June 12, 2003

Dr. Inés R. Triay, Manager
Carlsbad Field Office
U.S. Department of Energy
P.O. Box 3090
Carlsbad, NM 88221

Dear Dr. Triay:

As you are aware, the Environmental Protection Agency (EPA) has been monitoring changes to the performance assessment baseline established in the original certification for the Waste Isolation Pilot Plant (WIPP). In updating the Department of Energy’s performance assessment computer system, Sandia National Laboratories (SNL) staff have conducted computer code qualification testing of the performance assessment codes to establish a verifiable baseline that complies with EPA requirements. For the new OpenVMS 7.3-1 Operating System (OS) and new Compaq ES40 hardware platform, EPA has completed its technical review of the records of the tests conducted to re-qualify 27 WIPP performance assessment computer codes and three libraries, accessed by the performance assessment computer codes, from the baseline established in the certification.

The EPA’s technical review of OpenVMS 7.3-1 OS and new Compaq ES40 hardware platform is discussed in detail in the enclosed report. In summary, the Agency has been able to verify that, for the OpenVMS 7.3-1 OS and Compaq ES40 hardware only, the WIPP performance assessment computer codes have been adequately qualified for use in compliance performance assessment calculations. During our initial review, Agency staff informally transmitted to your staff some concerns, listed here in Section 6 of the attached report. All of these concerns were ultimately resolved to our satisfaction.

At the close of our review, Department of Energy (DOE) added new hardware, the Compaq ES45, to the performance assessment computing cluster. The EPA was unable to complete an adequacy review of the recently added Compaq ES45 hardware configuration for two primary reasons. First, a preliminary review of the regression testing of computer codes on the Compaq ES45 platform showed that the regression tests were compared with test cases run on the Compaq ES40 with OpenVMS 7.3-1, an operating system which had not yet been approved by EPA and therefore did not constitute an acceptable testing benchmark. With today’s approval of the Compaq ES40 and OpenVMS 7.3-1, it is now appropriate for SNL to compare the Compaq ES45 results to Compaq ES40 with OpenVMS 7.3-1 operating system; however,
SNL documentation needs to be updated accordingly. Second, the absence of the DIFFERENCE files, in a readily reviewable format, as was used in the Compaq ES40 and OpenVMS 7.3-1 documents, does not allow an independent review of DOE's conclusions. We plan to evaluate the adequacy of the ES45 hardware during our review of the Compliance Recertification Application.

If you have any questions, please contact Betsy Forinash at (202) 564-9310.

Sincerely,

Frank Marcinowski, Director
Radiation Protection Division

Enclosure

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REVIEW OF WIPP PERFORMANCE ASSESSMENT
COMPUTER CODE MIGRATION

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Under
Contract 68-D-00-210
Work Assignment 2-08 Task 4 TD No. 2

Prepared for:
U.S. Environmental Protection Agency
Office of Radiation and Indoor Air
Washington, DC 20460

Mr. Charles O. Byrum
Work Assignment Manager

June 10, 2003
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EXECUTIVE SUMMARY

As part of the Waste Isolation Pilot Plant (WIPP) certification process, the Department of Energy (DOE) conducted a Performance Assessment (PA) to show compliance with EPA’s disposal regulations and compliance criteria at 40 CFR 194. As required by 40 CFR 194, the DOE must demonstrate, on an ongoing basis, that performance assessment computer software is in compliance with regulations outlined in Section 194.23 - Models and Computer Codes. Since EPA’s certification of the DOE WIPP Compliance Certification Application (CCA), DOE has added computer hardware and upgraded the computer software. In order to maintain compliance with Sections 194.22 and 194.23, DOE is required to conduct testing on the computer codes to ensure that they still function properly on new hardware and software. EPA reviewed the testing performed by DOE to demonstrate continued compliance with the addition of computer hardware and upgraded software.

During EPA’s initial review the Agency found seven preliminary concerns that DOE needed to resolve before the agency could approve the migration of the computer codes. The preliminary concerns are listed below and discussed in detail in Section 6 of this report:

1) Incremental Regression Testing
2) Acceptance Criteria of Regression Tests
3) Testing of Existing Functionality
4) Testing of New Functionality
5) Traceability of Computer Code/Libraries
6) Traceability within CMS Framework
7) Adequacy of Functional Tests

Through the course of our review, we determined that DOE had adequately addressed these preliminary concerns. We can now conclude that DOE’s modifications to their code migration activities have satisfactorily solved the concerns identified above, and the 27 computer codes and three libraries migrated to the Compaq ES40 with OpenVMS 7.3-1 are approved for use in compliance calculations for the WIPP performance assessment. Changes to the operating system, to computer codes, and new hardware - such as the Compaq ES45 - will be reviewed again for the recertification. EPA expects that the required future documentation would include the DIFFERENCE files presented in a format similar to that presented for the Compaq ES40 tests.
1.0 INTRODUCTION

This report describes results of the U.S. Environmental Protection Agency (EPA) review of performance assessment computer code development and testing activities performed by the U.S. Department of Energy (DOE) since the original certification of the Waste Isolation Pilot Plant (WIPP). The ability of the WIPP facility to meet the Agency's certification requirements was demonstrated in part through the use of a series of performance assessment computer codes that are documented in the Department's Compliance Certification Application (DOE 1996).

As part of the WIPP certification process, the DOE conducted a Performance Assessment (PA) to show compliance with our disposal regulations. As required by the regulations, the DOE must demonstrate on an ongoing basis that performance assessment computer software is in compliance with regulations outlined in §194.22 - Quality Assurance and §194.23 - Models and Computer Codes. Examples of software that must meet the compliance criteria are:

- scientific or engineering software used to assess the performance of a site,
- scientific or engineering software used to analyze data for, or produce input (parameters) to, a performance assessment calculation,
- software that is used in managing information or augmenting mission essential decisions, and
- software used to collect data (e.g., far-field, near-field, engineered barriers).

DOE executes the PA conceptual models through software applications with parameter value inputs on an infrastructure composed of computers and operating systems that must be periodically updated. For the certification application, performance analyses were run on the DEC Alpha Cluster using the OpenVMS operating system, version 6.1. In 1999 the operating system was updated from OpenVMS 6.1 to 7.1, and a year later from OpenVMS7.1 to 7.2. In the summer of 2001, the FORTRAN compiler available on the cluster was upgraded to version 7.4A. In August 2002, the operating system was upgraded to an Open VMS 7.3-1 operating system.

In addition to software upgrades, the DOE has made hardware upgrades. The DEC Alpha Cluster was the main platform for performance analyses for the WIPP during CCA. The cluster consisted of 11 DEC Alpha 2100 computers with 44 processors. In September 2001, a single Compaq Alpha ES40 computer was added to the WIPP PA hardware cluster. In August 2002, the DEC Alphas were replaced by a Compaq ES40. For the Compliance Recertification Application (CRA) PA, DOE intends to use Open VMS 7.3-1 as the operating system in conjunction with the Compaq ES40. To ensure that each code will function correctly on the ES45 platform running OpenVMS 7.3-1, each of the WIPP PA codes has undergone regression testing by DOE.
Although a single Compaq ES45 running OpenVMS 7.3-1 has recently been added and this configuration could be used for preparing the CRA, it was not included in this review. The Agency was unable to complete an adequacy review of the ES45 hardware configuration for two primary reasons. First, after a preliminary review of the regression testing of computer codes on the ES45 platform, the Agency found that the regression tests were compared with the same test cases run on the COMPAQ ES40 with OpenVMS 7.3-1, rather than tests performed with OpenVMS 6.1. Second, the Agency also found that the documentation supporting DOE's conclusions was inadequate. The absence of the DIFFERENCE files, in a readily reviewable format, does not facilitate an independent review of DOE's conclusions.

This report documents the results of the Agency's assessment performed to determine whether the observed DOE PA code activities comport with the compliance criteria requirements for §194.22 and §194.23. Specifically, EPA's evaluation addressed whether these changes have materially affected the Agency's original determination that the computer codes were adequate to support the certification decision.

The report is divided into five sections. Following this Introduction (Section 1), a Background section (Section 2) presents the approach that DOE has taken to meet the compliance criteria requirements for the computer codes. The Background section is followed by a summary of DOE's code migration approach and conclusions (Section 3). Section 4 presents the general approach that EPA followed to review DOE's code migration activities. Section 5 summarizes each of the computer codes and libraries that were migrated to the ES40 with the OpenVMS 7.3-1 operating system. Section 6 provides the summary and conclusions. References are provided at the end of each section.

2.0 BACKGROUND

In §194.22, the EPA required that the Department of Energy (DOE) implement a Quality Assurance program. This program, at a minimum, must meet the requirements of the American Society of Mechanical Engineers' (ASME) "Quality Assurance Program Requirements for Nuclear Facilities" (NQA-1-1989 edition), ASME's "Quality Assurance Requirements of Computer Software for Nuclear Facility Applications" (NQA-2a-1990 addenda, part 2.7 to ASME NQA-2-1989 edition), and ASME's "Quality Assurance Program Requirements for the Collection of Scientific and Technical Information on Site Characterization of High-Level Nuclear Waste Repositories" (NQA-3-1989 edition, excluding Section 2.1(b) and (c)). These ASME documents present criteria which require the establishment and execution of Quality Assurance programs for all aspects of the WIPP disposal system that affect the containment of waste.

2.1 Software Qualification

To demonstrate that computer software is in compliance with disposal regulations outlined in
§194.22, the DOE established a life-cycle management process for the software used to support their PA. Their qualification approach for the software follows the life-cycle phases outlined in ASME NQA-2a-1990 addenda, part 2.7 which are:

- Planning,
- Requirements,
- Design,
- Implementation,
- Validation,
- Installation and Checkout,
- Maintenance, and
- Retirement.

The life cycle phases are implemented using an iterative or sequential approach, following the process flowchart below (Figure 1). Each phase and associated documentation shown in Figure 1 are discussed in the following sections.

![Flowchart of DOE's Software Development Process](image)

**Figure 1** Major Components of DOE's Software Development Process.
**Planning Phase**

A Software QA Plan (SQAP) is produced during the planning phase for new software development (Figure1). Software under configuration control and developed within the scope of these QA requirements does not require a stand alone SQAP. Following the development of the SQAP, a strict sequence of performing activities is not required, provided that all specified requirements for each phase are met and the intent of the requirements are not subverted. SQAPs may be written for an individual code or a set of codes.

**Requirements Phase**

The documents produced during the requirements phase is the Requirements Document & Verification and Validation Plan (RD/VVP)(Figure1), which is a single document that identifies the computational requirements of the code (e.g., SECOFL2D must be able to simulate groundwater flow under steady-state conditions). The RD/VVP also describes how the code will be tested to ensure that those requirements are satisfied.

**Design Phase**

The Design document (DD)(Figure1), produced during the design phase, provides the following information (as applicable):

- Theoretical basis (physical process represented),
- Mathematical model (numerical model),
- Control flow and logic,
- Data structures,
- Functionalities and interfaces of objects, components, functions, and subroutines, and
- Ranges for data inputs and outputs, in a manner that can be implemented into software.

More than one design document may be created during software development. For example, a high-level design may be developed to match the code design to the requirements, and to define the overall architecture of the code (define modules and subroutines and their purpose, data structures, and what routine calls what routine, etc.). Another detailed design document may be developed to define how the modules will function in detail, define call interfaces between routines, defines data types, etc. A detailed design as its name implies, is very detailed down to level of almost writing the code (pseudocode). These design documents may be combined into a single document.

