0.41             |                  |
| , en              | · 12                                             |                                       | +4.5 (-<br>62 (-<br>13 (-                |                |            | 1361 3<br>1361 3 |                       |                            |                   |                      | )<br>         |                | ,        | 7 (C)          |              | 10              | ï          |       | 3                |                  |                  |
|                   | 3.4                                              |                                       | 000                                      | 0 10 G         | £          | - Paris          | 3.63                  |                            | 111 12<br>113 (11 |                      | 3.0           | ro co          | 62.0     | 5 5            | (3 C         | 63              | . č        | 10    | Ö                | ÷ 0              | , (3             |
| f.                | e.                                               |                                       | ्रापुर                                   | T***           | F -+ -     | *3- * ·          | TT TE                 | TT T                       |                   |                      | T -T          |                |          | r r            | -177         | - T             | -          | r r   | 24.              | 4 1              |                  |
|                   |                                                  | ir.                                   | 10 m 10                                  | i i i          | т. г.<br>Г |                  | U IU                  | a i                        | 1, 1              | i in ci              |               | 1 12           | Tra tr   | ; ;;           |              |                 | 71 U       | r -r  | T                |                  | 4                |
| gare, in a        |                                                  | 4.3%                                  | of the fig                               | 1.1.           | ( - 1 -    | 16.19            | 144                   | 1 17 1                     | · Úw              | 1,41 s               | 15-1          | !              |          | 144            | 1            | 1 - 1           | 9.         | 1 - 1 |                  |                  | 1 <del>-</del> 1 |
| Š                 | 1155 (A)                                         | 19 (19)                               | COL                                      | ) eve          | 5.00 E.C.  |                  | <b>1</b> ( )=         | · 0                        | / ) C             | , ,                  | ş. ş          | ¥.,            |          | 1. 1           | 4            |                 | 4)         | i Ç   | ij.              |                  |                  |
| ji.               |                                                  | 15872                                 |                                          |                |            |                  |                       |                            |                   |                      |               | 10.3           |          |                |              | r vije<br>Listo |            |       |                  |                  |                  |
| 61                | 0.000 (A)    | 1.                                    |                                          |                |            |                  |                       |                            |                   |                      | i. ;          | 在<br>被         |          |                |              |                 | Pau II.    |       |                  |                  |                  |
| 41                |                                                  |                                       | 7-41                                     | (E)            | 1 . 1 .    | 19 百             | A (1)<br>373          | e ( <del>ri</del><br>rije) | 1 5 C<br>113 TJ   | ) (*1/-)<br>t - #, - | r . 1         | - <b>*</b> ( * | 15 A. C. | 3 ()<br>1 , 1  | orer<br>orer | ) (65)<br>  (3) | ć∮.<br>co∵ | J (1) | €.3<br>(**)      | نر ي.<br>پيس     | ר יין<br>נויין   |
|                   | The Samuel Co                                    |                                       |                                          | ن از           |            |                  | 52/1r                 |                            |                   |                      | 7.1           | 4.6            | Ž,       |                | 10           |                 |            | -2    | de),             |                  |                  |
| L<br>A            | i, dil. 197                                      | 0                                     | 464                                      |                |            | 43-17            | 143 (                 | . 366-1                    | . (*              | :                    |               | 37 (S)         | , a 7    | T ea           | PAN A        | r.est           | 61.        | 4.1   | ( P. 1           | ્રે<br>(•        | 1 ÷ 1            |
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|                   | 1377                                             | 6                                     | 000C                                     |                | V. C . C   | 111              | 100                   | ( 1 Y Y                    | r'n r''           |                      | 3 ( )         | 1              | 1 1      | 1 ( )          | - 5          | F Y 30 11       | 1.         | 200   | 1.3              |                  | ) C.)            |
|                   | 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1          |                                       | i či či i<br>i urion                     | ጉርጥ ሆ          | 174 (194   | 1,413.4          | $\alpha \cdot \alpha$ | E1 1 1 1 1 1               | 403.46            | 15.1.20.14           | 17.17.1       | 110.115        | 16.3.~41 | F 1            | CHT          |                 | 1.0        |       | 110.00           |                  |                  |
| ប្រាស់<br>ពីទី ទី | 7 V 3 G 16 V                                     |                                       |                                          |                | 7.77       | 430              |                       |                            | 7.71              | 2                    |               | 特领             |          | ŗ              |              |                 |            | 表级    | $\mathbb{R}^{n}$ | 4,47             |                  |
|                   | (; 0<br>() -r                                    |                                       | 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1 | * # 15 TO 10   |            |                  | ATT IN                | ****                       |                   |                      | 3. 支<br>3. 数  |                |          |                |              |                 |            |       |                  |                  |                  |
| គ ្រ 🔆 🖫          | de Carlo                                         | 的现在分<br>其他的                           | റെറ                                      | 3 5 7          |            |                  | 50                    | 130                        | רי כו             | . C.                 | 3 I           | , 4 , 4        |          | , 1            |              | L . 34          |            |       |                  |                  |                  |
| 4, 0, 4 (D)       |                                                  |                                       | <b>小</b> 多是                              |                |            |                  |                       |                            |                   |                      |               |                |          |                |              |                 |            |       |                  |                  |                  |
| 5.000             | (L)          | 14.                                   | Cr in i                                  | o or r         | 11400      | n i              | r ( s                 | ୍ତି (<br>ସେଠାର             | 10 C              | co'a                 | ,             | · 1            | 1957     | ,<br>, , ,     | r ta e       | - r x           |            | i iii | 0                | ر.<br>(۱)        | )<br>1 Li 1      |
|                   | A. W.                                            |                                       |                                          |                |            | 場が               |                       | miri                       | 133.              |                      | \$            |                | - 19 (9) | 1.4            |              |                 | rç         |       | 304              |                  |                  |
|                   |                                                  |                                       |                                          |                |            |                  |                       |                            |                   |                      |               |                |          |                |              |                 |            |       |                  |                  |                  |

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# Figure 6.1-4 (Page 1 of 2)

# Listing of Four Rows of AKX Values from LOCAL TEST, ASC

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   7.4882095+02
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                                      9.038485-01
  45
  47 40 8.78533E-01
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# Figure 6.1-4 (Page 2 of 2) Listing of Four Rows of AKX Values from LOCAL\_TEST.ASC

|                                        | 2000 000<br>300            | + + -                           | 3 (1)                                      |                   | 0.747242+03                                                           | 13 43                | .5164-5-33/                                 |
|----------------------------------------|----------------------------|---------------------------------|--------------------------------------------|-------------------|-----------------------------------------------------------------------|----------------------|---------------------------------------------|
| 7                                      |                            | 5.4184                          | 5 <u>5</u> 243                             | 47.               | 1.975768+02                                                           | 3 45 1               | .50 <b>9</b> 955-00                         |
|                                        |                            | : 13 Bb3                        | (E-NE/S                                    |                   | 71.963.98E+&1                                                         | ° 6 . % . 4 ° ∞8     |                                             |
| 9                                      | 47                         |                                 |                                            |                   | 9.460105-01                                                           |                      | . 22 J. |
|                                        | * 취급하다.<br>- 300명 #115 : 1 | (3) / 22 3 A<br>- X - X 3 3 3 4 |                                            |                   | 2 747245-03<br>1 975765-02<br>9 63285-31<br>6 65285-31<br>1 872355-02 |                      | s.secc<br>                                  |
|                                        |                            | ovivate<br>3 o gerb             | 0 Br 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 |                   | 120275+03                                                             |                      | (03585B-03                                  |
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| -/4                                    | 17                         | 12,5120                         | 42.02                                      | 3-2 4-7           | 21,21,44,35,432                                                       | 125 m 2 km 2         | .,92329 <b>8-</b> 83                        |
| ************************************** | 17                         | 0,0250                          | 5E422,                                     | 280 47            | 7,189638+01                                                           | - 29 . 4 /           | .659.45+01<br>.04812E+03                    |
| 4155. Television                       | 47                         |                                 | 28+01<br>95.60                             |                   | 9.98037E+71<br>1.63961E+03                                            |                      | .46651E#82                                  |
| 35                                     | 17                         |                                 | วิธี-จั้ว                                  | 37 47             | 1.474665400                                                           |                      | _70553 <b>5</b> 463                         |
| 39                                     | 47                         | 1.5.2                           | 5E+92                                      | 40 7.49           |                                                                       |                      |                                             |
| 12:                                    |                            | 5 5 5 5                         | 115+00°                                    | 43 47             | 2.44703E-00                                                           | 144 47 669<br>47= 40 | 7.141268-71<br>3.403398-71                  |
| 3                                      |                            |                                 | JE - 94                                    | · 30 · · · (3/-5) | 3.60999E=11                                                           |                      |                                             |

# Figure 6.1-5

# (Page 1 of 3) Listing of SF2D1 TEST READ 1.FOR

```
RROGRAM TEST READ :

7. 649-94 ELUSH S DOMERISKS
THIS PROPAM WAS WRITTEN FOR THE SINGLE PUPPOSE OF
SERVEYING SINARY OUTPYT RECM SECORUSE
SOFT FISH FAMORE OF SPECIFIEL ARRAYS ARE PRINCED TO THE
SUTPYTHE FOR VERIFICATION BY INSPECTION
                      Reads London pubperty file FORGE (CAT: written for SET FEED and comparable (25 into an ABC) into the Sile of the Sile of the Longon Sale of the FORGE CAT and the user's choice of output file names.
                        IMBUICIT COUBUE PRECISION A-H.O-IN
                      dimension TMPARR(0:130,0:130)
                       CHARACTER*50 INFILE, OUTRILE
                     TATA ISECO2 10/
TATA ISECO2 10/
                 aggin Procesumed.
                      WRITELO, ', 'Encorcipe name of the shput tile.'
PREAD S. A ' TAFILE
TREN UNITERSECON FILE=CNRILE, STATUS*'SUD', READONLY,
FORME:UNFORMATIES';
                         WRITE of the came of the capput files:
                          READ FINANT CURFILE
                         JREMOUNTTHIDETY_GREG, FILEFOUTFILE, STATUSH'NEW'
          THE SELECTION OF THE SERVICE CONTRACTOR OF THE SELECTION 
        ASS FORMAT STAIN LREIS S.
ASS FORMAT DIE, TREIS S.
           RDUM2, RDUM2
        READ(ISECO2) TL. JS
. . READ(ISECO2) RDUM1, RDUM2, RDUM3
READ(ISECO2) RDUM1, RDUM2, RDUM3
     C:.../.1+D-arrays
               Read x-coordinates
READ(ISECO2)
    C ... Read y-coordinates
                      READ(ISECO2)
     C....Read delta x's
                         READ (ISECOS)
    C. . . Fead deita y s
                            READ (ISECOL)
           ....2-D arrays
     C. Read & relative offsets
                READ(ISECO2)
    C. ... Fead y relative offsets
           READ(ISECO2)
    SC .... READ AND ECHO THESE FOR TEST 6-9-94
```

# Figure 6.1-5 (Page 2 of 3)

# Listing of SF2D1 TEST READ 1.FOR

```
WRITE ILEQUIRES(1);
      LODE FORMAT TO THE SAME AND THE
                    Wedte lotal-afeda.
      CONFORMAT CONTRACT CO
                  S((1,j,TMPARR(I,J)^{\dagger}SCF, I=31,30), J=28,28)
       - READ AND BOND THESE FOR TREET. 6-9-44
   ntormation
                    WRSTS SEFELERES, 114
FORMAT 1, 3,880 E
WRSTS SEFEL SEEG 158
  JANEAR TARABATA DA BESTA DESENDADA DESTA SE
એ.. aread and etho These for Test: 6-9-84ન
                  ..Read Eluid compressibility
READ(ISECO1) ((TMRARR(I,J),I=0,IL+14,J=0/JL+11)
                      WRITE (DDFIL_GREG, 120)
 129 FORMAT (' ((2,j,alpha (2,j)), (2=1,10), (3=1,2)
                       WRITE (IDFIL GREG, 953)
S + (1, j), TMPARR(\frac{1}{2}), SCE, I = 1, IC, J = 1, 1
                         WRITE (IDFIL GREG ) 221).
         132 FORMAT (/ [(d); alpha(1, j), l=21, 30), j=28,28);)
                         WRITE (IDFIL GREG, 953)
                     $((1,),TMPARR(1,U) *SCF, 1=21,30), J=28,28)
                         WRITE (IDFIL GREG, 124)
       124 FORMAT (* ((1,j,alpha(1,j), 1=41, 50), j=57,57).)
WRITE (12816_2886,953)
                      S((1,j),TMPARR(1,J),SCE,[1+4],50), J=57,57)
 C. READ AND ECHO THESE FOR TEST 6-9-94
 C.....Read porosity
                         READ(ISECOL) ((TMPARR(I,3), I=0, Ib+1), J=0, Jb+1)
          WRITE (IDFIL GREG, 190)
130 FORMAT (% ((1.) 5 Chi 1.5); 1= 1.10), j = 1. (1))
                         WRITE (IDFIL GREG: 18
```

# NEORMATION ON

# Figure 6.1-5 (Page 3 of 3) Listing of SF2D1\_TEST\_READ\_LFOR

```
WRITE GDETLIGREG, 451
John Johnson J. J. Jel (18)
                  WRITE COFILLIRES, 132
            PORMATA TO TO THE PORMATA PROPERTY OF THE PORMATA PROP
  1=225.8007.5=28.08.4
Read specific storage
READ(ISECO1)
         Read agultar sconicivosy
READ ISECCO
             Real aquitet this ness
           Read adu far bortom
REAO SECON
Read well rouge recharge sept
READ ISENT
               .Read fluet canducts.cty
READ(fe8ct
                .Read river head
                    READ (ISECC.)
                   Read river bectom
                    READ (SSECOL)
                   Read constant head
READWISECOL
                    STOP MOST_READ_ : MORNAL TOWALSTION SNS
```

# Figure 6.1-6 (Page 1 of 3)

# Listing of SF2D1 TEST\_READ.OUT

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ABOTT POTENT FROM FILE SECOL RESIDENTEST ORP
THEE POLE BOUTAINS SPECIFIC PANSES THAT WILL BE SED FOR TURRFICATIONS
THE SAME TO BE THE SECOND OF THE SECOND O
  ...957005-05
  1.689008-05
  1.33900E-37
1.32900E-37
1.42400E+37
  u-<u>67500E-67</u>
2-35500E-25
  1.3050 UE-25

1.3700 UE-05

15800 E-06

139800 E-06

1.39800 E-06

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1.35500 E-10

1.35500 UE-10

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# Figure 6.1-6 (Page 2 of 3) Listing of SF2D1\_TEST\_READ.OUT

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# Figure 6.1-6 (Page 3 of 3) Listing of SF2D1\_TEST\_READ,OUT

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# Figure 6.1-7

# SF2D1 PRESECOFL TEST.INP

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# 7.0 RELATED TESTING DOCUMENTATION

Table 7-1
Documentation Related to the Testing of PRESECOFL2D

| Test Item                          | Description                                                                              | SCMS Filename                                                                                             |
|------------------------------------|------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| Test Log                           | Issues and events that arose during the testing of PRESECOFL2D version 4,02ZO            | SF2D1_TESTLOG.1XT                                                                                         |
| FLINT Output                       | Output generated as a result of running the source code analyzer, FORTRAN-Lint           | SFIDI_FLINT.OUT                                                                                           |
| Scripts used                       | Command files used to build the executables, and the run the PCA analysis and test cases | SF2D1_BUILD.COM<br>SF2D1_MMS<br>SF2D1_BUILD.LOG<br>SF2D1_TESTCASE_PCA_CUM.COM<br>SF2D1_TEST_NODBG_RUN.COM |
| SCA Output                         | Output generated as a result of running the source code analyzer, DECset-SCA             | SF2D!_SCA_MOD_NOT_REF.TXT<br>SF2D1_CALLTREE.TXT<br>SF2D1_MODULES.OUT                                      |
| PCA Output                         | Output generated as a result of running the program coverage analyzer, DECset-PCA        | SF2D1_PCA.LOG<br>SF2D1_TEST_COVER.TXT<br>SF2D1_COVERAGE_CUM.TXT<br>SF2D1_COVERAGE.TXT                     |
| Input Files                        | Input files required to perform both the PCA analysis and the functional testing.        | SF2D1_PRESECOFL.INP<br>SF2D1_REGION_TEST.CDB<br>SF2D1_LOCAL_TEST.CDB                                      |
| Testing Tools                      | Source codes of utility programs used during testing                                     | SF2D1_READ_PRP.FOR<br>SF2D1_TEST_READ_1.FOR                                                               |
| Input Files for Testing Tools      | Input files on which testing tools operate                                               | SF2D1_REGION_TEST.PRP<br>SF2D1_LOCAL_TEST.PRP                                                             |
| Output Files from Testing<br>Tools | Output files resulting from running the testing tools.                                   | SF2D1_REGION_TEST.ASC<br>SF2D1_LOCAL_TEST.ASC<br>SF2D1_TEST_READ.OUT                                      |
| Requirements Document              | A list of the requirements for PRESECOFL2D                                               | N/A                                                                                                       |
| Verification and Validation Plan   | A description of the testing strategy for PRESECOFL2D                                    |                                                                                                           |
| Implementation Document            | Source code listing and a description of the executable generation                       | N/A                                                                                                       |
| User's Guide                       | Instruction for using PRESECOFL2D                                                        | N/A                                                                                                       |

# 8.0 CONCLUSION

The testing for PRESECOFL2D as prescribed in the Verification and Validation Plan has been completed and all acceptance criteria have been satisfied. The test case provided in Section 6 provide complete coverage of all functional requirements as described in Section 6.

# 9.0 REFERENCES

- 1) WIPP-PA Qualification Guide for Pre-existing Software, Version 2.0, dated 8/24/95.
- 2) WIPP-PA Implementation Document for PRESECOFL2D Version 4.02ZO, WPO# 23296
- 3) WIPP-PA Requirements Document for PRESECOFL2D Version 4.02ZO WPO# 23318
- 4) Rechard, R.P., ed. 1992, User's Manual for CAMCON: Compliance Assessment Methodology Controller Version 3.0. SAND 90-1983, Albuquerque, NM: Sandia National Laboratories.
- 6) WIPP-PA User's Manual for PRESECOFL2D Version 4.02ZO, WPO# 23297

# INFORMATION ONLY

# 10.0 APPENDICES

# APPENDICES A - Reviewer's Forms

See attached

# WASTE ISOLATION PILOT Sandia PLANT Laboratories

# Validation Document Reviewer's Form

Form Number: 452

Effective: 7/31/95

|                                                                                                                                                                                                                              | Procedure: 19                                                                                                                                                                           | <u>9-1</u> F                                                                                                | Revision:                                                                       |                                                  | Pag           | е     | ofi_          |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------|--------------------------------------------------|---------------|-------|---------------|
| WPO Number:                                                                                                                                                                                                                  | 23319                                                                                                                                                                                   |                                                                                                             | Software Cl                                                                     | assification: _                                  | <i>5</i> /J/L | -54   |               |
| Reviewer Instruction Check the "Yes" box Check the "No" box for Check the "N/A" box Check the "N/R" box For multiple reviewer, Prior to sign-off of the that "Yes" or "N/A" mexplaining the reason This form shall be income | for each item reviewer for each item which refor items that are not for items not reviewers, each reviewer shall Validation Document, ay be checked, or a new for the non-conformation. | quires furthe<br>applicable.<br>d (only if thei<br>l complete a<br>, all "No" iten<br>nemo from th<br>ance. | r work<br>re are multiple<br>Validation Doo<br>ns shall be ap<br>ne DM shall be | cument Revie<br>propriately add<br>attached to t | _e .          |       | sponsor NO NO |
| Are all tests iden<br>significant inputs                                                                                                                                                                                     | ation Completeness<br>tified in the VVP docu<br>and outputs, and the<br>rations used to run the                                                                                         | imented, incl<br>hardware ac                                                                                | nd                                                                              | ∑ Yes                                            | ☐ No          | ☐ N/A |               |
| <ul> <li>nand calculation</li> <li>calculations using</li> <li>empirical data</li> </ul>                                                                                                                                     | its compared to at lea                                                                                                                                                                  | en problems,<br>es and/or tec                                                                               | , <sup>5</sup>                                                                  | ⊠ Yes                                            | ∏ No          | N/A   | N/R           |
| 3. Peer Review If test cases did n                                                                                                                                                                                           | not provide sufficient v<br>r review performed?                                                                                                                                         |                                                                                                             | as a                                                                            | Yes                                              | □ No ;        | ∑ N/A | ☐ N/R         |
| 4. Test Documenta Do the tests-meet                                                                                                                                                                                          | ition Acceptability<br>I the acceptance crite                                                                                                                                           | ria identified                                                                                              | in the VVP?                                                                     | X Yes                                            | ☐ No [        | N/A   | ☐ N/R         |
| 5. Test Documenta<br>Are the tests docu<br>can be repeated?                                                                                                                                                                  | ition Repeatability<br>umented in sufficient o                                                                                                                                          | detail such th                                                                                              | at they                                                                         | ⊠ Yes                                            | ☐ No [        | N/A   | N/R           |
| 6. Computer File D<br>Are the test case<br>Validation Docum                                                                                                                                                                  | input and output files                                                                                                                                                                  | included in t                                                                                               | he                                                                              | ⊠ Yes                                            | No [          | □ N/A | □ N/R         |
| Are the validation                                                                                                                                                                                                           | ry of Documentation<br>methods, test data, notest that can be undestent individual?                                                                                                     | esults and co                                                                                               | onclusions<br>independent                                                       | ⊠ Yes                                            | ☐ No [        | □ N/A | N/R           |
| C. David () Reviewer Name (printed)                                                                                                                                                                                          | odegraff.                                                                                                                                                                               | <u></u>                                                                                                     | •                                                                               | yslegraf                                         | <u>/</u>      | // C  | Det 95        |

# WASTE ISOLATION PILOT

# Review Comment (Software)

| ational PLANT                         |                                       | Form Number: 25                       | <b>39</b>                         | Effective: 7/31/95 |
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| Laboratories                          | Procedure:                            | QAP 19-1 Revision                     | n:                                | Page of2           |
| File Code: SWCF-                      | A                                     | 1.1.6.9                               |                                   | PA SET             |
|                                       |                                       | WBS #(s)                              | -                                 | Alpha Code         |
| Keywords: (Used for                   | unique identific                      |                                       |                                   |                    |
| PRESEC                                | FLZO,                                 | SF201                                 |                                   |                    |
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| SECTION                               | · · · · · · · · · · · · · · · · · · · | <u> </u>                              |                                   |                    |
| 1. Software Name:                     | -                                     | Version ID:                           | Versio                            | n Date:            |
| PRESECOFI                             | 20                                    | 4.02                                  | Version                           | 5/20/57            |
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| 2. Type of Comment:                   | (check one)                           | Required                              | Suggested                         | Εποι               |
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| Validat                               | tion Docu                             | ment, pg 5 Se                         | Tan 17                            | Document Document  |
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# WASTE ISOLATION PILOT **PLANT**

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# Review Comment (Software)

Form Number: 299

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| File Code: SWCF-                                         | A                           | 1.1.6.                        | 9                                   |                        |                                                                  | PA                                |
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| SECTION I                                                | <del></del>                 |                               |                                     |                        |                                                                  | >                                 |
| 1. Software Name:                                        | :                           | Version ID:                   |                                     |                        | Version Date:                                                    | J. /                              |
| PRESECUE                                                 | LZD                         | 4.02                          |                                     |                        | Version Date:                                                    | 20/99                             |
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# Review Comment (Software)

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| SECTION                                                                                                             |                        |                                          |                                            |
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| PRESECOFLZD                                                                                                         | 4.02                   | Version Da                               | 120/94                                     |
| 2. Type of Comment: (check one)                                                                                     | Required               | Suggested                                | Error                                      |
| Software Type: (check or.e)                                                                                         | Commercial             | Developed                                | System                                     |
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| 4. Comment: (check one, attach pag<br>Validation Do                                                                 | nes as needed)         | Technical  Table 4.1                     | Document                                   |
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| SECTION II                                                                                                          |                        |                                          |                                            |
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# WASTE ISOLATION PILOT

Randia PLANT ational Laboratories

# Review Comment (Software)

Form Number: 299

Effective: 7/31/95

|                      | Procedure.         | QAP 19-1       | Revision:                             |             |              | Page1_      | of               |
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| SECTION              |                    |                |                                       |             |              | <del></del> |                  |
| 1. Software Name:    |                    | Version ID:    |                                       |             | 1/2          |             | <del></del>      |
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# APPENDIX B: PRIMITIVE BASELINE DOCUMENT

The following pages from the verification section primitive baseline documentation currently stored in SWCF as a part of the prior QA efforts. The basis of the current regression testing is to duplicated the results from prior testing. This was done by reproducing the results found in the baseline documentation. This reproduction is found in Figure 6.1-2.

FigureB-1
(Page 1 of 3)
Pages 4-6 of the Verification Section of the Primitive Baseline

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Page 4 of 11
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FigureB-1
(Page 2 of 3)
Pages 4-6 of the Verification Section of the Primitive Baseline

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# FigureB-1 (Page 3 of 3) Pages 4-6 of the Verification Section of the Primitive Baseline

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EPA Comment Enclosure 2, Pages 3-4 194.23(a)(3)(iv)

#### **Comment Text**

Section 194.23(a)(3)(iv) requires "computer models accurately implement the numerical models" and are free of coding errors and produce stable results.

Appendix PAR identifies the assigned values for both longitudinal and transverse dispersivity in the Culebra as 0.0. Although this value would appear to lead to conservative results by reducing the amount of surface area available for matrix diffusion, there is insufficient evidence presented in the CCA that the SECOTP code will provide stable solutions at such low dispersivities. In fact, in a letter from James McCord to James Ramsey (Sandia National Lab), provided as an attachment to the Parameter Record Package for non-Salado longitudinal dispersivity, Dr. McCord states "Assuming that the numerical codes used correctly solve the governing partial differential equations, simulations using local dispersivities less than or equal to 2 m will yield results consistent with field scale dispersive spreading observations as reported by Gelhar et al. (1992)."