**Implementation Phase**

The following documents are produced during the implementation phase:

*User’s Manual (UM)* - describes the code’s purpose and function, mathematical governing equations, model assumptions, the user’s interaction with the code, and the models and methods
employed by the code (Figure 1). The User’s Manual generally includes:

- The numerical solution strategy and computational sequence, including program flowcharts and block diagrams;

- The relationship between the numerical strategy and the mathematical strategy (i.e., how boundary or initial conditions are introduced);

- A clear explanation of model derivation. The derivation starts from generally accepted principles and scientifically proven theories. The User’s Manual justifies each step in the derivation and notes the introduction of assumptions and limitations. For empirical and semi-empirical models, the documentation describes how experimental data are used to arrive at the final form of the models. The User’s Manual clearly states the final mathematical form of the model and its application in the computer code;

- Descriptions of any numerical method used in the model that goes beyond simple algebra (e.g., finite-difference, Simpson’s rule, cubic splines, Newton-Raphson Methods, and Jacobian Methods). The User’s Manual explains the implementation of these methods in the computer code in sufficient detail so that an independent reviewer can understand them; and.

- The derivation of the numerical procedure from the mathematical component model. The User’s Manual gives references for all numerical methods. It explains the final form of the numerical model and its algorithms. If the numerical model produces only an intermediate result, such as terms in a large set of linear equations that are later solved by another numerical model, then the User’s Manual explains how the model uses intermediate results. The documentation also indicates those variables that are input to and output from the component model.

Implementation Document (ID) - provides the information necessary for the re-creation of the code used in the 1996 WIPP Performance Assessment calculation (Figure 1). Using this information, the computer user can reconstruct the code or install it on an identical platform to that used in the 1996 WIPP PA calculation. The document includes the source-code listing, the subroutine-call hierarchy, and code compilation information.

Validation Phase
The validation phase consists of executing and reviewing the test cases identified in the approved VVP to demonstrate that the developed software meets the requirements defined for it in the RD (Figure 1). The Validation Document (VD), produced during this phase, summarizes the results of the testing activities prescribed in the Requirements Document and Verification and Validation Plan documents for the individual codes and provides evaluations based on those results. The Validation Document contains listings of sample input and output files from computer runs of a model. The Validation Document also contains reports on code verification, bench marking, and validation, and also documents results of the quality assurance procedures.

**Installation and Checkout Phase**

The following documents are produced during the installation and checkout phase:

- The Installation and Checkout (I&C) Form NP 19-1-8
- The Access Control Memorandum and
- The Approved Users Memorandum

**Production Software and/or Baseline Document Change Control**

When changes to the software baseline occur the Change Control Form, Form NP 19-1-9, is used. Types of changes that may be implemented are:

- Major changes - include new requirements, new design, new models, new implementation, require a new baseline (i.e., SQAP, RD, DD, VVP, ID, UM, VD) to be documented. In addition to revising every baseline document a change control form and the Installation and Checkout Form are used.

- Minor changes - do not affect the requirements or design and can be documented with addenda (no more than three addenda’s per baseline document) or page changes to the affected baseline document, in addition to the Change Control form and the Installation and Checkout Form.

- Patch changes - can be used for very small fixes to the code usually one or two lines of source code or expanding a fields character length etc. Patch changes can be documented and tested with the Change Control Form and Installation & Checkout Form.

**System Software and Hardware Change Control**

**Coding Documentation Standards.** Any change to software must be accompanied by
documentation describing the change, the date the change was made, and the name of the person responsible for implementing the change. This documentation should be clearly identified, and placed in the code in the vicinity of the change, as well as at the top of the code prior to the first executable line. The code reviewer shall determine if this documentation is clear and sufficient.

**Significant System Software or Hardware Changes.** The Code Team/Sponsor (single-user systems) or System Administrator (multi-user systems) proposes significant system software or hardware changes using the Change Control Form NP 19-1-9. Examples of significant changes to system software or hardware:

- changes to the operating system such that the version or level identifier changes
- changes to the Central Processing Unit (CPU)
- database management system change

In general, changes are significant if they impact the results generated by production software or cause recompilation of production software.

**Software Problem Report (SPR).** Whenever a software problem is identified, the Code Team/Sponsor evaluates the problem to determine if it is indeed a problem (as opposed to user error) (Figure 1). If it is a problem, the SPR process is followed.

The Code Team/Sponsor shall classify the problem as major if it could significantly impact previous uses of code or if it will require significant modification to the software; otherwise it is classified as minor. For major problems, the Responsible Manager identifies affected users to be notified of the problem, and designate qualified personnel to identify and evaluate the impact of the software problem. The affected analyses is revised necessary, and the evaluation and resolution of the software problem shall be documented in Part II of the Software Problem Report and Evaluation Form. For minor problems, this evaluation can be performed by the Code Team/Sponsor.

**Configuration Management (Configuration Identification and Status Accounting).** This section provides the process for defining the configuration of software products, establishing software configuration baselines, and tracking the status of baseline changes. A software configuration baseline consists of the source code and baseline documents, providing objective evidence of technical adequacy.

The SCM Coordinator maintains a Software Baseline List, and make it available upon request. The SCM Coordinator performs a completeness review to ensure compliance with the procedure, and to ensure that necessary components of configuration
management are present.

For Compliance Decision, the Software Baseline List contains:

- code name and version,
- code version date,
- code Team/Sponsor name,
- code classification,
- RD version,
- VVP version,
- DD version,
- ID version,
- UM version,
- VD version,
- list of approved users (may be listed by name, organization, group, or task, etc...)
- list of approved system software/hardware configurations,
- list of outstanding Software Problem Report (SPR) numbers, and
- status of approved changes which are in process.
- I&C date

Retirement Phase

To retire a code, the Code Team/Sponsor issues a memorandum to the SCM Coordinator requesting that the code be retired, and provide a reason for the retirement. The SCM Coordinator marks the code as retired in the baseline software list. The System Administrator and/or Code Team/Sponsor shall take action to prevent the use of the retired code. This could involve removal of the software from the computer or the changing of execution privileges.

2.2 Post CCA SQA Upgrades and Documentation

Since the time of certification, the DOE has implemented upgrades to the software operating systems and computer hardware which are documented in the following reports:

- Summary of Performance Assessment System Upgrades Since the Compliance Certification Application

- Analysis Package for AP-042 (documents the upgrade from Open VMS operating
software from Version 6.1 to Version 7.1)

- Analysis Package for Regression Testing the Upgrade to OpenVMS Version 7.2 on the WIPP DEC Alpha Cluster

- Analysis Package for Regression Testing for the Compaq Alpha ES40 Hardware Upgrade on the WIPP DEC Alpha Cluster

- Analysis Package for Regression Testing for the upgrade of Operating System to Open VMS 7.3-1 and Hardware to HP Alpha ES45

For the upgrades to the operating system and hardware on which the PA codes run, regression testing was performed to demonstrate that the codes still produce acceptable output. Regression testing, as a discipline, consists of running a set of one or more tests for a computer program and verifying that the output produced in the tests is within previously specified acceptable limits.

EPA has reviewed the documentation that DOE has developed to assess whether the computer codes still meet the requirements specified in §194.22 and §194.23 of the Rule. In addition to the references cited above, the EPA reviewed User’s Manuals, Validation Documents, Implementation Documents and Requirements Document & Verification and Validation Plans for each code. Since all of the of the code modifications that have been made since certification are documented on Change Control, Software Installation and Checkout Forms, these forms have also been reviewed by EPA.

3.0 OVERVIEW OF DOE’S COMPUTER CODE MIGRATION ACTIVITIES

As mentioned in Section 1.0, in August 2002, the operating system was upgraded to OpenVMS 7.3-1, and the DEC Alpha 2100s replaced by a Compaq ES40. This configuration will be used for preparing the Compliance Recertification Application (CRA). EPA will evaluate additional computer code changes when the CRA is submitted by DOE. Because of these changes, regression testing has been conducted by DOE for 27 PA software codes and 3 libraries on the Compaq ES40 using the OpenVMS 7.3-1 operating system to ensure that each code continues to satisfy all the criteria in its requirements documents.

The requirements documents for each software code specifies the validation criteria for the code and the test cases that demonstrate compliance with these criteria. Sandia National Laboratories used regression testing to determine whether each code could satisfy the criteria in its requirements documents when run in the current computing configuration. The regression test
was conducted by running every validation test for each code in the current computing configuration (OpenVMS 7.3-1 running on the Compaq ES40) and comparing the code’s output to the output from the code’s validation tests. The differences between the two sets of output were then analyzed. Any numerical differences between code outputs were evaluated to determine if the code output met the code’s acceptance.

### Table 3.1. Codes Versions in the VMS 7.3-1 Regression Test

<table>
<thead>
<tr>
<th>Code Name</th>
<th>Version</th>
<th>Code Name</th>
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<td>2.35</td>
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#### 3.1 DOE’s Test Methodology

The test methodology and acceptance criteria described in AP-089 were implemented by DOE for these regression tests and the results are presented in Section 5 of this document. The regression tests involved running each code on the ES40 with OpenVMS 7.3-1. Every test case from each code’s requirements document was run, and the results were compared to test results from the validation of that code. The result was a comprehensive analysis of every test case and
every acceptance criterion for each software code.

Whenever possible, the regression test methodology used the VMS DIFFERENCE command to compare output from the regression testing to output from previous validations. The DIFFERENCE command compares two files and identifies records that are different in the two files. The DIFFERENCE command was not used to compare binary output data. Binary output data, from both the regression testing and from previous validations, were often processed through other software codes to produce ASCII files that could be compared using the DIFFERENCE command.

In some cases, comparison using the DIFFERENCE was not appropriate or possible. For example, the code BLOTCDDB produces plots using the Adobe POSTSCRIPT language. These plots were compared visually to verify that the plots were correct. In a few cases, output from the code validation tests was not available electronically. In these cases, output was compared to printed information in the code’s validation report.

Differences that involve dates and times, file and directory names, user names, platform names, system version numbers and execution statistics were termed acceptable. Differences in numerical output required analysis to determine the origin of the differences and whether the differences affect the code’s performance. Numerical differences were determined to be acceptable if the analysis judged that the output, although different, still met the acceptance criteria for the code.

After concluding a code meets the acceptance criteria specified in its requirements documents, a Software Installation and Checkout Form was completed for each code. The I&C documents that a code’s regression test results meet the acceptance criteria specified in its requirements documents, managements approval of the installation of the software and the Software Configuration Management (SCM) Coordinator’s approval of the release of the code as production baseline software.

3.2 DOE’s Conclusions

Table 3.2 summarizes results from the regression testing of 27 software codes qualified by DOE. With the exception of BRAGFLO, DOE’s initial examination of the results found all differences in numerical output to be acceptable. BRAGFLO Test Case 6 showed a large number of numerical differences that required a separate analysis to show that BRAGFLO met the acceptance criteria for this test case. DOE concluded that all other differences were acceptable; DOE found that these differences were limited to differences in code run date and times,
directory or file names, user names, platform names, system version numbers or execution statistics.