The Department needs to provide evidence that the numerical solver method implemented in the SECOTP code correctly solves the partial differential equations at the dispersivities of 0.0 over the range of Courant numbers used in the CCA.

# **DOE** Response

Numerical approximations of advection-dominate transport problems may result in spatial oscillations near regions where the concentration gradients are steep. These oscillations (commonly referred to as undershoot and overshoot) are caused by the inability of second order numerical approximations to accurately propagate short wavelength harmonics. The phenomenon becomes more apparent when the local Peclet number exceeds a value of 10 because the short wavelength harmonics become increasingly important (Huyakorn and Pinder, 1983, p. 206). The Peclet number, which is inversely proportional to the dispersion coefficient, is quite large when the dispersivities are set equal to zero.

In most transport simulators this phenomenon is addressed by enhancing spatial discretization and/or introducing numerical dispersion by reducing the order of the numerical approximation (upwind or upstream weighting discretization schemes).

Fully-weighted upwind schemes do not have undershoot and overshoot problems, but numerical dispersion is often quite large and the resulting solution may not be accurate. To avoid oscillatory behavior limit numerical dispersion, a total variation diminishing (TVD) flux limiter scheme is invoked in SECOTP2D. The underlying concept is the application of upwinding techniques where needed to the degree necessary to prevent non-physical oscillations. A discussion of TVD including references is found on page 7 of the WIPP PA User's Manual for SECOTP2D, Version 1.30 (Appendix SECOTP2D of the CCA).

In the CCA, zero dispersivity coefficients were used in both the longitudinal and transverse directions. The dispersion coefficients are extremely small, but non-zero, due to contributions from the molecular diffusion component. Because the SECOTP2D results did not exhibit oscillatory behavior, the CCA runs are in and of themselves a test of the stability of SECOTP2D and demonstrate that zero dispersivities are not a problem for SECOTP2D.

#### Reference:

Huyakorn, P.S., and G.F. Pinder, 1983. Computation Methods in Subsurface Flow, Academic Press, Inc., New York, NY. (Textbook)

EPA Commen Enclosure 2, I 194.23(a)(3)(i)

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### Comment Tex

194.23(a)(3)(iv)

Section 194.23(a)(3)(iv) requires "computer models accurately implement the numerical models."

In regard to the BRAGFLO computer code, Appendix MASS states "Approximating convergent and divergent flow around the intrusion borehole and the shaft creates two narrow necks in the otherwise fairly uniform width grid in the region representing the repository. In the undisturbed performance scenario and under certain conditions in other scenarios, flow in the repository may pass laterally through these necks. In reality, these necks do not exist. Their presence in the model is expected to have a negligible or conservative impact on model predictions compared to predictions that would result from use of a more realistic model geometry." The text further states that "The time scale involved and the permeability contrast between the repository and surrounding rock are sufficient that lateral flow that may occur in the repository is restricted by the rate at which liquid gets into or out of the repository, rather than the rate at which it flows through the repository." To support this contention, a grid study comparing a two-dimensional and three-dimensional model was performed and included as MASS Attachment 4-1. The results of this analysis indicate that under undisturbed performance the grids would provide similar answers. However, the models were parameterized such that, in both cases, brine did not flow up the borehole following an intrusion and therefore, the adequacy of the grid under disturbed conditions cannot be evaluated.

The Department needs to provide a similar analysis that is representative of an intrusion scenario in which brine reaches the Culebra. That is, the pressures in the repository have to be high enough so brine from the repository reaches the Culebra.

# DOE Response:

The modeling study documented in Appendix MASS, Attachment MASS 4-1, demonstrates that a 2D grid set up with radial flaring is adequate in approximating the behavior of the 3D system. The critical performance measure is not what in particular happened (e.g., brine flow reaching the Culebra), but that all representative measures of fluxes be comparable in both models. As demonstrated in the plots at the back of MASS Attachment 4-1, this is the case. Note that in addition to examining the effects of a 2D representation of the 3D system, the study documented in MASS

Attachment 4-1 also favorably benchmarked the BRAGFLO code against the TOUGH2 code, which uses quite different numerical approaches in solving similar multiphase flow equations and in defining WIPP-specific processes.

The calculations performed were appropriate for the determination because the geometries are comparable to those used in the CCA and the parameter values used in the codes are similar to the median values used in the CCA performance assessment (at the time the simulation was executed, the values used were median values in the SNL WIPP performance assessment database). To select a case in which brine flow occurred up the borehole, more extreme values than the medians would have to be selected for some variables. As indicated in the DOE response to the EPA comment on grid geometry, page 8 of enclosure 1, 194.23(a)(3)(iv), part (2), the use of median values for model geometry comparison studies has been recommended as appropriate by EPA representatives.

EPA Comment Enclosure 2, page 4 194.23(c)(2)

#### Comment Text

194.23(c)(2)

Section 194.23(c)(2) requires, among other things, "...reports on code verification, benchmarking, validation, and quality assurance procedures."

The Requirements Document and the Verification and Validation Plan for the NUTS computer code establishes the criterion that "the integrated sum of releases passing any point of interest should be less than the integrated release from the repository." However, this does not prove that mass is being conserved, nor is evidence of mass balance provided elsewhere in the documentation.

The Department needs to perform a mass balance analysis on the NUTS computer code.

# **DOE** Response

Inspection of the material balance variables associated with the ASCII outputs provided in the Requirements Document and the Verification and Validation Plan (RD/VVP) for all test cases, except Test case #5, show that material is conserved. Results of Test case #5 were reported in Computational Data Base (CDB) files rather than ASCII files, and therefore are not readily available for inspection of material balance. Results of the four other test cases, as reported in the RD/VVP, are sufficient to demonstrate mass balance.

All the ASCII output files reported in the RD/VVP for the NUTS computer code contain the Material Balance Error in terms of the variables mentioned in the response to Item (5) in the comment in Enclosure 1, page 9. However, these variables are not reported in the CDB files.

EPA Comment Enclosure 2, Pages 5-6 194.23(c)(2)

### Comment Text

194.23(c)(2)

Section 194.23(c)(2) requires, among other things, "...reports on code verification, benchmarking, validation, and quality assurance procedures."

The GRASP\_INV computer code user's manual describes a number of test problem computer runs. However, none of the test runs is similar to the way in which the code is implemented in the performance assessment. It is also never stated in the documentation that the GRASP-INV code has been tested in a manner in which it will be implemented in the performance assessment.

The Department needs to provide evidence that the GRASP-INV code was tested in a manner in which it will be implemented in the performance assessment, and provide a sample computer run that corresponds to the CCA results.

# DOE Response:

The test runs for GRASP-INV were conducted in a manner similar to that used for CCA PA code implementation. The documentation which describes test problem 16 for the GRASP-INV, Version 2.01, Version Date 8/21/95, Requirements Document and Verification & Validation Plan and GRASP-INV, Version 2.01, Version Date 8/21/95, Validation Document describe the specifications and results of a test problem which is functionally similar to the CCA PA application of GRASP-INV. Test problem 16 contains the 1992 Culebra model grid but uses a two categorical transmissivity classification. The test problem includes steady-state calibration to the 1992-selected steady-state heads as well as a demonstration of the functionality of the transient-calibration process. Thus, only minor differences exist between Test problem 16 and the CCA application of GRASP-INV. Specifically these differences are:

- 1) the CCA PA model used different boundary conditions,
- 2) the CCA PA model used different categorical and continuous variable variograms.
- 3) the CCA PA model used a finer finite-difference grid,
- 4) the CCA PA model used qualified data, and

5) the CCA PA model assigned weights to the observed steady-state head data.

With the exception of number 5 above, the functionality of the code tested in Test Problem 16 was identical to the application of the code during the CCA PA. In response to number 5, the end-to-end test problem being executed in response to the request in Enclosure 2, page 5, first 194.23(c)(2) citation, addresses this concern.

EPA Comment Enclosure 2, page 9 194.34(c)

#### Comment Text

# 194.34(c)

Section 194.34(c) requires documentation of computational techniques used in generating complementary, cumulative distribution functions.

Although the general approach to sampling of parameters is described briefly in Chapter 6, the User's Manual for Latin Hypercube Sampling (LHS), and Appendix PAR, no detailed discussion of the LHS procedure is included. The User's Manual contains a brief discussion of the advantages of this approach, but it does not clearly describe the implementation of the method.

The Department needs to provide a detailed discussion of the LHS procedure and its implementation.

# **DOE Response**

As the comment notes, Latin Hypercube sampling is described in Chapter 6, the User's Manual for Latin Hypercube Sampling, and Appendix PAR. Additional information about the theory and application of LHS is described in references cited in those portions of the CCA, as appropriate.

The attached text provides additional background information on the use of LHS. Details of the application of LHS in the CCA follow.

For the purposes of creating samples for the CCA performance assessment analysis, the LHS code and its preprocessor, PRELHS, were run in the production mode by the CCA\_MASTERs using their execution scripts. PRELHS was run to extract distribution information from the INGRES database and write it out to a file that served as the input file for LHS. At that point, the official execution scripts called the LHS code in order to create the actual samples. Three official samples were created, one for each of the three sample replicates described in the CCA documentation. At that point, the sampled information was available for use by client codes, either in its existing form or after postprocessing. The LHS sample files are not saved into the CMS after creation and are deleted. This is done because the sample files are easy to recreate if needed from PRELHS input files and INGRES database views, which were saved in the electronic archives.

# Description of the steps LHS goes through to create a sample

Following is a listing of the steps performed by the LHS code as it creates a sample. It is meant to show the order of how things are accomplished in the LHS process.

- 1. First, coding is invoked to open and name the input file, output file, and various scratch files used by LHS.
- Then, a subroutine is called to read the LHS input file containing the information extracted from the INGRES database for each distribution to be sampled. Further information is read defining execution flags and parameters for the upcoming run, along with any specified correlation among distributions.
- 3. Next, subroutines are called to write a banner to the output file followed by an echoed table of the distribution information and execution flags specified on the input file.
- 4. Following that, if the user has specified a correlation structure, then the correlation matrix is echoed and checked to make sure that it is positive definite. The Cholesky factorization is computed to be used later as part of the process for inducing the desired correlation structure.
- 5. At this point, subroutines are called to sample the distributions identified in the input file. For the case of the 57 distributions of interest in the LHS sample created for the CCA performance assessment, each distribution was fully evaluated in the order it appears in the input file, independent of any of the other distributions.
- 6. With the sampled values in hand, the next task is to call subroutines designed to arrange the sampled values to match the desired correlation structure as specified in the input file. For cases where no correlation structure was defined in the input file, LHS will arrange the sampled values in a way that minimizes correlations between distribution pairs. Correlations are implemented based on the ranks of the sampled distributions rather than on raw distribution values.
- 7. The final task is to call subroutines designed to write the sample values for each of the distributions to output files. Furthermore, depending on the execution keywords specified in the input file, other output tables may be

created containing sample ranks on a vector by vector basis. Additional output may be produced containing correlation tables based on both rank and raw data and histogram plots for each distribution sampled.

# Sampling Techniques used in the WIPP Compliance Certification Application

February 24, 1997 Memorandum

Jon C. Helton Sandia National Laboratories

# 1 Sampling Procedures

Extensive use is made of sampling procedures in the CCA performance assessment (PA). In particular, random sampling is used in the generation of individual CCDFs (i.e., for integration over the probability space ( $\hat{S}_{st}$ ,  $\hat{S}_{st}$ ,  $p_{st}$ ) for stochastic uncertainty) and Latin hypercube sampling is used for the assessment of the effects of imprecisely-known analysis inputs (i.e., for integration over the probability space ( $\hat{S}_{su}$ ,  $\hat{S}_{su}$ ,  $p_{su}$ ) for subjective uncertainty). Due to the importance of sampling procedures in this PA, brief descriptions are given for random sampling, importance sampling and Latin hypercube sampling, which are probably the most widely used sampling techniques. For notational convenience, assume that the variable under consideration is represented by

$$\mathbf{x} = [x_1, x_2, ..., x_{nV}] \tag{1.1}$$

and that the corresponding probability space is  $(S, \mathcal{S}, p)$ .

In random sampling, sometimes also called simple random sampling, the observations

$$\mathbf{x}_{k} = [x_{k1}, x_{k2}, ..., x_{k,nV}], \ k = 1, 2, ..., nR,$$
(1.2)

where nR is the sample size, are selected according to the joint probability distribution for the elements of  $\mathbf{x}$  as defined by  $(S, \mathcal{S}, p)$ . In practice,  $(S, \mathcal{S}, p)$  is defined by specifying a distribution  $D_j$  for each element  $x_j$  of  $\mathbf{x}$ . Points from different regions of the sample space S occur in direct relationship to the probability of occurrence of these regions. Further, each sample element is selected independently of all other sample elements. As illustrated in Fig. 1.1 for  $x_1 = U$ ,  $x_2 = V$ , nV = 2 and nR = 5, the numbers RU(1), RU(2), ..., RU(5) are sampled from a uniform distribution on  $\{0, 1\}$  and in turn lead to a sample U(1), U(2), ..., U(5) from U based on the cumulative distribution function for U. Similarly, the numbers RV(1), RV(2), ..., RV(5) lead to a sample V(1), V(2), ..., V(5) from V. The pairs

$$\mathbf{x}_k = [U(k), V(k)], k = 1, 2, ..., nR = 5,$$
 (1.3)

then constitute a random sample from  $\mathbf{x} = [U, V]$ , where U has a normal distribution on [-1, 1] and V has a triangular distribution on [0, 4].

Random samples are generated in an analogous manner when x has a dimensionality greater than 2 (e.g., nV = 100). Specifically, if the elements of x are represented by U, V, ..., W and a random sample of size nR is to be generated, then random numbers RU(1), RU(2), ..., RU(nR) are sampled uniformly from [0,1] and used to obtain corresponding values U(1), U(2), ..., U(nR) for U, random numbers RV(1), RV(2), ..., RV(nR) are sampled

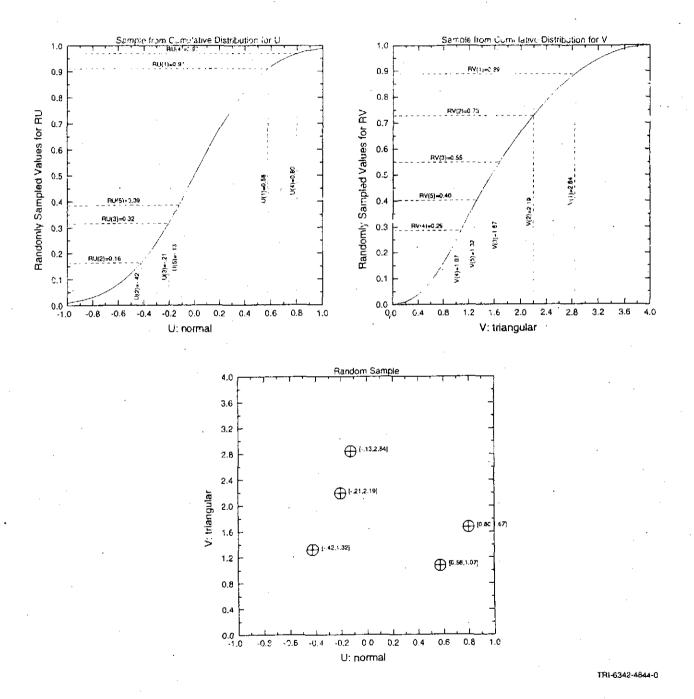


Fig. 1.11 Example of random sampling to generate a sample of size nR = 5 from  $\mathbf{x} = [U, V]$  with U normal on [-1, 1] (mean = 0, 0.01 quantile = -1, 0.99 quantile = 1) and V triangular on [0, 4] (mode = 1).

uniformly from [0,1] and used to obtain corresponding values V(1), V(2), ..., V(nR) for V, and so on, with the process continuing through all elements of x and ending with the selection of random numbers RW(1), RW(2), ..., RW(nR) from [0,1] and the generation of the corresponding values W(1), W(2), ..., W(nR) for V. The vectors

$$\mathbf{x}_k = [U(k), V(k)], ..., W(k)], k = 1, 2, ..., nR,$$
 (1.3a)

then constitute a random sample from  $\mathbf{x} = [U, V, ..., W]$ .

In random sampling, there is no assurance that points will be sampled from any given sub-region of the sample space S. Also, it is possible for an inefficient sampling of S to occur due to several sampled values falling very close together. The preceding problems can be partially ameliorated by using importance sampling. With this technique, S is exhaustively divided into a number of nonoverlapping subregions (i.e., strata)  $S_i$ , i = 1, 2, ..., nS. Then,  $nS_i$  values for  $\mathbf{x}$  are randomly sampled from  $S_i$ , with the random sampling carried out in consistency with the definition of  $(S, S, \rho)$  and the restriction of  $\mathbf{x}$  to  $S_i$ . The resultant vectors

$$\mathbf{x}_{k} = [x_{k1}, x_{k2}, ..., x_{k,nV}], \ k = 1, 2, ..., \sum_{i=1}^{nS} nS_{i}$$
 (1.4)

then constitute an importance-based sample from S (i.e., a sample obtained by importance sampling). Typically, only one value is sampled from each  $S_i$ , with the result that the sample has the form

$$\mathbf{x}_{k} = [x_{k1}, x_{k2}, ..., x_{k,nV}], \quad k = 1, 2, ..., nS,$$
(1.5)

The name importance sampling derives from the fact that the  $S_i$  are in part defined on the basis of how important the  $\mathbf{x}$ 's contained in each set are to the final outcome of the analysis. Often, importance sampling is used to assure the inclusion in an analysis of  $\mathbf{x}$ 's that have high consequences but low probabilities (i.e., the probabilities  $p(S_i)$  are small for the  $S_i$  that contain such  $\mathbf{x}$ 's). When importance sampling is used, the probabilities  $p(S_i)$  and number of observations  $nS_i$  taken from each  $S_i$  must be folded back into the analysis before results can be meaningfully presented.

Several examples of importance sampling for  $\mathbf{x} = [U, V]$  are given in Fig. 1.2. The two top frames are for strata of equal probability (i.e., all  $p(S_i)$  are equal). For two uniform distributions, this results in all strata having the same area (upper left frame). For two nonuniform distributions, different strata can have different areas even though they have the same probability (upper right frame). The two lower frames are for strata of unequal probability. In this case, the variable distributions and the strata probabilities interact to determine the area of the strata. However, it is important to recognize that specifying variable distributions, number of strata and strata probabilities does not uniquely define an importance sampling procedure; rather, there are many ways in which the strata  $S_i$  can be defined

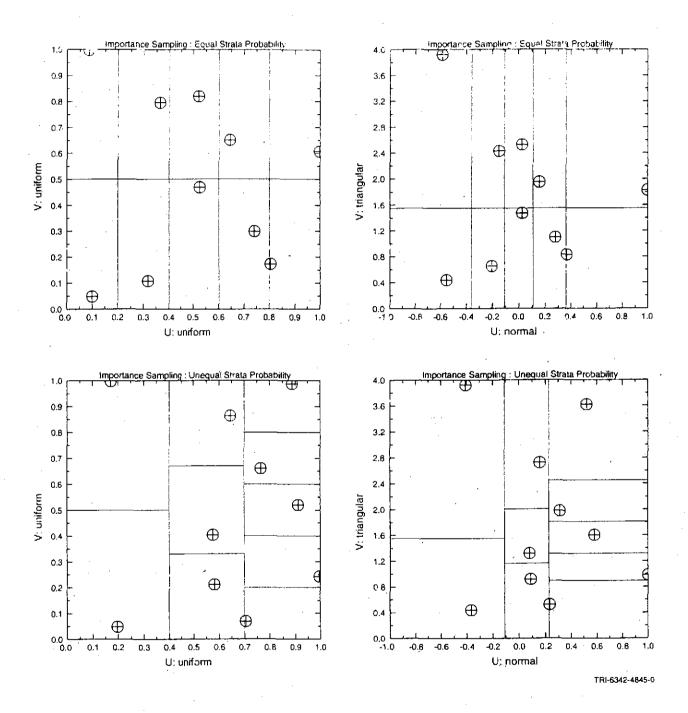


Fig. 1.2. Examples of importance sampling with ten strata (i.e., nS = 10), one random sample per strata (i.e.,  $nS_i = 1$ ), equal strata probability (i.e.,  $p(S_i) = 1/10$ , upper frames), unequal strata probability (i.e.,  $p(S_i) = 0.2, 0.2, 0.1, 0.1, 0.1, 0.06, 0.06, 0.06, 0.06, 10$  (left frames) and U normal on [-1, 1] (mean = 0, 0.01 quantile = -1, 0.99 quantile = 1) and V triangular on [0, 4] (mode = 1) (right frames)

that are consistent for the preceding constraints. In particular, appropriate definition of strata will depend on specific properties of individual analyses. Similar ideas also hold for more than two variables, in which case the strata become enclosed volumes in a space with the same dimension as **x**.

Importance sampling operates to ensure the full coverage of specified regions in the sample space. This idea is carried farther in Latin hypercube sampling to ensure the full coverage of the range of each variable. Specifically, the range of each variable (i.e., the  $x_j$ ) is divided into nLHS intervals of equal probability and one value is selected at random from each interval. The nLHS values thus obtained for  $x_1$  are paired at random without replacement with the nLHS values obtained for  $x_2$ . These nLHS pairs are combined in a random manner without replacement with the nLHS values of  $x_3$  to form nLHS triples. This process is continued until a set of nLHS nV-tuples is formed. These nV-tuples are of the form

$$\mathbf{x}_{k} = [x_{k1}, x_{k2}, ..., x_{k,nV}], \ k = 1, ..., nLHS,$$
 (1.6)

and constitute the LHS. The individual  $x_j$  must be independent for the preceding construction procedure to work; a method for generating Latin hypercube and random samples from correlated variables has been developed by Iman and Conover (1982) and will be discussed briefly. Latin hypercube sampling is an extension of quota sampling (Steinberg 1963) and can be viewed as an n-dimensional randomized generalization of Latin square sampling (Raj 1968).

The generation of an LHS of size nLHS = 5 from  $\mathbf{x} = [U, V]$  is illustrated in Fig. 1.3. Initially, the ranges of U and V are subdivided into five intervals of equal probability, with this subdivision represented by the lines that originate at 0.2, 0.4, 0.6 and 0.8 on the ordinates of the two upper frames in Fig. 1.3, extend horizontally to the cumulative distribution functions, and then drop vertically to the abscissas to produce the 5 indicated intervals. Random values U(1), U(2), ..., U(5) and V(1), V(2), ..., V(5) are then sampled from these intervals. The sampling of these random values is implemented by (1) sampling RU(1) and RV(1) from a uniform distribution on [0, 0.2], RU(2) and RV(2) from a uniform distribution on [0.2, 0.4], and so on and (2) then using the cumulative distribution functions to identify (i.e., sample) the corresponding U and V values, with this identification represented by the dashed lines that originate on the ordinates of the two upper frames in Fig. 1.3, extend horizontally to the cumulative distribution functions, and then drop vertically to the abscissas to produce U(1), U(2), ..., U(5) and V(1), V(2), ..., V(5). The generation of the LHS is then completed by randomly pairing (without replacement) the resulting values for U and V. As this pairing is not unique, many possible LHSs can result. Two such LHSs are shown in the lower two frames in Fig. 1.3, with one LHS resulting from the pairings [U(1), V(2)], [U(2), V(5)], [U(3), V(3)], [U(4), V(1)], [U(5), V(3)] (lower left frame) and the other LHS resulting from the pairings [U(1), V(1)], [U(1), V(1)], [U(1), V(1)], [U(1), V(1)].

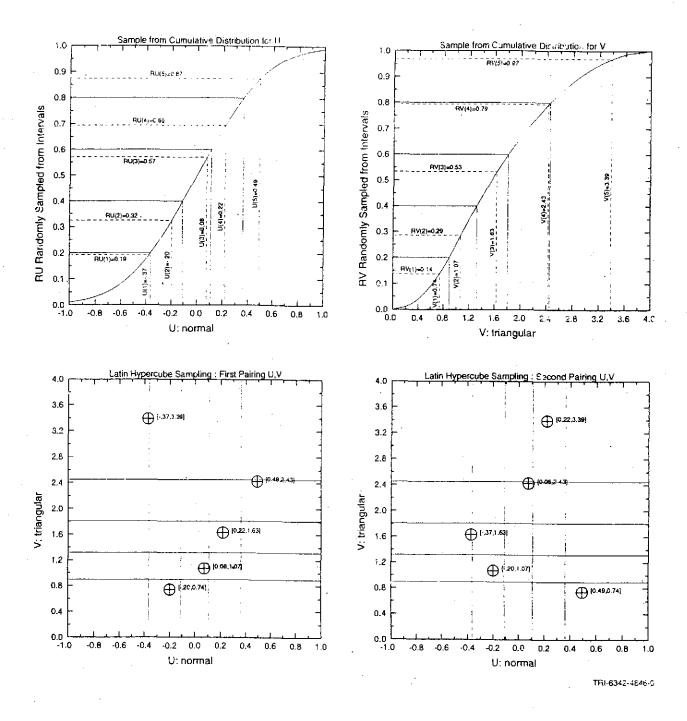


Fig. 1.3. Example of Latin hypercube sampling to generate a sample of size nLHS = 5 from  $\mathbf{x} = [U, V]$  with U normal on [-1, 1] (mean = 0, 0.01 quantile = -1, 0.99 quantile = 1) and V triangular on [1, 4] (mode = 1).