BRAGFLO 4.10, Test Case 6 showed a large number of numerical differences between the output from OpenVMS 7.3-1 and the output from the code’s validation tests. The large number of differences precluded analysis of the differences to determine whether the code meets the acceptance criteria for this test case. Consequently, the output of Test Case 6 was analyzed by DOE separately to determine whether the code meets its acceptance criteria when run on the ES40 with OpenVMS 7.3-1. DOE concluded that, in fact, the results of BRAGFLO for Test Case 6 did meet the acceptance criteria. Since all differences between the results of these regression tests, run in OpenVMS 7.3-1 on the Compaq ES40, and the results of previous validations are acceptable, DOE concluded that all 27 software codes meet the acceptance criteria specified in their respective requirement documents, and thus DOE assumed that they are validated on the Compaq ES40 with OpenVMS 7.3-1.

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<th>Acceptable Numerical Differences</th>
<th>Unacceptable Differences</th>
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4.0 EPA's REVIEW APPROACH

The Agency's review has been conducted by a team consisting of Agency and contractor personnel, and coincides with a parallel review of changes to the parameter data base. The review was initiated in July 2002 with preparatory activities and assembly of background information. The computer codes are maintained in Carlsbad by the Department's WIPP science advisor, Sandia National Laboratories (SNL).

The Agency's review has been conducted in several stages, recognizing that changes in the assessment approach might be required, depending upon the results obtained. The following preparatory activities were conducted before conducting on site reviews:

- Tabulation of EPA's code acceptance criteria that had been developed by the Agency during the CCA.
- Preparation of a list of computer code life-cycle documentation (e.g., Verification & Validation Plans, Change Control and Error Reporting forms etc.) that the Agency would like to review.
- Preparation of a draft checklist for reviewing the ability of the performance assessment codes to meet the quality assurance criteria.
- Preparation a list of computer codes (e.g., BRAGFLO, NUTS, SECOTP) that are the most difficult to qualify and therefore, would be reviewed first.

Since DOE was still in the process of deciding which codes were to be qualified in OpenVMS 7.3-1 on the Compaq ES40, EPA's early review focused on the approach that DOE had taken in the past to migrate the computer codes to OpenVMS 7.1 and 7.2. This approach allowed the EPA to provide interim guidance during DOE's migration from OpenVMS 7.2 to OpenVMS 7.3.

The following on-site review activities were conducted by EPA:

- Received an overview presentation by SNL personnel describing the computer code migration activities.
- Obtained and reviewed the adequacy of documentation describing the computer code migration activities.
- Reviewed the adequacy of testing performed to demonstrate consistency of code output under different operating/hardward systems.
• Reviewed and evaluated the traceability of the code migration information.

• Review the ability of performance assessment codes to accurately reproduce output obtained under the software/hardware configurations in place during the CCA. access input parameters from the new database.

Initial meetings with Department and SNL personnel were held in Carlsbad during the week of August 5, 2002. Additional meetings were held in Carlsbad during the weeks of October 21, 2002, November 18, 2002, and February 10, 2003, for the purpose of completing the review. During these meetings, an overview of the computer code qualification activities was presented by SNL and documentation describing the computer code qualification activities was obtained and reviewed. An initial evaluation of the adequacy of physical documentation was reviewed at the Carlsbad Records Center. Remote access to the computer codes was requested to facilitate the review. In addition to the on-site reviews, offsite activities were conducted that included the review of relevant documents (e.g., Change Control and Error Reporting Forms, Code Tracking Sheets, Validation Documents), recreation of selected DIFFERENCE files, review of all DIFFERENCE files for all test cases for each of the 27 computer codes and 3 libraries that DOE tested. The results of these activities are summarized in Section 5, below.

5.0 SUMMARY OF INDIVIDUAL COMPUTER CODE MIGRATION

The following section presents the results of EPA’s computer code migration analysis for each individual code examined. Specific software and hardware configurations used in the CCA PA are reviewed, followed by the regression test methodology, EPA’s analysis of the testing, and EPA’s conclusion.

5.1 ALGEBRACDB

This section presents the regression test results for the ALGEBRACDB Version 2.35 code. ALGEBRACDB is a utility code that adds, removes, or manipulates data on CAMDAT database (CDB) files. The data manipulations to be performed are expressed as algebraic equations involving the existing and/or newly created data.

5.1.1 Introduction
ALGEBRACDB 2.35 was used in the WIPP Compliance Certification Application (CCA) PA. ALGEBRACDB 2.35 was validated in January 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of ten Test Cases (1 through 10) met the acceptance criteria
defined in the RD/VVP for ALGEBRACDB 2.35 (document Version 1.00 [2]). In January 1997 ALGEBRACDB was re-evaluated, and DOE determined that several requirements, previously identified as “Functionality Not Tested” in the RD/VVP (document Version 1.00), were in-fact in need of testing. DOE generated five additional Test Cases (11 through 15) to address these parameters and validated on a DEC Alpha 2100 with OpenVMS 6.1 [3] by demonstrating that the results met the acceptance criteria defined in the RD/VVP for ALGEBRACDB 2.35 (document Version 1.01[3]). When combined together, document Versions 1.00 and 1.01 of the RD/VVP describe all the requirements and testing of ALGEBRACDB 2.35.

5.1.2 Test Methodology
The tests for this code comprised the fifteen test cases described in the Requirements Document & Verification and Validation Plan for ALGEBRACDB Version 2.35 (RD/VVP) (both document Versions 1.00 [3] and 1.01 [4]). The first 10 tests are described in document Version 1.00 and the remaining 5 cases are included in document Version 1.01. Regression test results from ALGEBRACDB 2.35 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of ALGEBRACDB 2.35 run on a DEC Alpha 2100 with OpenVMS 6.1, as documented in the Validation Document for ALGEBRACDB Version 2.35 (VD) (both document Versions 1.00 [5] and 1.01 [6]). CAMDAT database files (CDB) are produced in fourteen of the RELATE test cases. The output CDB files are converted from a binary, CDB, file to an ASCII file for comparison during the validation process. In the previous ALGEBRACDB 2.35 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [5]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Section 5.10, GROPECDB). For DOE’s regression test, GROPE 2.12 is used to convert the CDB output files from ALGEBRACDB 2.35 in OpenVMS 7.3-1, as well as ALGEBRACDB 2.35 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

The regression test methodology used the VMS DIFFERENCE command to compare output from ALGEBRACDB 2.35 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of ALGEBRACDB 2.35 with OpenVMS 6.1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files. Records with differences are grouped into sections; a section begins with a record that is different between the two files, and ends with the first subsequent record where the two files agree. In the output of the DIFFERENCE command, sections are separated by rows of 12 asterisks; inside a section, the records from the two files are separated by a row of 6 asterisks. At the end of the DIFFERENCE output, the utility reports the number of sections and the number of records in which differences were found.
5.1.3 EPA’s Conclusions
EPA found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, platform names, system version numbers, the directory and file names. The comparison found no differences in the numerical output of ALGEBRACDB 2.35. The Agency concludes that ALGEBRACDB 2.35 meets the acceptance criteria in the RD/VVP and is validated for WIPP PA use on the ES40 with OpenVMS 7.3-1.

5.1.4 References


5.2 BLOTCDB
This section presents DOE’s regression test results for the BLOTCDB Version 1.37 code. BLOTCDB 1.37 plots the mesh and results from finite-element and finite-difference analysis programs. BLOTCDB plots all intermediate and final results from all main modules used to
perform the WIPP PA. BLOTCDB directly reads a computational database (CDB) file and plots: (1) the computational mesh with contoured analysis results, (2) grid distance versus any variable, and/or (3) any variable versus any other variable. BLOTCDB produces mesh plots with various representations of the analysis output variables and can also produce X-Y curve plots of the analysis variables.

5.2.1 Introduction

BLOTCDB 1.37 was validated in May of 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of six test cases met the acceptance criteria defined in the RD/VVP [1,2]. BLOTCDB 1.37, running on the OpenVMS 6.1 operating system, was validated for use in the Compliance Certification Application (CCA). The code has not been revised since the initial validation.

5.2.2 Test Methodology

The tests for this code comprised the six test cases described in the Requirements Document & Verification and Validation Plan for BLOTCDB Version 1.37 (RD/VVP) [1]. Regression test plots from BLOTCDB 1.37 run on the ES40 with OpenVMS 7.3-1 were visually compared by DOE to plots from the validation tests of BLOTCDB 1.37 run on a DEC Alpha 2100 with OpenVMS 6.1.

Validation of BLOTCDB 1.37 running on a Compaq ES40 using OpenVMS 7.3-1 was also accomplished by visually comparing output plot files to the corresponding output plot files from the previous validation of BLOTCDB 1.37 running on a DEC Alpha 2100 using OpenVMS 6.1. These files were identified in BLOTCDB 1.37 RD/VVP [1] as necessary to determine that the test case met its acceptance criteria.

5.2.3 Test Results

The six test cases for BLOTCDB 1.37 were executed on the Compaq ES40 with OpenVMS 7.3-1. The output plot files from the original validation of BLOTCDB 1.37 running OpenVMS 6.1 were not retained electronically. Therefore, DOE visually compared the output plot files from the test cases to the corresponding plot files from the previous validation of BLOTCDB 1.37 illustrated as figures in the validation document [2]. DOE believes that the comparison found that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names.
5.2.4 EPA’s Conclusions

After conducting a visual comparison of the output plot files, EPA has found that all differences between the results of BLOTCDB 1.37 in OpenVMS 7.3-1 and BLOTCDB 1.37 in OpenVMS 6.1 are acceptable, therefore EPA concludes that BLOTCDB 1.37 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.2.5 References


5.3 BRAGFLO

This section presents the regression test results for the BRAGFLO Version 4.10 code. BRAGFLO is a program used to study two-phase (brine and gas), three-dimensional isothermal flow in porous media. It has been developed specifically for use in assessing the performance of the WIPP, particularly the flow behavior in the immediate vicinity of the repository. The physical model is described by material balance equations for brine and gas, Darcy’s law, and two phase fluid properties. The numerical model includes a cell-centered finite difference discretization, Newton solution of the nonlinear constitutive equations, and linear equation solvers necessary for the Newton iteration. Various submodels specific to WIPP include a pressure-induced fracture treatment, creep closure of the repository, and gas generation resulting from corrosion and biodegradation of waste components.

5.3.1 Introduction

Since the CCA PA, the BRAGFLO code has undergone a series of revisions. Versions 4.00 and 4.01 of BRAGFLO were used in the WIPP CCA. BRAGFLO 4.00 was used to calculate Salado flow; BRAGFLO 4.01 was used to calculate direct brine releases. These codes were validated on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of each test case met the
acceptance criteria defined in the RD/VVPs [3, 4, 5, 6].

BRAGFLO 4.10 was created to combine the capabilities of both BRAGFLO 4.00 and BRAGFLO 4.01 into a single code version. No new functionality was added [1]. BRAGFLO 4.10 was validated on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of each test case met the acceptance criteria defined in the RD/VVP [3].

DOE ran the OpenVMS 7.3-1 tests using the FORTRAN 7.3 Run-Time Library (RTL) instead of the current version of the RTL, version 7.4A. The date and time functions in the RTL changed between version 7.3 and 7.4A, and BRAGFLO 4.10 does not run with the new date and time functions. Accordingly, BRAGFLO 4.10 is run using the FORTRAN 7.3 RTL by implementing the procedure described in [7].

BRAGFLO 4.10 has one open problem report [8]. BRAGFLO 4.10 uses an outdated list-directed I/O format that allows space-padded fields. Many of the input files for the BRAGFLO 4.10 test cases were generated by PREBRAG 6.00 and include space-padded fields. To allow BRAGFLO 4.10 to read these input files, each input file is modified by a conversion script, EVAL_BF2_CONVERT_INPUT.COM, to remove extraneous spaces from the input file. The test input files for this analysis required the use of this conversion script.