The generation of an LHS for nV > 2 proceeds in a manner similar to that shown in Fig. 1.3 for nV = 2. The sampling of the individual variables for nV > 2 takes place in exactly the same manner as shown in Fig. 1.3. However, the nV variables define an nV-dimensional solid rather than a 2-dimensional rectangle in the plane. Thus, the two lower frames in Fig. 1.3 would involve a partitioning of an nV-dimensional solid rather than a rectangle.

Random sampling is the preferred technique when sufficiently large samples are possible because it is easy to implement, easy to explain, and provides unbiased estimates for means, variances and distribution functions. The possible problems with random sampling derive from the rather vague phrase "sufficiently large" in the preceding sentence. When the underlying models are expensive to evaluate (e.g., many hours of CPU time per evaluation) or estimates of extreme quantiles are needed (e.g., the 0.999999 quantile), the required sample size to achieve a specific purpose may be too large to be computationally practicable. In the CCA PA, random sampling is used for the estimation of CCDFs (i.e., integration over  $(\delta_{sh}, \delta_{sl}, p_{st})$ ) because it was possible to develop a computational strategy that allowed the use of a sample of size nS = 10000 to estimate an exceedance probability of 0.001 (i.e., the 0.999 quantile of the distribution of normalized releases to the accessible environment).

When random sampling is not computationally feasible for the estimation of extreme quantiles, importance sampling is often employed. However, the use of importance sampling on nontrivial problems is not easy due to the difficulty of defining the necessary strata and also of calculating the probabilities of these strata. For example, the fault and event tree techniques used in probabilistic risk assessments for nuclear power stations and other complex engineered facilities can be viewed as algorithms for defining importance sampling procedures. The bettom line is that the definition and implementation of an importance sampling procedure is not easy. Further, without extensive a priori knowledge, the strata may end up being defined much more finely than is necessary, with the result that the importance sampling procedure ends up requiring more calculations than the use of random sampling to calculate the same outcomes. For example, the numbers of strata in the importance sampling procedure used to estimate CCDFs in the 1991 and 1992 preliminary WIPP PAs (Helton and Iuzzolino 1993) greatly exceeds the size of the random samples used in the CCA PA to estimate CCDFs. The unequal strata probabilities also make the outcomes of analyses based on importance sampling inconvenient for use in sensitivity analyses (e.g., how does one interpret a scatterplot or a regression analysis derived from results obtained from an importance sampling procedure). For the preceding reasons, importance sampling was not used in the PA for the CCA.

Latin hypercube sampling is used when large samples are not computationally practicable and the estimation of very high quantiles is not required. The preceding is typically the case in uncertainty and sensitivity studies to assess the effects of subjective uncertainty. First, the models under consideration are often computationally demanding, with the result that the number of calculations that can be performed to support the analysis is necessarily limited. For example, the totality of the model calculations (i.e., BRAGFLO, NUTS, PANEL, GRASP\_INV, SECOFL2D, SECOTP2D, CUTTINGS\_S, BRAGFLO\_DBR) in the CCA PA is too extensive to permit the generation of

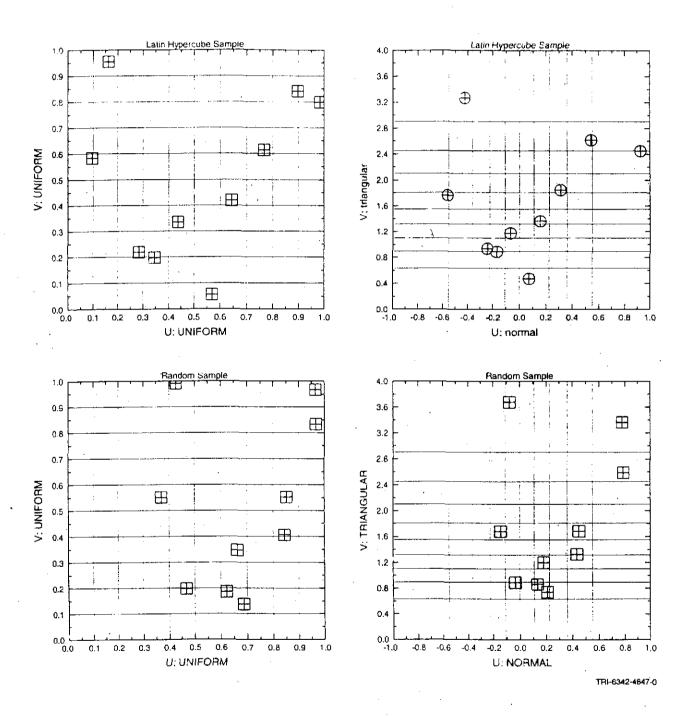


Fig. 1.4. Examples of Latin hypercube and random sampling to generate a sample of size 10 from variables U and V with (1) U and V uniform on [-1, 1], and (2) U normal on [-1, 1] (mean = 0, 0.01 quantile = -1, 0.99 quantile = 1) and V triangular on [0, 4] (mode = 1).

thousands of CCDFs in an uncertainty/sensitivity study to assess the effects of subjective uncertainty. Second, the estimation of very high quantiles is generally not required in an analysis to assess the effects of subjective uncertainty. Typically, a 0.90 or 0.95 quantile is adequate to establish where the available information indicates a particular analysis outcome is likely to be located; in particular, a 0.99, 0.999 or 0.9999 quantile is probably not needed in assessing the effects of subjective uncertainty.

Desirable features of Latin hypercube sampling include unbiased estimates for means and distribution functions and dense stratification across the range of each sampled variable (McKay et al. 1979). In particular, uncertainty and sensitivity analysis results obtained with Latin hypercube sampling have been observed to be quite robust even when relatively small samples (i.e., nLHS = 50 to 200) are used (Iman and Helton 1988, 1991; Helton et al. 1995).

For perspective, Latin hypercube and random sampling are illustrated in Fig. 1.4 for two different distribution pairs. To facilitate comparisons, the grid that underlies the LHSs is also shown for the random samples, although it plays no role in the actual generation of these samples. The desirability of Latin hypercube sampling derives from the full coverage of the range of the sampled variables; specifically, each equal probability interval for U and also each probability interval for V has exactly one value sampled from it. In contrast, the random sampling makes less efficient use of the sampled points, with the possibility existing that significant parts of a variables range will be omitted and that other parts will be overemphasized. The enforced stratification in Latin hypercube sampling prevents such inefficient samplings while still providing unbiased estimates for means and distribution functions.

The outcome of the enforced stratification associated with Latin hypercube sampling is that estimates of means and distribution functions tend to be more stable when generated by Latin hypercube sampling than by random sampling. Here, stability refers to the amount of variation between results obtained with different samples generated by the particular sampling technique under consideration. This stability can be illustrated by comparison of estimates of the CDF for the simple function

$$f(U, V) = U + V + UV \tag{1.6}$$

obtained with Latin hypercube and random sampling under the assumption that U and V are uniformly distributed on [0, 2]. In particular, each sampling technique is used to generate 100 samples of size 10 and also 100 samples of size 100 from U and V. Each sample gives rise to an estimated CDF for f (Fig. 1.5). The goal is to compare the variability between the estimates obtained with Latin hypercube and random sampling. Presenting plots similar to those in Fig. 1.5 for 100 CDFs at a time is not very informative because the CDFs tend to turn into a solid black mass. A more informative presentation is to summarize the distributions of CDFs with mean and percentile curves. The location of the percentile curves then provides an indication of how stable the estimates of the CDFs are. In particular, limited separation between low and high percentiles (e.g., the 10th and 90th) indicates that the sampling

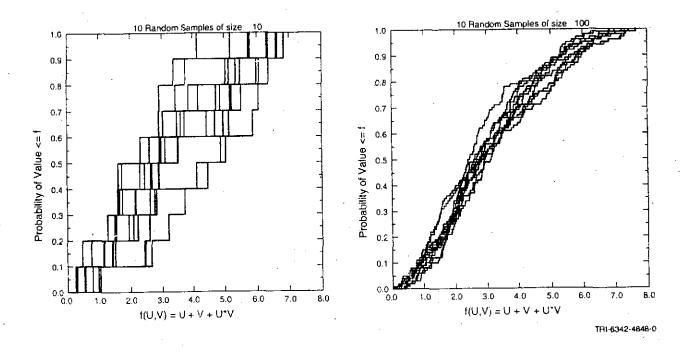


Fig. 1.5. Example CDFs for f(U, V) = U + V + UV estimated with random samples of size 10 and 100 under the assumption that U and V are uniformly distributed on [0, 2].

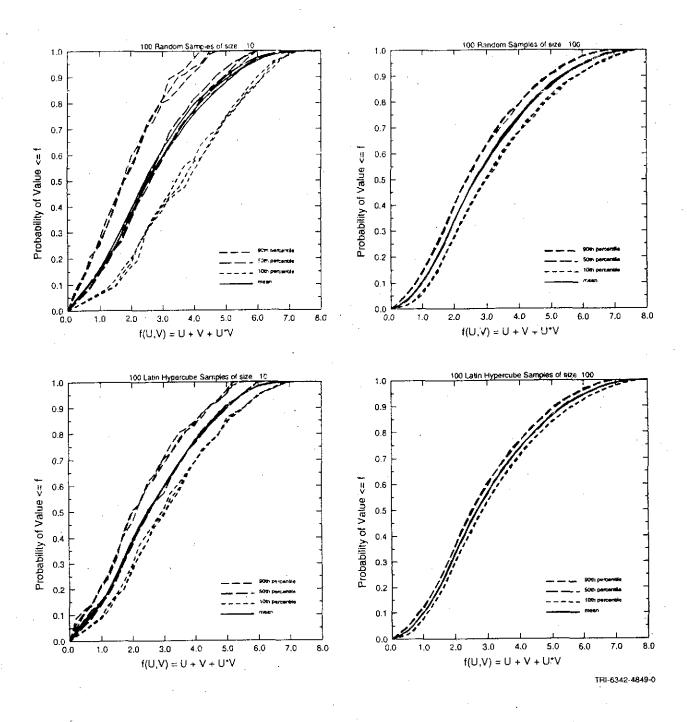


Fig. 1.6. Summary of distribution of CDFs for f(U, V) = U + V + UV estimated with 3 replications of 100 Latin hypercube and random samples of size 10 and 100 under the assumption that U and V are uniformly distributed on  $\{0, 2\}$ .

procedure is providing stable estimates of the CDF (i.e., there is little variability in the estimated CDF from one sample to the next); in contrast, a large spread between low and high percentiles indicates that the sampling procedure is not providing stable estimates of the CDF (i.e., there is substantial variability in the estimated CCDF from one sample to the next). The previously indicated 100 samples of size 10 and 100 are summarized in this manner in Fig. 1.6. Further, the analysis was replicated three times to give three estimates of the 10th percentile, three estimates of the 50th percentile, and so on. As examination of Fig. 1.6 shows, Latin hypercube sampling is producing CDF estimates that are more stable than those produced by random sampling (i.e., the spread between the 10th and 90th percentile curves is tighter for Latin hypercube sampling than for random sampling). The stability of the mean and percentile estimates across the three replicates indicates that the observed stability is real rather than a chance occurrence associated with a particular set of 100 Latin hypercube or random samples.

From the perspective of uncertainty and sensitivity analysis, the full stratification over the range of each sampled variable is a particularly desirable property of Latin hypercube sampling. In a large analysis such as the CCA PA, there are potentially hundreds of predicted variables that will be examined at some point in the uncertainty and sensitivity analysis. Further, it is likely that almost every sampled variable will be important with respect to at least one of these predicted variables. With Latin hypercube sampling, every variable gets equal treatment (i.e., full stratification) within the sample; should a variable be important with respect to a particular output variable, it has been sampled in a way that will permit this importance to be identified. In contrast, it is very difficult to design an importance sampling procedure that provides acceptable results for a large number of sampled and predicted variables. In one sense, Latin hypercube sampling can be viewed as a compromise importance sampling procedure when a priori knowledge of the relationships between the sampled and predicted variables is not available. When random sampling is used with a small sample size in an analysis that involves a large number of sampled and predicted variables, the possibility exists that the chance structure of the sample will result in a poor representation of the relationships between some of the sampled and predicted variables. Such poor relationships can also occur for Latin hypercube sampling when several sampled variables affect a given predicted variable, but are less likely to do so than is the case with random sampling.

For reasons just outlined, the CCA PA uses Latin hypercube sampling to determine the effects of subjective uncertainty (i.e., to integrate over  $(S_{su}, S_{su}, P_{su})$ ). In particular, Latin hypercube sampling is felt to be the most appropriate procedure to use to meet the requirement in 40 CFR 194.34(b) that "Computational techniques, which draw random samples from across the entire range of the probability distributions developed pursuant to paragraph (b) of this section, shall be used in generating CCDFs and shall be documented in any compliance application."

# 2 Correlation Control (Adapted from Sect. 3.2 of Helton 1993)

Control of correlation within a sample can be very important. If two or more variables are correlated, then it is necessary that the appropriate correlation structure be incorporated into the sample if meaningful results are to be obtained in subsequent uncertainty/sensitivity studies. On the other hand, it is equally important that variables do not appear to be correlated when they are really independent.

It is often difficult to induce a desired correlation structure on a sample. Indeed, most multivariate distributions are incompatible with the majority of correlation patterns that might be proposed for them. Thus, it is fairly common to encounter analysis situations where the proposed variable distributions and the suggested correlations between the variables are inconsistent; that is, it is not possible to have both the desired variable distributions and the requested correlations between the variables.

In response to this situation, Iman and Conover (1982) have proposed a method of controlling the correlation structure in random and Latin hypercube samples that is based on rank correlation (i.e., on rank-transformed variables) rather than sample correlation (i.e., on the original untransformed data). With their technique, it is possible to induce any desired rank-correlation structure onto the sample. This technique has a number of desirable properties: (1) It is distribution free. That is, it may be used with equal facility on all types of distribution functions. (2) It is simple. No unusual mathematical techniques are required to implement the method. (3) It can be applied to any sampling scheme for which correlated input variables can logically be considered, while preserving the intent of the sampling scheme. That is, the same numbers originally selected as input values are retained; only their pairing is affected to achieve the desired rank correlations. This means that in Latin hypercube sampling the integrity of the intervals is maintained. If some other structure is used for selection of values, that same structure is retained. (4) The marginal distributions remain intact.

For many, if not most, uncertainty/sensitivity analysis problems, rank-correlation is probably a more natural measure of congruent variable behavior than is the more traditional sample correlation. What is known in most situations is some idea of the extent to which variables tend to move up or down together; more detailed assessments of variable linkage are usually not available. It is precisely this level of knowledge that rank correlation captures.

The following discussion provides an overview of the Iman/Conover procedure for inducing a desired rank correlation structure on either a random or a Latin hypercube sample. A more detailed discussion of the procedure is given in the original article. The procedure begins with a sample of size m from the n input variables under consideration. This sample can be represented by the  $m \times n$  matrix

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix}$$
(2.1)

where  $x_{ij}$  is the value for variable j in sample element i. Thus, the rows of **X** correspond to sample elements, and the columns of **X** contain the sampled values for individual variables.

The procedure is based on rearranging the values in the individual columns of X so that a desired rank correlation structure results between the individual variables. For convenience, let the desired correlation structure be represented by the  $n \times n$  matrix

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ \vdots & \vdots & & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{bmatrix}$$
(2.2)

where  $c_{kl}$  is the desired rank correlation between variables  $x_k$  and  $x_l$ .

Although the procedure is based on rearranging the values in the individual columns of **X** to obtain a new matrix **X**\* that has a rank correlation structure close to that described by **C**, it is not possible to work directly with **X**. Rather, it is necessary to define a new matrix.

$$\mathbf{S} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1n} \\ s_{21} & s_{22} & \cdots & s_{2n} \\ \vdots & \vdots & & \vdots \\ s_{m1} & s_{m2} & \cdots & s_{mn} \end{bmatrix}$$
(2.3)

that has the same dimensions as X, but is otherwise independent of X. Each column of S contains a random permutation of the m van der Waerden scores (Conover 1980)  $\Phi^{-1}(i/m+1)$ ,  $i=1,2,\ldots,m$ , where  $\Phi^{-1}$  is the inverse of the standard normal distribution. The matrix S is then rearranged to obtain the correlation structure defined by C. This rearrangement is based on the Cholesky factorization (Golub and van Loan 1983) of C. That is, a lower triangular matrix P is constructed such that

$$C = PP^{T}$$
 (2.4)

This construction is possible because C is a symmetric, positive-definite matrix (Golub and van Loan 1983, p. 88).

If the correlation matrix associated with S is the  $n \times n$  identity matrix (i.e., if the correlations between the values in different columns of S are zero), then the correlation matrix for

$$S^* = SP^T \tag{2.5}$$

is **C** (Anderson 1984, p. 25). At this point, the success of the procedure depends on the following two conditions: (1) that the correlation matrix associated with **S** be close to the  $n \times n$  identity matrix; and (2) that the correlation matrix for **S**<sup>\*</sup> be approximately equal to the rank correlation matrix for **S**<sup>\*</sup>. If these two conditions hold, then the desired matrix **X**<sup>\*</sup> can be obtained by simply rearranging the values in the individual columns of **X** in the same rank

order as the values in the individual columns of S\*. This is the first time that the variable values contained in X enter into the correlation process. When X\* is constructed in this manner, it will have the same rank correlation matrix as S\*. Thus, the rank correlation matrix for X\* will approximate C to the same extent that the rank correlation matrix for S\* does.

The condition that the correlation matrix associated with S be close to the identity matrix is now considered. For convenience, the correlation matrix for S will be represented by E. Unfortunately, E will not always be the identity matrix. However, it is possible to make a correction for this. The starting point for this correction is the Cholesky factorization for E:

$$\mathbf{E} = \mathbf{Q}\mathbf{Q}^{\mathsf{T}} \tag{2.6}$$

This factorization exists because E is a symmetric, positive-definite matrix. The matrix S\* defined by

$$\mathbf{S}^{\star} = \mathbf{S}(\mathbf{Q}^{-1})^{\mathsf{T}}\mathbf{P}^{\mathsf{T}} \tag{2.7}$$

has C as its correlation matrix. In essence, multiplication of S by  $(Q^{-1})^T$  transforms S into a matrix whose associated correlation matrix is the  $n \times n$  identity matrix; then, multiplication by  $P^T$  produces a matrix whose associated correlation matrix is C. As it is not possible to be sure that E will be an identity matrix, the matrix  $S^*$  used in the procedure to produce correlated input should be defined in the corrected form shown in (2.7) rather than in the uncorrected form shown in (2.5).

The condition that the correlation matrix for S\* be approximately equal to the rank correlation matrix for S\* depends on the choice of the scores used in the definition of S. On the basis of empirical investigations, Iman and Conover (1982) found that van der Waerden scores provided an effective means of defining S, and these scores are incorporated into the rank correlation procedure in the widely used LHS program (Iman and Shortencarier 1984). Other possibilities for defining these scores exist, but have not been extensively investigated. The user should examine the rank correlation matrix associated with S\* to ensure that it is close to the target correlation matrix C. If this is not the case, the construction procedure used to obtain S\* can be repeated until a suitable approximation to C is obtained. Results given in Iman and Conover (1982) indicate that the use of van der Waerden scores leads to rank correlation matrices for S\* that are close to the target matrix C.

Additional information on the Iman/Conover (i.e., restricted pairing) technique to induce a desired rank-correlation structure is given in the original article. The results of various rank-correlation assumptions are illustrated in Iman and Davenport (1982). The LHS (Latin Hypercube Sample) program generates both random and Latin hypercube samples with user-specified rank correlations between variables.

### 3 Sample Size for Incorporation of Subjective Uncertainty

The guidance in 40 CFR 194.34(d) states that "The number of CCDFs generated shall be large enough such that, at cumulative releases of 1 and 10, the maximum CCDF generated exceeds the 99th percentile of the population of CCDFs with at least a 0.95 probability." For a Latin hypercube or random sample of size n, the preceding guidance is equivalent to the inequality

$$1 - 0.99^n > 0.95, (3.1)$$

which results in a minimum value of 298 for n. In consistency with the preceding result, the 1996 CCA PA uses an LHS of size 300 to integrate over the probability space  $(S_{su}, \mathcal{L}_{su}, p_{su})$  for subjective uncertainty. Actually, as discussed in the next section, three replicated LHSs of size 100 each are used, which results in a total sample size of 300.

### 4 Statistical Confidence on Mean CCDF

The guidance in 40 CFR 194.34(f) states that "Any compliance assessment shall provide information which demonstrates that there is at least a 95 percent level of statistical confidence that the mean of the population of CCDFs meets the containment requirements of § 191.13 of this chapter." Given that Latin hypercube sampling is to be used, the confidence intervals required in 194.34(f) can be obtained with a replicated sampling technique proposed by R.L. Iman (1982). In this technique, the LHS in Eq. (1.6) is repeatedly generated with different random seeds. These samples lead to a sequence  $\overline{P}_r(R)$ , r = 1, 2, ..., nR, of estimated mean exceedance probabilities, where  $\overline{P}_r(R)$  defines the mean CCDF obtained for sample r (i.e.,  $\overline{P}_r(R)$  is the mean probability that a normalized release of size R will be exceeded) and nR is the number of independent LHSs generated with different random seeds. Then,

$$\overline{P}(R) = \sum_{r=1}^{nR} \overline{P_r}(R) / nR \tag{4.1}$$

and

$$SE(R) = \left\{ \sum_{r=1}^{nR} \left[ \overline{P}_r(R) - \overline{P}(R) \right]^2 / nR(nR - 1) \right\}^{1/2}$$
 (4.2)

provide an additional estimate of the mean CCDF and an estimate of the standard error associated with the mean exceedance probabilities. The t-distribution with nR-1 degrees of freedom can be used to place confidence intervals around the mean exceedance probabilities for individual R values (i.e., around  $\overline{P}(R)$ ). Specifically, the 1- $\alpha$  confidence interval is given by  $\overline{P}(R) \pm t_{1-\alpha/2}$  SE(R), where  $t_{1-\alpha/2}$  is the 1- $\alpha/2$  quantile of the t-distribution with

nR-1 degrees of freedom (e.g.,  $t_{1-\alpha/2} = 4.303$  for  $\alpha = 0.05$  and nR = 3). The same procedure can also be used to place pointwise confidence intervals around percentile curves.

### 5 Generation of LHSs

The LHS program (Iman and Shortencarier 1984) was used to produce three independently generated LHSs of size nLHS = 100 each, for a total of 300 sample elements. Each individual replicate is an LHS of the form

$$\mathbf{x}_{\text{su},k} = [\mathbf{x}_{k1}, \mathbf{x}_{k2}, ..., \mathbf{x}_{k,nV}], k=1,2,...,nLHS=100.$$
 (5.1)

In the context of the replicated sampling procedure described in Sect. 4, nR = 3 replicates are being used with each replicate of size 100. For notational convenience, the replicates are designated by R1, R2 and R3 for replicates 1, 2 and 3, respectively.

At the beginning of the analysis, only the 31 variables that are used as input to BRAGFLO had been fully specified (i.e., their distributions  $D_j$  had been unambiguously defined); the remaining variables were still under development. To allow the calculations with BRAGFLO to proceed, the previously indicated LHSs were generated from nV = 75 variables, with the first 31 variables being the then specified inputs to BRAGFLO and the remaining 44 variables being assigned uniform distributions on [0, 1]. Later, when the additional variables were fully specified, the uniformly distributed variables were used to generate sampled values from them consistent with their assigned distributions. This procedure allowed the analysis to go forward while maintaining the integrity of Latin hypercube sampling procedure for the overall analysis.

With nV = 75 in the LHSs and 31 variables already assigned, 44 additional variables were available for incorporation into the analysis. To assure that the number of available positions in the LHSs was not exceeded, each group of investigators developing characterizations of variable uncertainty was assigned a maximum number of variables that they could elect to have incorporated into the analysis, with the sum of these maximums being less than 44. Ultimately, 26 additional variables were selected for incorporation into the analysis, which produced the 57 variables sampled in the CCA PA.

The restricted pairing technique described in Sect. 3 was used to induce requested correlations and also to assure that uncorrelated variables had correlations close to zero. Due to the sequential manner in which the variables were developed, it was actually only the first 31 variables used as input to BRAGFLO that could have specified non-zero correlations. The correlations for the remaining variables were controlled in the sense that they were forced to be close to zero.

The variable pairs (ANHCOMP, ANHPRM), (HALCOMP, HALPRM) and (BPCOMP, BPPRM) were assigned rank correlations of -0.99, -0.99 and -0.75, respectively. Further, all other variable pairs were assigned rank

correlations of zero. The restricted pairing technique was quite successful in producing these correlations. Specifically, the correlated variables have correlations that are close to their specified values and uncorrelated variables have correlations that are close to zero.

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EPA Comment Enclosure 2, Page 11 194.44

#### **Comment Text**

# Engineered Barriers

#### 194.44

Section 194.44 requires that the disposal system incorporate engineered barriers designed to prevent or substantially delay the movement of radionuclides towards the accessible environment.

While the inclusion [of] magnesium oxide (MgO) as a backfill material will improve repository performance, the Department must provide an engineered design which supports the assumptions about the performance of MgO. The evidence must support the assumptions used in PA.

The Department must provide an engineering design which provides the method of placement and quantity emplaced such that the MgO will be distributed as assumed in the conceptual models to support the reaction of MgO to be as predicted in the expected WIPP repository environment. The Department must also provide information which demonstrates that the excess volume proposed to be emplaced can actually be accommodated and whether it covers the uncertainties in the actual geochemical process.

# **DOE Response**

The DOE will respond to this comment in two parts: Part I will address the physical placement of MgO within the repository and address the stated concern regarding the distribution of MgO being consistent with the conceptual models assumed. Part II demonstrates that the excess volume can be emplaced and that the uncertainties in possible reactions has been considered in determining the quantity to be emplaced.