5.3.2 Test Methodology
The tests for this code comprised all twelve test cases described in the Requirements Document & Verification and Validation Plan for BRAGFLO Version 4.10 (RD/VVP) [1]. Regression test results from BRAGFLO 4.10 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of BRAGFLO 4.10 run on a DEC Alpha 2100 with OpenVMS 6.1 [2].

The regression test methodology uses the VMS DIFFERENCE command to compare output from BRAGFLO 4.10 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of BRAGFLO 4.10. For Test Cases 6 and 7, the number of numerical differences requires additional analysis techniques to determine if the differences are acceptable. Test Case 7 also required the use of three other WIPP PA codes: POSTBRAG 4.00, SUMMARIZE 2.20, and SPLAT 1.02. These three codes have been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Sections 5.17, 5.27, and 5.25 for POSTBRAG, SUMMARIZE and SPLAT, respectively). The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.
The validation test for test Case 6 compared BRAGFLO output with Excel spreadsheet calculations of appropriate variables for each of the functions listed in the Requirements Document & Verification and Validation Plan for BRAGFLO, Version 4.10 (RD/VVP) [1,12]. The acceptance criteria for Test Case #6 were independent calculations and manual inspection of the output to verify that BRAGFLO is performing the calculations correctly. DOE performed the independent calculations by using values of pressures and saturations reported in BRAGFLO output files.

5.3.3 Test Results

The twelve test cases for BRAGFLO 4.10 were executed on the Compaq ES40 with OpenVMS 7.3-1. Each test case generated output files, which were compared to the output files from the BRAGFLO 4.10 validation tests, executed on a DEC Alpha 2100 with OpenVMS 6.1. For all but Test Case 7, DOE used the DIFFERENCE command to compare output files. For Test Case 7, DOE used plots to compare output. Test Cases 2, 3, 8 and 9 produced output that was numerically identical to the output of the validation tests. Test Cases 1, 4, 5, 6, 7, 10, 11 and 12 showed differences in numerical output. DOE concluded that all other differences in output are acceptable; namely, that the differences are limited to code run date and time, file and platform names. EPA also found that all other differences in output are acceptable; namely, that the differences are limited to code run date and time, file and platform names.

Where the numerical output was different from the results of the validation tests, DOE determined if the VMS 7.3-1 output met the acceptance criteria specified in the BRAGFLO 4.10 RD/VVP [1]. For most test cases, the RD/VVP requires comparison of BRAGFLO results to hand calculations, values from other software, or the results of physical tests to validate BRAGFLO calculation methods. The acceptance criteria specify either agreement to within 10% of the comparative solution, or reasonable agreement, which relies on the expert opinion of the code sponsor. DOE applied the same standards to the numerical output that differed between BRAGFLO run on the Compaq ES40 with OpenVMS 7.3-1 and the validation tests of BRAGFLO 4.10. With the exception of Test Case 6, DOE concluded that all output that was different still met the acceptance criteria. EPA also found that all output (with the exception of Test Case 6) that was different still met the acceptance criteria.

For Test Case 6, the number of differences in the output will required a separate analysis (see Section 5.3.2) to determine if the OpenVMS 7.3-1 output meets the acceptance criteria for that test case. DOE concluded that the validation test demonstrated that BRAGFLO 4.10 met these criteria. Following the completion of that separate analysis, DOE concluded that BRAGFLO 4.10 satisfies the validation criteria in the BRAGFLO 4.10 RD/VVP [1], when run with OpenVMS.
7.3-1. EPA also found that BRAGFLO 4.10 satisfies the validation criteria in the RD/VVP [3], when run with OpenVMS 7.3-1.

5.3.4 EPA’s Conclusions
Since all differences are acceptable, EPA concludes that BRAGFLO 4.10 meets the acceptance criteria specified in the VVP [1], and thus is validated on the Compaq ES40 with OpenVMS 7.3-1.

5.3.5 References


5.4 CCDFGF

This section presents the regression test results for the CCDFGF Version 3.01 code. The CCDFGF code assembles the results calculated by the other codes in the WIPP PA system to produce cumulative complementary distribution functions (CCDFs) of releases. Since the Compliance Certification Application (CCA) PA, the CCDFGF code has undergone a series of revisions. CCDFGF 1.01 was used in the WIPP CCA. Version 1.01 was validated on a DEC Alpha 2100 running OpenVMS 6.1 [3]. The validation demonstrated that the results of the four test cases met the acceptance criteria defined in the VVP for Version 1.01 [4].

5.4.1 Introduction

In 1996, CCDFGF was revised to Version 2.01 to improve and clarify the algorithm by which releases to the Culebra were calculated. CCDFGF 2.01 was validated on a DEC Alpha 2100 running OpenVMS 6.1 [5]. Test Cases 1-4, for the validation of CCDFGF 2.01, were identical to the test cases for the validation of CCDFGF 1.01 [6]. The acceptance criteria for these test cases were satisfied by showing that the output from CCDFGF 2.01 was identical to the output of the CCDFGF 1.01 validation tests.

In 1997, CCDFGF was revised to Version 3.00 to correct an error found in Version 2.01 and to add functionality required for the Performance Assessment Verification Test (PAVT). CCDFGF 3.00 was validated on a DEC Alpha 2100 running OpenVMS 6.1 [7]. Test Cases 1-4, for the validation of CCDFGF 3.00, were not identical to the test cases for the validation of CCDFGF 2.01 [6]. Rather, the test cases for CCDFGF 3.00 were modifications of those used for CCDFGF 2.01. The modified test cases examined the features added to CCDFGF for Version 3.00 and specified additional acceptance criteria for these features. The validation of CCDFGF 3.00 demonstrated by DOE’s analysis that the additional acceptance criteria were met. Consequently, the validation of CCDFGF 3.00 relies the combination of the validation of CCDFGF 2.01 and on the extensions to the test cases for CCDFGF 3.00.

CCDFGF was revised again in 1997 to Version 3.01, to add the capability of producing intermediate results for releases to and from the Culebra. Test Case 5 was added to validate this additional capability [2]. Since the revision consisted only of code to consolidate existing output

23
of CCDFGF, and previous testing had validated that existing output, the validation of CCDFGF 3.01 only examined Test Case 5 [8]. Consequently, the validation of CCDFGF 3.01 relies on the combination of the validation of CCDFGF 2.01, the extensions to the test cases for CCDFGF 3.00, and the additional test case for CCDFGF 3.01.

5.4.2 Test Methodology

The tests for this code comprised the test cases described in the Verification and Validation Plan for CCDFGF Version 3.00 (VVP) [1], and the additional test case for CCDFGF Version 3.01 in the addendum to the VVP [2]. Regression test results from CCDFGF 3.01 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CCDFGF 3.00 and 3.01 run on a DEC Alpha 2100 with OpenVMS 6.1. EPA’s review for CCDFGF also involved downloading and comparing the relevant files from SNL’s computers.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CCDFGF 3.01 on the Compaq ES40 running OpenVMS 7.3-1 to the output from previous validation tests. Because the validation of CCDFGF 3.01 was an extension of the validation of CCDFGF 2.01, the previous validation tests include the validation of CCDFGF 2.01 and CCDFGF 3.00, which were both validated on a DEC Alpha 2100 with OpenVMS 6.1.

For Test Cases 1 through 4, CCDFGF 3.01 results from the Compaq ES40 running OpenVMS 7.3-1 were compared to the validation test results for CCDFGF 3.00 running on a DEC Alpha 2100 with OpenVMS 6.1; for Test Case 5, CCDFGF 3.01 results from the Compaq ES40 running OpenVMS 7.3-1 were compared to the validation test results for CCDFGF 3.01 running on a DEC Alpha 2100 with OpenVMS 6.1. The VMS DIFFERENCE command compares two files and identifies records that are different between the two files.

5.4.3 Test Results

The five test cases for CCDFGF 3.01 were executed on the Compaq ES40 running OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of the appropriate version of CCDFGF by using the DIFFERENCE command. The output from the CCDFGF code is almost entirely numerical data. None of the output files contain code run dates or times, file or directory names, user names, platform names or system version numbers. Hence the comparison of output files found only differences in numerical output. The comparison found differences in the output of Test Cases 2, 3 and 5. The numeric differences in the output of Test Cases 2 and 5 resulted from a change to the FORTRAN FORMAT statement and were determined by EPA to be acceptable. The differences in the output of Test Case 3
resulted from the changes made between CCDFGF 3.00 and CCDFGF 3.01, and were also
determined by EPA to be acceptable.

5.4.4 EPA’s Conclusions
Since all differences are acceptable, EPA concludes that CCDFGF 3.01 meets the acceptance
criteria specified in the VVP [1, 2], and thus is validated on the Compaq ES40 with OpenVMS
7.3-1. EPA also strongly recommends as a process improvement that the DOE continue to test
CCDFGF by individually checking the contribution from each computer code that contributes to
the CCDFGF.

5.4.5 References

   CCDFGF Version 3.00”. Sandia National Laboratories. Sandia WIPP Central Files WPO
   # 45412.

   Plan for CCDFGF Version 3.01”. Sandia National Laboratories. Sandia WIPP Central
   Files WPO # 45412.

   1.01”. Sandia National Laboratories. Sandia WIPP Central Files WPO # 42042.

   CCDFGF Version 1.01”. Sandia National Laboratories. Sandia WIPP Central Files WPO
   # 42043.

   2.01”. Sandia National Laboratories. Sandia WIPP Central Files WPO # 42772.

   CCDFGF Version 2.01”. Sandia National Laboratories. Sandia WIPP Central Files WPO
5.5 CCDFSUM

This section presents the regression test results for the CCDFSUM Version 2.00 code. The CCDFSUM code plots the cumulative complementary distribution functions (CCDFs) for the releases calculated by the code CCDFGF.

5.5.1 Introduction

Since the Compliance Certification Application (CCA) PA, the CCDFSUM code has undergone a series of revisions. CCDFSUM 1.01 was used in the WIPP CCA. Version 1.01 was validated on a DEC Alpha 2100 running OpenVMS 6.1 under the requirements of QAP 9-1 (now NP 9-1) [2]. In 1996, CCDFSUM was revised to Version 2.00 to accommodate changes made in CCDFGF 3.00. CCDFSUM 2.00 was validated on a DEC Alpha 2100 running OpenVMS 6.1 [3].

5.5.2 Test Methodology

The tests for this code comprised the test cases described in the Verification and Validation Plan for CCDFSUM Version 2.00 (VVP) [1]. Regression test results from CCDFSUM 2.00 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CCDFSUM 2.00 run on a DEC Alpha 2100 with OpenVMS 6.1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CCDFSUM 2.00 on the Compaq ES40 running OpenVMS 7.3-1 to the output from previous validation tests. The VMS DIFFERENCE command compares two files and identifies records that are different between the two files.

5.5.3 Test Results

The VVP for CCDFSUM 2.00 lists a total of nine test cases, however, CCDFSUM is run only in the first test case. The other eight test cases specify comparison of the output of the first test case with different criteria. These test cases do not exercise any function of the code. For this regression test, DOE believes (and EPA agrees) that it is sufficient to run only the first test case and compare its output with the output of the previous validation test.

The first test case was executed on the Compaq ES40 with OpenVMS 7.3-1. The output files were compared to the corresponding output files from the validation of CCDFSUM 2.00 by using the DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run dates and times. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run dates
and time.

5.5.4 EPA’s Conclusions
EPA has found that all differences in output are acceptable; namely, that the differences are limited to code run dates and times. The comparison found no differences in the numerical output of CCDFSUM 2.00. EPA concludes that CCDFSUM 2.00 meets the acceptance criteria in the VVP and is validated for WIPP PA use on the ES40 with OpenVMS 7.3-1.

5.5.5 References


5.6 CUTTINGS_S
This section presents the regression test results for the CUTTINGS_S Version 5.04A code. The CUTTINGS_S (CUSP) code was written to calculate the quantity of radioactive material (in Curies) brought to the surface from a radioactive waste disposal repository as a consequence of an inadvertent human intrusion through drilling. The code determines the amount of material removed from the repository by several release mechanisms, and decays the material to the time of intrusion.

5.6.1 Introduction
Since the Compliance Certification Application (CCA) PA, the CUTTINGS_S code has undergone a series of revisions. CUTTINGS_S 5.03 was used in the WIPP CCA. Version 5.03 was validated in May 1996 on a DEC Alpha 2100 with OpenVMS 6.1. The validation was accomplished by demonstrating the results of the six test cases met the acceptance criteria defined in the RD/VVP [4].

In July 1997 CUTTINGS_S was revised to Version 5.04 and was validated on a DEC Alpha 2100 with OpenVMS 6.1. Test Cases 1-6 for the validation of CUTTINGS_S 5.04 were identical
to test cases for the validation of CUTTINGS_S 5.03. The acceptance criteria for these test cases were satisfied by showing that the output from CUTTINGSS_S 5.04 was identical to the output of the CUTTINGS_S 5.03 validation tests. New Test Cases 7-9 were validated by demonstrating the output of Test Cases 7–9 met the acceptance criteria defined in the RD/VVP for CUTTINGS 5.04 [3].

In January 2001, CUTTINGS_S was revised to 5.04A to remove references to unused libraries. Although, SDBREAD_LIB and the INGRES library, are not used in PA calculations, CUTTINGS_S 5.04 checks for their availability and will not run if they are absent. Since these libraries are no longer present on the system, it was necessary to eliminate the linkages. The following quotation from the change control form explains the revisions:

“CUTTINGS_S Version 5.04 was mistakenly linked with SDBREAD_LIB and an INGRES library. Although SDBREAD_LIB and the INGRES library are not used, the INGRES system must be installed on the system for Version 5.04 to run. The linked software is no longer available on the system, so CUTTINGS_S will be relinked to remove these libraries.

There are no source changes between CUTTINGS_S Version 5.04A and Version 5.04. The only difference is that CUTTINGS_S Version 5.04A will not be linked with SDBREAD_LIB and the INGRES library. The code will now be linked with the standard libraries CAMDAT_LIB, CAMCON_LIB, and CAMSUPES_LIB. (The library .OLB files that were used for Version 5.04 will not be used for Version 5.04A.” [5]

5.6.2 Test Methodology
The tests for this code comprised the nine test cases described in the Requirements Document & Verification and Validation Plan for CUTTINGS_S Version 5.04 [RD/VVP] [3]. Regression test results from CUTTINGS_S 5.04A run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CUTTINGS_S 5.04A run on a DEC Alpha 2100 with OpenVMS 7.2-1.

Since DOE did not regression test CUTTINGS_S 504A on the ES40 with OpenVMS 7.3-1 directly to the validation tests of CUTTINGS_S 5.04A run on a DEC Alpha 2100 with OpenVMS 6.1, it was necessary for EPA to further review the results of DOE’s earlier migration tests[1,2]. EPA’s review for CUTTING_S also involved downloading and comparing the relevant files from SNL’s computers. That review indicated that there were no numerical or
other significant differences between CUTTINGS_S 5.04A run on a DEC Alpha 2100 with OpenVMS 7.2-1 and CUTTINGS_S 5.04 run with OpenVMS 6.1 on the same hardware. EPA therefore concludes, that DOE’s approach is acceptable (in which regression test results from CUTTINGS_S 5.04A run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CUTTINGS_S 5.04A run on a DEC Alpha 2100 with OpenVMS 7.2-1).

CAMDAT database files (CDB) are produced in the first eight CUTTINGS_S 5.04A test cases. The output CDB files are converted from a binary, CDB file to an ASCII, using the code GROPE output file for comparison during the validation process. In the previous CUTTINGS_S 5.04A validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [7]. Following the same process described in Section 5.10, GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 [part of DOE’s regression testing program]. For DOE’s regression test of CUTTINGS_S 5.04A, GROPE 2.12 was used to convert the CDB output files from CUTTINGS_S 5.04A in OpenVMS 7.3-1, as well as CUTTINGS_S 5.04A in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

5.6.3 Test Results
The nine test cases for CUTTINGS_S 5.04A were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared by DOE to the corresponding output files from the validation of CUTTINGS_S 5.04A on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics.

5.6.4 EPA’s Conclusions
There were no numerical differences between CUTTINGS_S 5.04A run on a DEC Alpha 2100 with OpenVMS 7.2-1 and CUTTINGS_S 5.04 run with OpenVMS 6.1 on the same hardware. Since all differences between the results of CUTTINGS_S 5.04A, in OpenVMS 7.3-1 and OpenVMS 6.1, are acceptable, EPA concludes that CUTTINGS_S 5.04A meets the acceptance criteria specified in the RD/VVP [3], and thus is validated on the Compaq ES40 with OpenVMS 7.3-1.4.
5.6.5 References


5.7 EPAUNI

This section presents the regression test results for the EPAUNI Version 1.14 code. EPAUNI calculates the number of Environmental Protection Agency (EPA) units per unit volume and associated volumetric weighting for each contact-handled (CH) transuranic (TRU) waste stream. EPAUNI is also used to calculate the WIPP scale average EPA units per unit volume for remotely handled (RH) TRU waste streams destined for disposal at the WIPP facility. EPA units are calculated only for the key radionuclides that are responsible for 99% of the activity in the waste. The dominant radionuclides in the CH waste are Am241, Pu238, Pu239, Pu240, and U234. Two parent radionuclides (Pu241 and Cm244), which produce Am241 and Pu240, respectively, are also accounted for in the CH waste calculations. The calculations for RH waste include three additional radionuclides: Cs137, Sr90 and U233.

5.7.1 Introduction

EPAUNI 1.14 was used in the WIPP CCA PA. The code was validated in June 1997 on a DEC Alpha 2100 with OpenVMS 6.1. Validation of Version 1.14 was accomplished by demonstrating
that the results of five test cases met the acceptance criteria defined in the VVP for EPAUNI 1.14 [1].

5.7.2 Test Methodology
The tests for this code comprise the five test cases described in the *Verification and Validation Plan* for EPAUNI Version 1.14 (VVP) [1]. Regression test results from EPAUNI 1.14 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of EPAUNI 1.14 run on a DEC Alpha 2100 with OpenVMS 6.1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from EPAUNI 1.14 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of EPAUNI 1.14. The VMS DIFFERENCE command compares the two files and identifies records that are different in the two files.

5.7.3 Test Results
The five test cases for EPAUNI 1.14 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared by DOE to the corresponding output files from the validation of EPAUNI 1.14 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE’s comparison found no differences in the output files. EPA also found that there were no differences in the output files.

5.7.4 EPA’s Conclusions
Since there are no differences between the results of EPAUNI 1.14, in OpenVMS 7.3-1, and EPAUNI 1.14, in OpenVMS 6.1, EPA concludes that EPAUNI 1.14 meets the acceptance criteria specified in the VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.7.5 References

5.8  FMT

This section presents the regression test results for the FMT Version 2.40 code. FMT 2.40 calculates the chemical equilibrium in high-inoic-strength geochemical systems at 25 °C. FMT 2.40 also predicts solubility behavior of Am(III), Th(IV) and Np(V) in brines such as those found in Castile, Rustler, and Salado Formations near the WIPP. The executable used in the test is FMT 2.00 was validated in November 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of nine test cases met the acceptance criteria defined in the RD/VVP for FMT 2.00 [3,4].

5.8.1  Introduction

In August 1996, FMT was revised to Version 2.10 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [5]. Test cases identical to the nine test cases for the validation of FMT 2.00 were run. The acceptance criteria for these test cases were satisfied through regression testing that the output from FMT 2.10 was identical to the output of the FMT 2.00 validation tests.

In September 1996, FMT was revised to Version 2.20 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [6]. It was determined at that time that the only test cases needed for validation were Test Cases 1, 2, 6 and 7. Test cases identical to these four test cases for the validation of FMT 2.10 were run. The acceptance criteria for these test cases were satisfied through regression testing which found that the output from FMT 2.20 was identical to the output of the FMT 2.10 validation tests. Test Case 1 also underwent some additional evaluation to ensure it met the acceptance criteria defined in the RD/VVP for FMT 2.20 [7].

In January 1997, FMT was revised to Version 2.30 and was validated on a DEC Alpha 2100 with OpenVMS 7.1 [8]. The four test cases previously identified (Test Cases 1, 2, 6 and 7) were re-named as Test Cases 1 through 4 and three additional test cases (labeled as Test Cases 5, 6 and 7) were generated. Test Cases 1 through 4, identical to the four test cases for the validation of FMT 2.20 were run. The acceptance criteria for Test Cases 1 through 4 were satisfied through regression testing. The regression testing found the output from FMT 2.30 was identical to the output of the FMT 2.20 validation tests. Test Cases 5, 6 and 7 were validated by demonstrating the results of the three test cases met the acceptance criteria defined in the RD/VVP for FMT 2.30 [9].

In October 1998, FMT was revised to Version 2.40 and was validated on a DEC Alpha 2100 with OpenVMS 7.2 [2]. In addition to the seven test cases from the previous validation, one additional test case was added (Test Case 8). The code was validated by demonstrating the output of the
eight FMT 2.40 test cases met the acceptance criteria defined in the RD/VVP for FMT 2.40 [1].

5.8.2 Test Methodology

The tests for this code comprised the eight test cases described in the Requirements Document & Verification and Validation Plan for FMT Version 2.40 RD/VVP [1]. Regression test results from FMT 2.40, run on the ES40 with OpenVMS 7.3-1, were compared to results from the validation tests of FMT 2.40, run on a DEC Alpha 2100 with OpenVMS 6.1 [2]. EPA’s review for FMT also involved downloading and comparing the relevant files from SNL’s computers.

The regression test methodology uses the VMS DIFFERENCE command to compare output from FMT 2.40 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the previous validation of FMT 2.40. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.8.3 Test Results

The eight test cases for FMT 2.40 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the eight cases were compared by DOE to the corresponding output files from the validation of FMT 2.40 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to file and directory names. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics.

5.8.4 EPA’s Conclusions

Since all differences between the results of FMT 2.40, in OpenVMS 7.3-1, and FMT 2.40, in OpenVMS 6.1, are acceptable, EPA concludes that FMT 2.40 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS Version 7.3-1.

5.8.5 References


5.9 GENMESH

This section presents the regression test results for the GENMESH version 6.08 code. GENMESH 6.08 constructs a right-hand, Cartesian, rectangular finite-difference grid in one, two, or three dimensions as defined by a user input file. In addition to establishing mesh connectivity and node coordinates, the program also sets material regions, geometry flags for node or element boundary conditions, and element attributes associated with the cell size. In WIPP PA application, GENMESH is the first module run for setting up a computational model. GENMESH is used to establish the computational grid or mesh containing nodes, elements, and material regioning information. The output from GENMESH is the preliminary CAMDAT or "CDB" binary file. These CAMDAT files are the essence of the WIPP PA system, because all PA codes read and write to and from these CAMDAT files.