Uncertainty in the geochemical reactions that may occur is not covered as part of the response to this EPA comment. Rather, uncertainty in geochemical reactions is being addressed in response to a different EPA comment through direct experimental demonstration of the efficacy of MgO. It is important to remember that the MgO backfill is an assurance measure intended to satisfy, in part, the requirement to include an engineered barrier in the disposal system.

# Part I- Engineering Design for MgO placement

The method of MgO placement and quantity are described in Section 3.3.3 of the CCA. Preliminary placement test have been performed using minisacks and supersacks in the repository setting and demonstrate that backfill can be emplaced as described in Section 3.3.3 without significant impact to waste handling operations.

WIPP waste handling procedures WH-1011, Revision 2, dated October 1, 1996, describes the emplacement procedure for mini sacks of MgO in the void spaces between the waste drums in the 7-pack configuration. Current waste handling procedures for emplacement of waste in rooms are being modified to specify MgO placement with standard waste boxes (SWBs), MgO placement along the rib (space between the waste containers and the wall of the room), and super sack placement on top of waste containers. These procedures will provide those specific actions that must be performed such that the emplacement design specified in Section 3.3.3 will be achieved.

Part II- Consistency of emplacement method with conceptual models and consideration of uncertainty in determination of quantities of MgO to be emplaced.

The emplacement methodology described in Section 3.3.3 of the CCA was developed with specific consideration of the performance criteria required by the conceptual models relevant to MgO backfill. The assumptions in the conceptual models regarding MgO are covered in Sections 6.4.3.3 (Gas Generation), 6.4.3.3 (Chemical Conditions), 6.4.3.5 (Dissolved Actinide Source Term), and 6.4.3.6 (Colloidal Actinide Source Term), as well as Appendix SOTERM and Appendix BACK of the CCA. Additional discussions of MgO backfill can be found in Chapter 9, Section 9.3.1.2.10.2 and Appendix PEER, Section 1. The essential performance criteria relevant to placement of MgO are (1) that MgO be distributed in such a manner that the assumption of uniformity of chemical conditions through disposal rooms is valid, and (2) enough MgO is emplaced such that the consumption of all CO<sub>2</sub> produced is assured.

The MgO will be emplaced consistent with the design specified in Section 3.3.3. This design provides for MgO to be distributed throughout waste disposal rooms, including between waste drums and standard waste boxes. This distribution is sufficient to assure accessibility of MgO to chemical reactions taking place over the regulatory time scale. The Conceptual Model Peer Review Panel considered this in their examination of the MgO issue and found the emplacement design to be consistent with the conceptual model assumptions (Final Report, July 1996, page 3-154, Assumption (1)).

The quantity of MgO required to be emplaced to assure removal of CO<sub>2</sub> from the gas phase is based on calculations that consider all processes that might contribute to CO<sub>2</sub> production. These calculations are very conservative in that they utilize a maximum estimate of CO<sub>2</sub> production, a quantity that is unlikely to be attained. Based on the BIR and memoranda in the records center, the total number of moles of MgO required to react with the maximum possible amount of CO<sub>2</sub> generated is 9.85 x 10<sup>8</sup> moles. Using the appropriate conversion factors (40.3 gm/mole, 0.001 kg/gm, 2.202 kg/lb, 0.0005 lb/ton), at total of 43,700 tons of MgO are required to react with this maximum estimate of carbon dioxide production. Section 3.3.3 of the CCA documents that approximately 85,600 tons of backfill will be emplaced in the repository. Therefore, by dividing the mass of backfill to be emplaced (85,600 tons) by the maximum mass of MgO required to react with the maximum possible carbon dioxide production (43,700 tons), a 1.95 factor of safety results. In other words, 95% more MgO will be emplaced than is required to react with a conservative estimate of the maximum quantity of CO<sub>2</sub> production.

EPA Comment Enclosure 2, Page 11 194.51

# Consideration of Protected Individual

Section 194.51 requires, among other things, that exposure from all sources of radionuclide release from the disposal system to the accessible environment be examined.

Chapter 8 of the CCA provides a bounding analysis to demonstrate compliance with 40 CFR 191.15. However, the analysis only assumes exposure via consumption of potable water. It does not explicitly include the analysis of doses posed by other potential exposure pathways such as stock consumption or irrigation.

The Department needs to provide documentation which discusses why pathways other than consumption of potable water are not considered.

# DOE Response

The DOE has analyzed pathways other than the consumption of potable water as reported in the attached report, "Analysis Report for Estimating Dose from Cattle, Vegetable Consumption and Inhalation Pathways Utilizing Contaminated Water from the Top of the Salado, Culebra, and Selected Marker Beds for an Undisturbed Case Supporting Review Compliance Certification Application." The report shows that doses received from these pathways are indeed negligible and are bounded by the analysis conducted, described, and reported in Chapter 8 of the CCA. It is important to remember that these pathways are more unrealistic than the bounding case evaluated in the CCA.

Analysis Report for Estimating Dose from Cattle, Vegetable Consumption and Inhalation Pathways Utilizing Contaminated Water from the Top of the Salado, Culebra, and Selected Marker Beds for an Undisturbed Case Supporting Review Compliance Certification Application

# **Document Version 1.01**

### WBS # 1.2.01.5.3.1

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#### 1.0 Introduction

This analysis report summarizes the background, analysis procedure and results for the Waste Isolation Pilot Plant (WIPP) Repository dose calculation resulting from (1) consumption of beef cattle drinking water from a stockpond utilizing a contaminated ground-water source by a rancher residing at the location of the well; (2) consumption of crops irrigated from a contaminated ground-water source by a farm family residing at the location of the well; and (3) inhalation of resuspended irrigated soil. The requirements and standards which form the guidance for this calculation are set forth in the following paragraphs. This analysis represents a continuation of the drinking water pathway calculation, reported in Chapter 8 of the CCA.

# 1.1 Purpose of this Analysis and Background Information

The purpose of this analysis is to provide quantitative analysis of pathways for human exposure to radionuclides which potentially may be released through MB 139 (and Mbs 138, a & b) at the site boundary during 10,000 years of undisturbed performance. The CCA contained results of a conservative and bounding analysis of the hypothetical doses from consumption of contaminated drinking water, (Chapter 8, CCA). This analysis uses the same conservative and bounding assumptions used in the CCA to examine alternative exposure pathways. Specifically, this analysis presents dose calculations for ingestion pathways for beef and irrigated crops, and for the inhalation of resuspended particles of irrigated soil. These analyses were performed to address comments raised by the EPA in their review of the CCA [EPA-1].

The undiluted sources for this analysis appear in Table 1-1. A dilution factor of 52.4 was used for the purpose of achieving a potable water supply. This was based on a recommendation of 10,000 ppm (mg/L) TDS for potential drinking water sources contained in 40 CFR 191 (1993). However, in the NALCO Water Handbook [NA-1] a value of 500 ppm (mg/L) TDS is indicated as the level for potable water.

Three hundred realizations of the modeling system were generated during the CCA analyses for the containment requirements (Chapter 6, CCA). These same realizations were also used for individual and groundwater protection requirements (Chapter 8, CCA). These 300 realizations are comprised of three sets (or replicates) of one hundred realizations each, generated using the Latin Hypercube sampling technique. Of the 300 realizations, none show any radionuclides reaching the top of the Salado through the sealed shafts.

Nine of the 300 realizations show concentrations of radionuclides greater than zero reaching the accessible environment through the anhydrite interbeds. All of the remaining 291 realizations show that no radionuclides reach the accessible environment during the regulatory time frame of 10,000 years after repository closure through the anhydrite interbeds. A receptor in the accessible environment could not come in contact with the anhydrite interbeds located at a depth greater than 2000 feet. Table 1-1 shows the maximum concentrations of radionuclides calculated by the modeling evaluation as reaching the accessible environment in the nine non-zero realizations. The full range of

estimated values for radionuclide concentrations is from zero to the values shown in Table 1-1. The maximum concentration values shown in Table 1-1 occur 10,000 years after closure. These are the same values used in Chapter 8, CCA.

For the purposes of this analysis, the maximum concentration set, Replicate 3 Vector 64, was used to determine doses for the cattle, vegetable consumption, and inhalation pathways since this represents the largest concentration and gave the largest dose from drinking water as reported in Chapter 8, Table 8-2, CCA.

40 CFR Part 194.51 states that doses must be estimated for an individual who resides at the location in the accessible environment where that individual would be expected to receive the highest exposure from radionuclide releases from the disposal system. All potential pathways for exposure associated with the undisturbed performance of the repository must be assessed (40 CFR § 194.52).

Table 1-1. Maximum Concentrations of Radionuclides (Undiluted)
Within the Salado Interbeds at the Disposal System Boundary Occurring at
10,000 yrs. after Closure (Modified from Table 8-1, CCA)

| Realization<br>No. | Vector<br>No. <sup>(1)</sup> | Concentration (Curies/liter) |                          |                   |                          |                          |
|--------------------|------------------------------|------------------------------|--------------------------|-------------------|--------------------------|--------------------------|
|                    |                              | <sup>241</sup> Am            | <sup>239</sup> Pu        | <sup>238</sup> Pu | <sup>234</sup> U         | <sup>230</sup> Th        |
| 1                  | Replicate 1<br>Vector 46     | 1.36 x 10 <sup>-17</sup>     | 4.33 x 10 <sup>-12</sup> | N (2)             | 5.82 x 10 <sup>-13</sup> | 2.10 x 10 <sup>-1</sup>  |
| 2                  | Replicate 2<br>Vector 16     | N                            | 5.13 x 10 <sup>-14</sup> | N                 | 6.77 x 10 <sup>-15</sup> | 1.89 x 10 <sup>-1</sup>  |
| . 3                | Replicate 2<br>Vector 25     | N                            | 1.35 x 10 <sup>-15</sup> | - Ņ               | 1.65 x 10 <sup>-16</sup> | 7.00 x 10 <sup>-1</sup>  |
| 4                  | Replicate 2<br>Vector 33     | 1.32 x 10 <sup>-17</sup>     | 7.18 x 10 <sup>-14</sup> | N                 | 9.76 x 10 <sup>-15</sup> | 9.36 x 10 <sup>-1</sup>  |
| 5                  | Replicate 2<br>Vector 81     | N                            | 6.23 x 10 <sup>-18</sup> | N                 | N                        | N                        |
| 6                  | Replicate 2<br>Vector 90     | N                            | 5.20 x 10 <sup>-16</sup> | N                 | 7.40 x 10 <sup>-17</sup> | N                        |
| 7                  | Replicate 3<br>Vector 3      | 3.50 x 10 <sup>-18</sup>     | 3.08 x 10 <sup>-13</sup> | N <sub>.</sub>    | 4.32 x 10 <sup>-14</sup> | 1.07 x 10 <sup>-10</sup> |
| 8                  | Replicate 3<br>Vector 60     | 5.98 x 10 <sup>-17</sup>     | 7.41 x 10 <sup>-14</sup> | N                 | 9.09 x 10 <sup>-15</sup> | 2.30 x 10 <sup>-1</sup>  |
| 9                  | Replicate 3<br>Vector 64     | 5.42 x 10 <sup>-17</sup>     | 5.85 x 10 <sup>-12</sup> | N                 | 7.61 x 10 <sup>-13</sup> | 4.68 x 10 <sup>-13</sup> |
| 10-300             | -                            | N                            | N                        | N                 | N                        | N                        |

- 1. The procedure used to extract these values from the NUTS data is described in Appendix C.
- 2. Values less than 10<sup>-18</sup> curies per liter are considered to be negligible (N) relative to the other values and are not reported.

# 1.2 Bounding Analysis

Uncertainty in the calculation of radionuclide concentrations in the anhydrite interbeds is described in Section 6.1.2 ([CCA-1]). Additional uncertainty is involved in the calculation of doses resulting from the specified exposure pathways. Given this uncertainty, the DOE has elected to perform a bounding analysis using assumptions that do not represent reality, but that would result instead in a bounding estimate that is much greater than any reasonably expected dose to a receptor. If this unrealistic bounding analysis results in calculated doses to the receptor that are below the regulatory limit, compliance with the standard can be demonstrated.

The bounding analysis used for this assessment is based on the following factors and assumptions:

- 1. No specific transport mechanism is postulated. Instead, all of the contaminants reaching the accessible environment within the anhydrite interbeds during the year of maximum releases (10,000 years after closure) within the 10,000 year period, are assumed to be available to a receptor.
- 2. Brine derived from the anhydrite interbeds has total dissolved solids (TDS) concentrations of about 324,000 parts per million [BR-1]; this represents a concentration that is too high to be consumed by humans. For the bounding analysis, the calculation includes the dilution of this brine by a factor of 32.4 to a TDS concentration of 10,000 parts per million.
- 3. The resulting annual committed effective dose is calculated based on a 50-year dose commitment. Calculations were performed using the GENII-A dose code (Appendix GENII, CCA). A 50-year dose commitment is selected because this period is specified in Appendix B of 40 CFR Part 191.
- 4. The parameters associated with the individual receptors for each scenario appear in Tables 1-2, 1-3, and 1-4. Data related to food pathways, irrigation and inhalation were selected as representative values typical of the associated activities [NRC-1], [DOE-1], except where noted.

Table 1-2 GENII-A Input Parameters for Farm Family Scenario-Terrestrial Food Consumption Utilizing Irrigation from Ground Water Source.

| Food<br>Type | Grow<br>Time<br>Days | lrrigation<br>  Kate<br>  (cm/yr) | Time<br>monds | Yield<br>kg/m2 | Consumption<br>Heldup (days) | Consumption<br>Rate (kg/yr) |
|--------------|----------------------|-----------------------------------|---------------|----------------|------------------------------|-----------------------------|
| Leaf         | 90                   | 100                               | 6             | 1.5            | 14                           | 15                          |
| Root         | 90                   | 100                               | 6             | 4.0            | 14                           | 140                         |
| Fruit        | 90                   | 100                               | 6             | 2.0            | 14                           | 64                          |
| Grain        | 90                   | 100                               | 6             | 0.8            | 180                          | 72                          |

Table 1-3 GENII-A Input Parameters for Cattle Rancher Scenario.

| Food<br>Type | Consumption Rate<br>(kg/yr) | Consumption<br>Holdup (days) | Drinking<br>Water<br>Contamination<br>Fraction | Diet<br>Fraction | Grow<br>Time<br>days | Stored Feed<br>Irrigation<br>Rate (cm/yr) | Stored<br>Feed<br>Time<br>(months) | Stored<br>Feed<br>Vield<br>(kg/m3) | Stored<br>Feed<br>Storage<br>Time<br>(days) |
|--------------|-----------------------------|------------------------------|------------------------------------------------|------------------|----------------------|-------------------------------------------|------------------------------------|------------------------------------|---------------------------------------------|
| Beef         | 70                          | 34 .                         | 1                                              | 1                | 90                   | 100                                       | 6                                  | 0.8                                | 180                                         |

Table 1-4 GENII-A Input Parameters for Farm Family Inhalation Pathway

| Breathing Rate      | 270 cm <sup>3</sup> /sec. (Chronic) |
|---------------------|-------------------------------------|
| Inhalation Period   | 8760 hours/yr.                      |
| Mass Loading Factor | 1.0E-04 gm/m <sup>3</sup>           |

The mass loading factor is based on data representative of regional resuspension data for the 1991 to 1996 time period, Appendix-B and [AIRS-1]. Section 194.51 states that DOE shall assume that an individual resides at the single geographic point where that individual would receive the highest dose. With the bounding analysis, the DOE complies with the intent of this criterion, but the specific location of the receptor is not identified because all of the contaminants reaching the accessible environment within the anhydrite interbeds during the year of maximum releases are assumed to be directly available to the receptor, regardless of the location of the receptor. The well from which the receptor drinks is assumed to be located such that the contaminants reaching the anhydrite interbeds are delivered directly to the well. This well is the source of the

stockpond from which the cattle drink and from which irrigation for feed and vegetable crops is obtained. Additionally, an inhalation calculation for the farm family represents a pathway by which dried irrigated soil is resuspended above the farm area and inhaled by the farm inhabitants. The data used in this analysis appear in Tables 1-2, 1-3, and 1-4. Data related to food pathways, irrigation, and inhalation were selected as representative values typical of the associated activities [NRC-1], [DOE-1], except where noted.

The bounding analysis dose calculation was performed using the GENII-A code, Version 2.10 [GEN-1]. This program runs on the DEC Alpha System. Appendix GENII of the CCA [CCA-1] describes the modeling method. GENII-A incorporates dose-calculation guidance provided in Appendix B of 40 CFR Part 191.

# 1.3 Dose Calculation Results

The maximum doses calculated to result from the releases listed in Table 1-1 after applying the factors and assumptions listed above, are shown in Table 1-5. Because of the conservative and unrealistic assumptions underlying the analysis, the bounding doses are greater than any realistic doses that could be delivered to a receptor. The calculated bounding doses are well below the regulatory standard, which is an annual committed effective dose of 15 millirem. The full range of estimated radiation doses is from zero to some value less than the bounding values shown in Table 1-5

Table 1-5 Calculated Annual Committed Effective Doses at 10,000 yrs. after Closure

| Scenario.                 | Annual Committed Effective Dose (millirem) |
|---------------------------|--------------------------------------------|
| Farm Family<br>Inhalation | 3.1 x 10 <sup>-4</sup>                     |
| Farm Family<br>Ingestion  | 4.6 x 10 <sup>-1</sup>                     |
| Cattle Rancher            | 3.3 x 10 <sup>-8</sup>                     |

For comparison, the maximum dose reported in the CCA for the drinking water pathway is 4.7 x 10<sup>-1</sup> millirem/yr, (Table 8-2 of the CCA).

# 2.0 Summary of Compliance with the Individual Protection Standard

In performing the compliance assessment, the DOE applied a bounding-analysis approach using unrealistic assumptions that result in the over-estimation of potential doses and contaminant concentrations. This conservative approach assumes that all contaminants reaching the accessible environment are directly available to a receptor. Using this very conservative approach, the calculated maximum potential dose to an individual would be about one-thirtieth of the individual protection standard.

# 3.0 Software Used for Analysis

NUTS [NU-1]

GENII-A . Version 2.10 [GEN-1], [GEN-2], [GEN-3]

This program runs on the DEC Alpha System under VMS Operating system. This analysis was performed by Leo J. Rahal, the code sponsor.

# 3.1 Point of Contact

Code Sponsor: **GENII-A** Leo J. Rahal, Org. 6849, Geo-Centers Inc. (505) 766-9629 The GENII-A code was run on the DEC Alpha system using VMS. The calculations were performed by Leo J. Rahal, the code sponsor.

Radionuclide source data were obtained from the **NUTS [NU-1]** output through the **Compliance Assessment Methodology Controller** (CAMCON) library data access process. All calculations were performed within the **Configuration Management System** (CMS) environment to ensure QA procedures are followed.

# 4.0 Calculational Procedure

The following information describes the calculation procedure used to evaluate doses at selected times and locations. These input and output files are listed in Appendix A, Table B-1. The Description column indicates the location, vector number and time for the input data obtained from the NUTS code. The output files are generated by running these input files according to the command given in Appendix A, i.e. @run\_gi2 100 where 100 is the number associated with the data file gi2\_calc100.inp for example. For the purpose of this analysis the time selected was 10,000 years after closure. 10,000 years is the cut-off time for required calculations. The 10,000 year period represents the time at which maximum values occur within the required 10,000 year period. The GENII-A [GEN-1] dose code determined the dose corresponding to this selected time.

### 5.0 References

- [AIRS-1] U.S. Environmental Protection Agency. 1992. National Air Data Branch. Aerometric Information Retrieval System. Total suspended particulate information for LEA County.
- [BR-1] Data taken from BRAGFLO output file relating to brine inventory at 10,000 years after closure for Replicate 1. Scenario 1 (Undisturbed Case), Vector 46. The file from which these data were taken is as follows: DISK\$TINA\_CCA, 19963:[BF.JDMILLE.CCA, 1996.POSTALG.R1S1]OSTALG\_CCA, 1996\_R1\_S1\_V046.CDB
- [CCA-1] Compliance Certification Application for the Waste Isolation Pilot Plant, United States Department of Energy Waste Isolation Pilot Plant, Carlsbad Area Office, Carlsbad, New Mexico, October 29, 1996.
- [DOE-1] Performance Assessment Task Team Progress Report . Radioactive Waste Technical Support Program, May 1994. DOE/LLW-157 Revision 1.
- [EPA-1] Letter from EPA, Mary D. Nichols to Alvin Alm, Department of Energy. December 19, 1996
- [GEN-1] WIPP PA User's Manual for GENII-A, Version 2.10. Document Version 1.00, WPO # 27751. November 13, 1995.
- [GEN-2] Napier, B.A., R.A. Peloquin, D.L. Strenge and J.V. Ramsdell. 1988. GENII-The Hanford Environmental Radiation Dosimetry Software System. Vol. 1: Conceptual Representation. PNL-6584, Vol. 1. Richland, WA: Pacific Northwest Laboratory.
- [GEN-3] Napier, B.A., R.A. Peloquin, D.L. Strenge and J.V. Ramsdell. 1988. GENII-The Hanford Environmental Radiation Dosimetry Software System Vol. 2: User's Manual. PNL-6584, Vol. 1. Richland, WA: Pacific Northwest Laboratory.
- [NA-1] The NALCO Water Handbook, Frank N. Kemmer, Nalco Chemical Company, McGraw-Hill Book Company, 1987, Pg. 35.2 Table 35.1A.
- [NRC-1] U.S. Nuclear Regulatory Commission, "Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50, Appendix I, "Regulatory Guide 1.109 (1997).
- [NU-1] WIPP PA User's Manual for NUTS, Version 2.02. Document Version 1.00, WPO # 37927. May 28, 1996.

# 6.0 Appendices

Appendix A: Listing of Input and Output Data Files for Dose Calculation: Marker Bcd 139 (Table A-1)

Table A-1 Input and Output Files for Dose Calculations (1)

| ANI'UT FILE              | OUTPUT FILE         | DESCRIPTION                                              |
|--------------------------|---------------------|----------------------------------------------------------|
| 1. gi2_calc311.inp       | gi2_calc311_trn:out | r3s1v064 10.000 yrs. MB139s (Farm Family-Food Ingestion) |
| 2 <u>zi2_cálc312.inp</u> | gi2_calc312_trn.out | r3s1v064 10,000 yrs. MB139s (Cattle Rancher)             |
| 3 gi2_calc812.inp        | gi2_calc812_trn.out | r3s1v064 10.000 yrs. MB139s (Farm Family-Inhalation)     |

#### Footnote 1:

To run these data files type the following command: RUN\_GI2 100 where 100 is the number associated with the data file GI2\_CALC100.INP, for example.

An output file GI2\_CALC100\_TRN.OUT, will be generated.

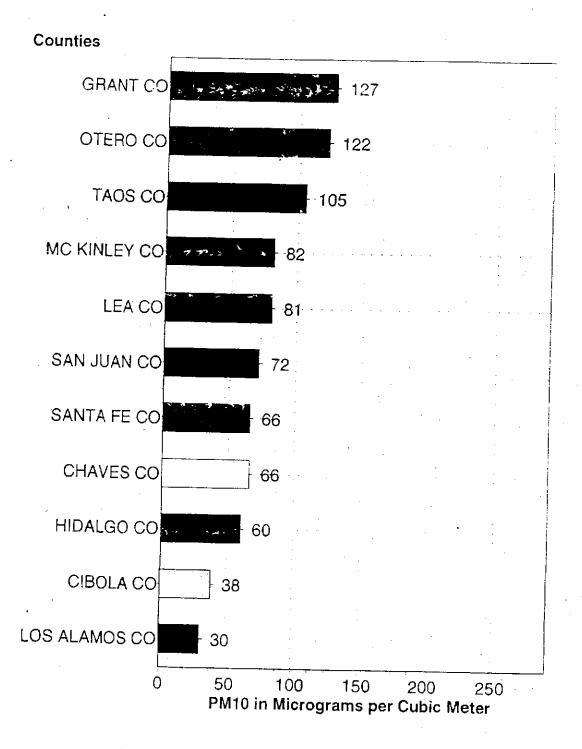
The edit command EDT filename was used to open and edit input and output files. Legend:

r3 replicate 3 of NUTS OUTPUT

s1 undisturbed case

v vector number

Appendix B: Graph of Mass Loading Data Token from 1991 to 1996 for Lea County.



# Appendix C: Procedure for Extraction of NUTS data used in this analysis.

The directory U1:[JDMILLE.TEST] contains the following files used in the extraction of data from NUTS:

- 1. PA\_NUTS\_ISO\_S1\_CONC.INP, the equation file, plus the NUTS.CDB ouput file are used to extract data from NUTS.
- 2. PA\_NUTS\_ISO\_CONC.COM is the command file for ALGEBRACDB [ALG-1] used to process these data.
- 3. The resulting CDB files are:

```
PA_NUTS_ISO_R1S1_CONC_V046.CDB
PA_NUTS_ISO_R2S1_CONC_V016.CDB
PA_NUTS_ISO_R2S1_CONC_V025.CDB
PA_NUTS_ISO_R2S1_CONC_V033.CDB
PA_NUTS_ISO_R2S1_CONC_V081.CDB
PA_NUTS_ISO_R2S1_CONC_V090.CDB
PA_NUTS_ISO_R3S1_CONC_V003.CDB
PA_NUTS_ISO_R3S1_CONC_V060.CDB
PA_NUTS_ISO_R3S1_CONC_V064.CDB
```

4. Selected times are obtained through processing by SUMMARIZE [SUM-1] , using the input file

# PA\_NUTS\_ISO\_S1\_CONC.SMZ

- 5. This output is transferred to an EXCEL spreadsheet form through multiple files, one for each vector. The EXCEL input file, containing all vectors is PA\_NUTS\_ISO\_S1\_CONC.TBL.
- 6. All files have been transferred to the CMS system.
- [ALG-1] <u>ALGEBRACDB</u>, WPO# 21247, 1995
- [SUM-1] <u>SUMMARIZE</u>, WPO# 21781, 1995