5.9.1 Introduction

GENMESH version 6.07ZO was validated in August 1995 on a DEC Alpha 2100 with
OpenVMS 6.1 by demonstrating that the results of nine test cases met the acceptance criteria defined in the RD/VVP for GENMESH 6.07ZO [2]. In January 1996, GENMESH was revised to Version 6.08 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [3,4]. Test cases identical to the test cases for the validation of GENMESH 6.07ZO were run. The acceptance criteria for these test cases were satisfied by showing that the output from GENMESH 6.08 was identical to the output of the GENMESH 6.07ZO validation tests. GENMESH 6.08 was used in the WIPP Compliance Certification Application (CCA).

5.9.2 Test Methodology

The tests for this code comprised the nine test cases described in the Requirements Document & Verification and Validation Plan for GENMESH Version 6.08 (RD/VVP) [1]. Regression test results from GENMESH 6.08, run on the ES40 with OpenVMS 7.3-1, were compared to results from the validation tests of GENMESH 6.08, run on a DEC Alpha 2100 with OpenVMS 6.1.

CAMDAT database files (CDB) are produced in each of the nine GENMESH test cases. The output CDB files are converted from a binary, CDB, file to an ASCII output file for comparison during the validation process. In the previous GENMESH 6.08 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [5]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the OpenVMS 7.3-1 Regression Test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from GENMESH 6.08 in OpenVMS 7.3-1, as well as GENMESH 6.08 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

During the validation of GENMESH 6.07ZO plots were generated for Test Cases 2-9 utilizing BLOTCDB 1.37. BLOTCDB 1.37 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the OpenVMS 7.3-1 Regression Test (see Section 5.2). The same CDB files used by BLOTCDB to generate plots were also converted to ASCII files utilizing GROPECDB (see above). Both the plots and the ASCII files were compared by DOE to the GENMESH input file as part of the validation of GENMESH 6.07ZO. Since both GROPECDB and BLOTCDB utilize the same input file and are compared to the same file for validation, for the purpose of the OpenVMS 7.3-1 Regression Test, DOE only compare the “GROPE” output files. This approach is considered acceptable by EPA.

5.9.3 Test Results

The nine test cases for GENMESH 6.08 were executed on the Compaq ES40 with OpenVMS
7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of GENMESH 6.08 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, directory and file names. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, directory and file names.

5.9.4 EPA’s Conclusions
Since all differences between the results of GENMESH 6.08, in OpenVMS 7.3-1, and GENMESH 6.08, in OpenVMS 6.1, are acceptable, EPA concludes that GENMESH 6.08 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.9.5 References


5.10 GROPECDB
This section presents the regression test results for the GROPECDB Version 2.12 code.
GROPECDB 2.12 allows a user to interactively look at the contents of an input CAMDAT Database (CDB) file. The user enters the commands either interactively from the keyboard or from an input command file. The outputs can either go to the screen or to a specified
file. GROPECDB 2.10 was used to convert binary CAMDAT database files to ASCII as part of the validation process for several WIPP PA codes at the time of the Compliance Certification Application (CCA).

5.10.1 Introduction
GROPECDB 2.12 was validated in June 1996, running on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of seven test cases met the acceptance criteria defined in the RD/VVP for GROPECDB 2.12. [1,2]. The code has not been revised since this validation.
In July 1997 a comparison of GROPECDB 2.10 output results to GROPECDB 2.12 (validated in June 1996) output results was performed [3]. DOE's evaluation concluded that the results were the same, with the exception of run time information (run date, directory names, file version numbers, and history comments).

5.10.2 Test Methodology
The tests for this code comprised the eight test cases described in the Requirements Document & Verification and Validation Plan for GROPECDB Version 2.12 (RD/VVP) [1]. Regression test results from GROPECDB 2.12 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of GROPECDB 2.12 run on a DEC Alpha 2100 with OpenVMS 6.1.
The regression test methodology uses the VMS DIFFERENCE command to compare output from GROPECDB 2.12 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of GROPECDB 2.12 running on a DEC Alpha 2100 with OpenVMS 6.1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.10.3 Test Results
The seven test cases for GROPECDB 2.12 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of GROPECDB 2.12 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names, platform names, system version numbers, and execution statistics. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names, platform names, system version numbers, and execution statistics.

5.10.4 EPA's Conclusions
Since all differences between the results of GROPECDB 2.12 in OpenVMS 7.3-1, and GROPECDB 2.12 in OpenVMS 6.1 were acceptable, EPA concludes that GROPECDB 2.12 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.10.5 References

5.11 ICSET
This section presents the regression test results for the ICSET Version 2.22 code. ICSET is a program that sets initial conditions in a Performance Assessment Computational Data Base (CDB) file in 1-D, 2-D, or 3-D. The ICSET array variables are, history, global, nodal, and element variable values, at the first time step (NSTEP=1) in a .CDB file. Both analysis array names and values are obtained from a user input file. In addition, any nodal or element variable (existing or new), can be linearly interpolated by specifying interpolation tables in the ICSET input text file.

5.11.1 Introduction
ICSET 2.21ZO, running on the OpenVMS 6.1 operating system, was validated in September 1995 [2]. The code has not been revised since this validation, but in 1996, a Change Control Form [3] was approved, revising the software version from 2.21 to 2.22 when new libraries were linked. ICSET 2.22 remains the current version of this software module.

5.11.2 Test Methodology
The tests for this code comprised the six test cases described in the Requirements Document & Verification and Validation Plan for ICSET Version 2.21ZO (RD/VVP) [2]. Regression test results from ICSET 2.22 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of ICSET Version 2.21ZO run on a DEC Alpha 2100 with OpenVMS 6.1.

CAMDAT database files (CDB) are produced in each of the six ICSET test cases. The output
CDB files are converted from a binary, CDB, file to an ASCII file for comparison during the validation process. In the previous ICSET 2.22 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from RELATE 1.43 in OpenVMS 7.3-1, as well as ICSET 2.22 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

5.11.3 Test Results
The six cases for ICSET 2.22 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of ICSET 2.21ZO running Alpha 2100 with OpenVMS 6.1 by using the DIFFERENCE command. The DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, and file names. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, and file names.

5.11.4 EPA’s Conclusions
Since all differences between the results of ICSET in OpenVMS 7.3-1 and OpenVMS 6.1, are acceptable, EPA concludes that ICSET 2.22 meets the acceptance criteria specified in the RD/VVP [1], and thus is validated on the Compaq ES40 with OpenVMS 7.3-1.

5.11.5 References


5.12 LHS

This section presents the regression test results for the LHS Version 2.41 code. The LHS program samples distributions of input parameters using either normal Monte Carlo sampling or efficient Latin Hypercube Sampling. LHS permits correlations (restricted pairings) between parameters. Latin Hypercube sampling reduces the minimum number of sample vectors [sv] required to about 4/3 * na, where na is the number of varying parameters. Only Latin Hypercube Sampling is used for WIPP PA.

5.12.1 Introduction

LHS Version 2.32ZO was validated in August 1996 on a DEC Alpha 2100 with OpenVMS 6.1 using ten test cases by demonstrating that the results of each test case met the acceptance criteria defined in the RD/VVP for LHS 2.32ZO [2,3].

In March 1996, LHS was revised to Version 2.41 and was validated on a DEC Alpha 2100 with OpenVMS 6.1. Test cases identical to the test cases for the validation of LHS 2.32ZO were run. The acceptance criteria for these test cases were satisfied by showing that the output from LHS 2.41 was identical to the output of the LHS 2.32ZO validation tests [1,4]. LHS 2.41 was used in the WIPP Compliance Certification Application (CCA).

5.12.2 Test Methodology

The tests for this code comprised the ten test cases described in the Requirements Document & Verification and Validation Plan for LHS Version 2.41 (RD/VVP) [1]. Regression test results from LHS 2.41 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of LHS 2.41 run on a DEC Alpha 2100 with OpenVMS 6.1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from LHS 2.41 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the previous validation of LHS 2.41. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.12.3 Test Results

The ten test cases for LHS 2.41 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of LHS 2.41 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. Test Case 1 shows a difference in the sampled value of one variable, but this difference is insignificant (see section 4.1). No other differences were found. DOE
concluded that all numerical differences were acceptable in the output of LHS 2.41. EPA also found that all the differences were acceptable in the output.

5.12.4 EPA's Conclusions
Since all differences between the results of LHS 2.41 in OpenVMS 7.3-1 and LHS 2.41 in OpenVMS 6.1 are acceptable, EPA concludes that LHS 2.41 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.12.5 References


* Note – Discrepancies exist within the Software Quality Assurance (SQA) package for LHS Version 2.41 documentation. Many of the documents incorrectly identify the current code as Version 2.40, as stated in the memo entitled “Correct Version Number for LHS” WPO # 38837. This discrepancy has been previously identified and documented and will be corrected during the next revision to the code documentation.

5.13 MATSET
This section presents the regression test results for the MATSET version 9.10 code. In WIPP PA applications, MATSET is executed after mesh generation (e.g., after running GENMESH). MATSET is used to set material property and attribute values used in the computational model. Property and attribute values are obtained from either the Performance Assessment Parameter
Database or directly from the MATSET input control file. The output from MATSET is written to a CAMDAT binary file.

5.13.1 Introduction
Since the Compliance Certification Application (CCA) the MATSET code has undergone a series of revisions. MATSET 9.0 was used in the WIPP CCA. MATSET 9.0 was validated in February 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of ten test cases met the acceptance criteria defined in the RD/VVP for MATSET 9.0. [2, 3]

In November, 2001 MATSET was revised to Version 9.10 and was validated on a DEC Alpha 2100 with OpenVMS 7.2-1 [1]. MATSET 9.10 accesses the new procedure-based Performance Assessment Parameter Database (PAPDB). It cannot read the databases accessed by previous versions of MATSET. Therefore, three new test cases (Test Cases 13 through 15) have been designed to verify that MATSET satisfies all of the requirements and additional functionality specified in Sections 2 and 3 of the VVP/VD [1]. Note that these test cases replace the test cases that were used to test previous versions of the code.

5.13.2 Test Methodology
The tests for this code comprised the three test cases described in the Verification and Validation Plan/Validation Document for MATSET Version 9.10 (VVP/VD) [1]. Regression test results from MATSET 9.10 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of MATSET 9.10 run on a DEC Alpha 2100 with OpenVMS 6.1.

CAMDAT database files (CDB) are produced in MATSET Test Cases 13 and 14. The output CDB files are converted from a binary, CDB file to an ASCII file for comparison during the validation process. In the previous MATSET 9.10 validation, the CDB files were converted using GROPE 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the OpenVMS 7.3-1 Regression Test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from MATSET 9.10 in OpenVMS 7.3-1, as well as MATSET 9.10 in OpenVMS 7.2-1, thereby eliminating the potential for differences because of different GROPE versions. The regression test methodology uses the VMS DIFFERENCE command to compare output from MATSET 9.10 on the Compaq ES40 with OpenVMS7.3-1 to the output from the previous validation of MATSET 9.10. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.13.3 Test Results
The three test cases for MATSET 9.10 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of MATSET 9.10 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers.

5.13.4 EPA's Conclusions
Since all differences between the results of MATSET 9.10, in OpenVMS 7.3-1, and MATSET 9.10 in OpenVMS 6.1 are acceptable, EPA concludes that MATSET 9.10 meets the acceptance criterion specified in the VVP/VD [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.13.5 References

5.14 NUTS
This section presents the regression test results for the NUTS Version 2.05A code. NUTS is a multidimensional, multicomponent radioactive material contaminant transport, single-porosity (SP), dual-porosity (DP), and dual-permeability (DPM) finite-difference simulator. The model simulates first order radioactive chain decay during radioactive material transport. However, the simulator is not limited to radioactive material transport, and any non-radioactive material can be included. Three types of sorption isotherms are considered to represent ion exchange between the solute and the surrounding formation; linear, Freundlich, and Langmuir equilibrium isotherms. Hydrodynamic dispersion is modeled with the assumption that the off diagonal dispersivities are
all zero. The solubility limits of the waste components, and their precipitation during migration are included in NUTS. The precipitate is allowed to undergo decay, and to redissolve in the brine if the concentration drops below the solubility limit. Multi-radioactive-site representations are also possible, in which case the contribution from each site to the component concentration and precipitation in each computational node can be found. A similar technique is used to handle the daughters generated from the decay of different parents. Many options for transport equation(s) discretization are included. In the implicit solution, the system of partial differential equations is solved sequentially to determine the contribution from parent radioactive material decay to the immediate daughter. In the sequential method, the solution proceeds progressively from the top of each radioactive material chain. Therefore, the contribution to any daughter from parent decay will be available. In addition, NUTS also accounts for thermal dependency of some properties.

5.14.1 Introduction
For the WIPP PA, the DOE intends to use NUTS for isothermal transport in the rock matrix. Consequently, the validation test demonstrated a subset of the capabilities of the NUTS code. For further details on NUTS features used in the Compliance Certification Application (CCA) calculations, refer to Table 1 in NUTS User’s Manual, Version 2.02. [5].

Since the CCA the NUTS code has undergone a series of revisions. NUTS Version 2.02 was used in the WIPP CCA. During the CCA, an error was found in NUTS 2.02; correction of this error resulted in NUTS Version 2.03 [6]. NUTS Version 2.05 was developed from NUTS 2.03 by adding the capability to calculate solubility limits with an implicit precipitation model [7]. NUTS Version 2.05A was developed from NUTS 2.05 to enable NUTS to run in OpenVMS 7.1 and subsequent operating systems [8]. NUTS 2.05A differs from NUTS 2.05 only in one subroutine that writes information records to the headers of output files [8]. Consequently, the RD/VVP for NUTS 2.05 [3] and the Validation Document (with addendum) for NUTS 2.05 [9, 10] are used for NUTS 2.05A.

The validation of NUTS 2.05A in Open VMS 7.2-1 was established by a sequence of regression tests. The results of the sequence of regression tests, from NUTS 2.02 in OpenVMS 6.1 to NUTS 2.05A in OpenVMS 7.2-1 are detailed in Annex A[1].

AP-089 [9], the planning document for this regression testing incorrectly identified SPR 99-001 [10] as an active problem report relating to NUTS 2.05A.

5.14.2 Test Methodology
The tests for this code comprised all test cases described in the *Requirements Document & Verification and Validation Plan for NUTS Version 2.05 RD/VVP*) [3]. Regression test results from NUTS 2.05A executed on the ES40 running OpenVMS 7.3-1 were compared to results from the installation and checkout tests of NUTS 2.05A executed on a DEC Alpha 2100 running OpenVMS 7.2, which served as the validation of NUTS 2.05A [4].

Since DOE did not regression test NUTS Version 2.05 run on the ES40 with OpenVMS 7.3-1 directly to the validation tests of NUTS Version 2.05, run on a DEC Alpha 2100 with OpenVMS 6.1, it was necessary for EPA to further review the results of DOE’s earlier migration tests[1,2]. That review indicated that there were no significant differences between NUTS Version 2.05, run on a DEC Alpha 2100 with OpenVMS 7.2-1 and NUTS Version 2.05, run with OpenVMS 6.1 on the same hardware. EPA therefore concludes, that DOE’s comparison approach is acceptable.

The regression test methodology uses the OpenVMS DIFFERENCE command to compare output from NUTS 2.05A on the Compaq ES40 running OpenVMS 7.3-1 to the output from the validation of NUTS 2.05A on a DEC Alpha 2100 running OpenVMS 7.2-1. This methodology is applied to all test cases for NUTS 2.05A except for Test Case 5. In addition, changes in output file format for Test Case 5 required a manual comparison out NUTS numerical output. Test Case 7 also required the use of three other WIPP PA codes: POSTBRAG 4.00, SUMMARIZE 2.20, and SPLAT 1.02. These three codes have been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Sections 5.17, 5.27, and 5.25 for POSTBRAG, SUMMARIZE and SPLAT, respectively.) EPA’s review for NUTS also involved downloading and comparing the relevant files from SNL’s computers.

CAMDAT database files (CDB) are produced in several of the test cases. The output CDB files are converted from a binary, CDB, file to an ASCII file for comparison during the validation process, by utility codes ALGEBRACDB and GROPECDB. Both codes have been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Sections 5.1 and 5.10 for ALGEBRACDB and GROPECDB, respectively). The OpenVMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.14.3 Test Results

Each test case generated output files, which were compared to the output files from the NUTS 2.05A validation tests, done in OpenVMS 7.2-1. In all test cases, the OpenVMS DIFFERENCE command was used to determine differences in text output. In addition, Test Case 5 produced CDB files, which were compared using ALGEBRACDB 2.35 and SUMMARIZE 2.20, and Test
Case 12 produced CDB files that were compared using GROPECDB 2.12. These other codes have been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the OpenVMS 7.3-1 Regression Test (see Sections 5.1, 5.27 and 5.10 for ALGEBRACDB, SUMMARIZE, and GROPECDB, respectively).

DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names, platform names and system version numbers.

EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names, platform names and system version numbers.

5.14.4 EPA’s Conclusions
Since all differences between the results of NUTS 2.05A, in OpenVMS 7.3-1, and NUTS 2.05A, in OpenVMS 7.2-1, are acceptable, EPA concludes that NUTS 2.05A meets the acceptance criteria specified in the RD/VVP [3], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.14.5 References


5.15 PANEL

This section presents the regression test results for the PANEL Version 4.00 code. PANEL takes
the source term data and computes the solubilities of the elements needed. PANEL also takes
brine flow and repository volume data from a CAMDAT database (CDB) file and computes the
amount of mobilized radioisotopes that leave the repository. PANEL 3.50ZO was validated in
September 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of
two test cases met the acceptance criteria defined in the RD/VVP for PANEL 3.50ZO [4,5].

In May 1996, PANEL was revised to Version 3.60 and was validated on a DEC Alpha 2100 with
OpenVMS 6.1. Test cases identical to the two test cases for the validation of PANEL 3.50ZO
were run. The acceptance criteria for these test cases were satisfied by showing that the output
from PANEL 3.60 was identical to the output of the PANEL 3.50ZO validation tests [6,7].
PANEL 3.60 was used in the WIPP Compliance Certification Application (CCA).

5.15.1 Introduction

In June 1998, PANEL was revised to Version 4.00 and was validated on a DEC Alpha 2100 with
OpenVMS 7.1 [8]. In addition to the two test cases from the previous validation, five more test
cases were added to the RD/VVP for Version 4.00 [3]. The acceptance criteria for Test Cases 1
and 2 were satisfied by showing that the output from PANEL 4.00 was identical to the output of
the PANEL 3.60 validation tests [7]. Test Cases 3-7 were validated by demonstrating the output
from PANEL 4.00 met the acceptance criteria defined in the RD/VVP for PANEL 4.00 [3].

5.15.2 Test Methodology

The tests for this code comprised the three test cases described in the requirements Document
and Verification and Validation Plan for PANEL Version 4.00 (RD/VVP) [3]. Regression test
results from PANEL 4.00, run on the ES40 with OpenVMS 7.3-1, were compared to results from
the validation tests of PANEL 4.00, run on a DEC Alpha 2100 with OpenVMS 7.1. Since DOE
did not regression test PANEL 4.00 run on the ES40 with OpenVMS 7.3-1 directly to the
validation tests of PANEL 4.00, run on a DEC Alpha 2100 with OpenVMS 6.1, it was necessary
for EPA to further review the results of DOE’s earlier migration tests[1,2]. That review
indicated that there were no numerical or other significant differences between PANEL 4.00, run
on a DEC Alpha 2100 with OpenVMS 7.1 and PANEL 4.00, run with OpenVMS 6.1 on the
same hardware. EPA therefore concludes, that DOE’s comparison approach is acceptable.

CAMDAT database files (CDB) are produced in each of the seven PANEL test cases. The output
CDB files are converted from a binary, CDB file to an ASCII file for comparison during the
validation process. In the previous PANEL 4.00 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [9]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 regression test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from PANEL 4.00 in OpenVMS 7.3-1, as well as PANEL 4.00 in OpenVMS 7.1, thereby eliminating the potential for differences because of different GROPE versions.

The regression test methodology uses the VMS DIFFERENCE command to compare output from PANEL 4.00 on the Compaq ES40 with OpenVMS7.3-1 to the output from the previous validation of PANEL 4.00.

5.15.3 Test Results
The seven test cases for PANEL 4.00 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of PANEL 4.00 on a DEC Alpha 2100 with OpenVMS 7.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers.

5.15.4 EPA’s Conclusions
Since all differences between the results PANEL 4.00, in OpenVMS 7.3-1, and PANEL 4.00, in OpenVMS 7.1, are acceptable, EPA concludes that PANEL 4.00 meets the acceptance criteria specified in the RD/VVP [3], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.15.5 References


5.16 PCCSRC

This section presents the regression test results for the PCCSRC Version 2.21 code. The statistical code, PCCSRC, evaluates parameter importance by reporting the partial correlation coefficients (PCC) and standardized regression coefficients (SRCs) on either the raw or ranked data. The absolute values of the standardized regression coefficients (or mathematically related partial correlation coefficients) can be used to measure parameter importance.

5.16.1 Introduction

PCCSRC Version 2.21 was validated in May 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of four test cases met the acceptance criteria defined in the RD/VVP for PCCSRC Version 2.21 [1,2].

5.16.2 Test Methodology

The tests for this code comprised the three test cases described in the Requirements Document & Verification and Validation Plan for PCCSRC version 2.21 RD/VVP) [1]. Regression test results from PCCSRC 2.21 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PCCSRC 2.21 run on a DEC Alpha 2100 with OpenVMS 6.1. The regression test methodology uses the VMS DIFFERENCE command to compare output from PCCSRC 2.21 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the original validation of PCCSRC 2.21.
5.16.3 Test Results
The four test cases for PCCSRC 2.21 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the original validation of PCCSRC 2.21 on a DEC Alpha 2100 with OpenVMS 6.1 by using the DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics.

5.16.4 EPA’s Conclusions
Since all differences between the results of PCCSRC 2.21, in OpenVMS 7.3-1, and PCCSRC 2.21, in OpenVMS 6.1, are acceptable, EPA concludes that PCCSRC 2.21 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.16.5 References

5.17 POSTBRAG
This section presents the regression test results for the POSTBRAG Version 4.00 code. POSTBRAG is a utility code that takes the binary output file generated by BRAGFLO and puts it into the CAMDAT output file format.

5.17.1 Introduction
For WIPP PA, POSTBRAG is used to create CAMDAT files, which are examined with BLOTCDB and/or GROPECDB. CAMDAT database files may also be referred to as CDB files. POSTBRAG 4.00 was validated in February, 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of two test cases met the acceptance criteria defined in the RD/VVP [1] for POSTBRAG 4.00. POSTBRAG 4.00 was used in the Compliance Certification Application (CCA). The code has not been revised since this validation. Previous to this version,
POSTBRAG Version 3.05ZO had a single test case validated to the acceptance criteria defined in the RD/VVP [3, 4] for POSTBRAG 3.05ZO.

5.17.2 Test Methodology
The tests for this code comprised the two test cases described in the requirements Document & Verification and Validation Plan for POSTBRAG Version 4.00 RD/VVP) [1]. Regression test results from POSTBRAG 4.00 run on the ES40 with OpenVMS 7.3-1 were compared by DOE to results from the validation tests of POSTBRAG 4.00 run on a DEC Alpha 2100 with OpenVMS 6.1.

Output files generated by POSTBRAG 4.00 in the OpenVMS 7.3-1 test were compared by DOE to the same output files from the previous validation. The files compared were those files identified in the initial validation as necessary to determine the test case met its acceptance criteria [1]. The test results generated in the OpenVMS7.3-1 test were visually compared by DOE to the hard copy test results found in the validation document [2].

5.17.3 Test Results
The two test cases for POSTBRAG 4.00 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were visually compared by DOE to the corresponding output files from the validation of POSTBRAG 4.00 on a DEC Alpha 2100 with OpenVMS 6.1. DOE concluded that their visual comparisons of the two files showed that all differences between the two files are acceptable as only the code run date and time, platform names, system version numbers, directory and file names are different. EPA conducted independent visual comparisons of the two files and also concludes that all differences between the two files are acceptable as only the code run date and time, platform names, system version numbers, directory and file names are different.

5.17.4 EPA's Conclusions
Since all differences between the results POSTBRAG 4.00, in OpenVMS 7.3-1, and POSTBRAG 4.00, in OpenVMS 6.1, are acceptable, EPA concludes that POSTBRAG 4.00 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.17.5 References
5.18 POSTLHS

This section presents the regression test results for the POSTLHS Version 4.07 code. The statistical code, POSTLHS, evaluates parameter importance by reporting the partial correlation coefficients (PCC) and standardized regression coefficients (SRCs) on either the raw or ranked data. The absolute values of the standardized regression coefficients (or mathematically related partial correlation coefficients) can be used to measure parameter importance.

5.18.1 Introduction

POSTLHS Version 4.06ZO was validated in October 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of two test cases met the acceptance criteria defined in the RD/VVP for POSTLHS 4.06ZO [1]. In February 1996, POSTLHS was revised to Version 4.07 and was validated on a DEC Alpha 2100 with OpenVMS 6.1. Test cases identical to the test cases for the validation of POSTLHS 4.06ZO were run. The acceptance criteria for these test cases were satisfied by showing that the output from POSTLHS 4.07 was identical to the output of the POSTLHS 4.06ZO validation tests [2]. POSTLHS 4.07 was used in the WIPP Compliance Certification Application (CCA).

5.18.2 Test Methodology

The tests for this code comprised the two test cases described in the Requirements Document & Verification and Validation Plan for POSTLHS 4.06ZO RD/VVP) [1]. Regression test results
from POSTLHS 4.07, run on the ES40 with OpenVMS 7.3-1, were compared to results from the validation tests of POSTLHS 4.07, run on a DEC Alpha 2100 with OpenVMS 6.1.

CAMDAT database files (CDB) are produced in each of the two POSTLHS test cases. The output CDB files are converted from a binary CDB file to an ASCII file for comparison during the validation process. In the previous POSTLHS 4.07 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [3]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from POSTLHS 4.07 in OpenVMS 7.3-1, as well as POSTLHS 4.07 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions. The regression test methodology uses the VMS DIFFERENCE command to compare output from POSTLHS 4.07 on the Compaq ES40 with OpenVMS7.3-1 to the output from the previous validation of POSTLHS 4.07.

5.18.3 Test Results
The two test cases for POSTLHS 4.07 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of POSTLHS 4.07 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics.

5.18.4 EPA’s Conclusions
Since all differences between the results of POSTLHS 4.07 in OpenVMS 7.3-1, and POSTLHS 4.07 in OpenVMS 6.1 are acceptable, EPA concludes that POSTLHS 4.07 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.18.5 References


5.19 POSTSECOTP2D

This section presents the regression test results for the POSTSECOTP2D Version 1.04 code. POSTSECOTP2D creates a new CAMDAT database (the WIPP Performance Assessment computational data base) from the output of the SECOTP2D computer program and the previous CAMDAT file. The program appends the computational database with ANALYSIS information output from the SECOTP2D code. Specifically, for each timestep of SECOTP2D output, POSTSECOTP2D writes values to the CAMDAT file. These values are written to the 'Analysis Results' section of the CAMDAT file: TIME, HIFLAG(=0), and ELEMENT variables (Species Concentrations and Darcy face velocities).

5.19.1 Introduction

Since the Compliance Certification Application (CCA) the POSTSECOTP2D code has undergone a series of revisions. POSTSECOTP2D Version 1.02, which was used in the WIPP CCA, was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of a test case met the acceptance criteria defined in the RD/VVP for POSTSECOTP2D 1.02 [3,4].

Validation was accomplished by demonstrating that the input data into POSTSECOTP2D 1.02 is the same as the output file to the CAMDAT database. The program ST2D3_VERIFY_RES (compiled and linked from ST2D3_VERIFY_RES.FOR) was executed to extract data corresponding to the data extracted from the output CAMDAT database file, ST2D3_SECOTP_TEST.CDB, with the above sequence of commands, and the data were compared and showed that POSTSECOTP2D correctly transfers data from the binary output file to the CAMDAT database. Only selected portions of each array written to the database were compared by DOE. If the entire contents of the database were compared to the results on the binary output file, a manual inspection of tens of thousands of numbers would have to be made. DOE points out that the magnitude of this task would be overwhelming. DOE also notes that the binary file has changed to a degree that computer differencing is not possible.
In June 1997, POSTSECOTP2D was revised to Version 1.04 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [1, 2]. Validation was accomplished by demonstrating that the results of the two test cases met the acceptance criteria defined in the RD/VVP for POSTSECOTP2D 1.02. Both test cases were different than had been used in the previous validation. Otherwise the methodology was the same as described above for version 1.02.

5.19.2 Test Methodology

The tests for this code comprised the two test cases described in the Requirements Document & Verification and Validation Plan for POSTSECOTP2D Version 1.04 (RD/VVP) [1]. Regression test results from POSTSECOTP2D 1.04 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of POSTSECOTP2D 1.04 run on a DEC Alpha 2100 with OpenVMS 6.1 [2].

CAMDAT database files (CDB) are produced in each of the two POSTSECOTP2D test cases. The output CDB files are converted from a binary, CDB, file to an ASCII file for comparison during the validation process. In the previous POSTSECOTP2D 1.04 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [5]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from POSTSECOTP2D 1.04 in OpenVMS 7.3-1, as well as POSTSECOTP2D 1.04 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

The regression test methodology uses the VMS DIFFERENCE command to compare output from POSTSECOTP2D 1.04 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the previous validation of POSTSECOTP2D 1.04 running on a DEC Alpha 2100 with OpenVMS 6.1.

5.19.3 Test Results

Two test cases for POSTSECOTP2D 1.04 were executed on the Compaq ES40 with OpenVMS 7.3-1, and the output files were compared to the corresponding output files from the validation of POSTSECOTP2D 1.04 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concludes that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file names, platform names, system version numbers and execution statistics. EPA also found that all differences in output are
acceptable; namely, that the differences are limited to code run date and time, file names, platform names, system version numbers and execution statistics.

5.19.4 EPA’s Conclusions
Since all differences between the results of POSTSECOTP2D 1.04, in OpenVMS 7.3-1, and POSTSECOTP2D 1.04 in OpenVMS 6.1 are acceptable, EPA concludes that POSTSECOTP2D 1.04 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.19.5 References

5.20 PREBRAG
This section presents the regression test results for the PREBRAG Version 6.00 code. PREBRAG is used to create BRAGFLO input files. PREBRAG reads specific data from an input CAMDAT file and, through instructions supplied in an ASCII input file, generates and ASCII BRAGFLO input file.

5.20.1 Introduction
Prior to the Compliance Certification Application (CCA) the PREBRAG code had undergone a single revision. PREBRAG 5.05ZO was validated [3] in September 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by acceptance testing a single test case, the output of which met the
acceptance criteria defined in the RD/VVP for PREBRAG 5.05ZO [4].

In February 1996, PREBRAG was revised to Version 6.00 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [1, 2]. PREBRAG 6.00 was used in the WIPP CCA. The validation test included the original test case defined for Version 5.05ZO, and an additional 2 test cases.

Acceptance of the added Test Cases 2 and 3, described in the RD/VVP for Version 6.00 [1], were satisfied by comparing output of the second test to the output of Test Case 1, while the acceptance criteria for Test Case 3 was satisfied by comparing its output to that of Test Case 2.

PREBRAG 6.00 has one open problem report [5]. PREBRAG 6.00 uses an outdated list-directed I/O format that allows space-padded fields. The output files from PREBRAG 6.00 validation and the VMS7.3-1 test include space-padded fields and cannot be read by BRAGFLO 4.10. There is no requirement for test output of PREBRAG to be read as input to BRAGFLO. To allow BRAGFLO 4.10 to read input files created by PREBRAG 6.00, a conversion script, EVAL_BF2_CONVERT_INPUT.COM, removes extraneous spaces from the input file. Use of this conversion script is not necessary for this regression test of PREBRAG 6.00.

5.20.2 Test Methodology

The tests for this code comprised the three test cases described in the Requirements Document & Verification and Validation Plan for PREBRAG Version 6.00 RD/VVP) [1]. Regression test results from PREBRAG 6.00 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PREBRAG 6.00 run on a DEC Alpha 2100 with OpenVMS 6.1 [2]. The regression test methodology uses the VMS DIFFERENCE command to compare output from PREBRAG 6.00 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of PREBRAG 6.00.

5.20.3 Test Results

PREBRAG is used to create BRAGFLO input files by reading specific data from an input CAMDAT file, and through instructions supplied in an ASCII input file, it generates an ASCII BRAGFLO input file. The test set for PREBRAG consists of three cases, which test the seventeen requirements of the RD/VVP [1]. The test cases for PREBRAG 6.00 were executed on the Compaq ES40 with OpenVMS 7.3-1, and output files were compared to the corresponding output files from the validation of PREBRAG 6.00 on a DEC Alpha 2100 with OpenVMS 6.1 by using the DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time. EPA also found that all
differences in output are acceptable; namely, that the differences are limited to code run date and time.

5.20.4 EPA’s Conclusions
Since all differences between the results of PREBRAG 6.00 in OpenVMS 7.3-1 and PREBRAG 6.00 in OpenVMS 6.1 are acceptable, EPA concludes that PREBRAG 6.00 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS Version 7.3-1.

5.20.5 References


5.21 PRELHS
This section presents the regression test results for the PRELHS Version 2.30 code. The PRELHS program extracts parameter distribution data requested by the user from the Performance Assessment Parameter Database and sets up the LHS (Latin Hypercube Sampling) input control file.

5.21.1 Introduction
Since the Compliance Certification Application (CCA) the PRELHS code has undergone a series of revisions. PRELHS Version 2.10 was used in the WIPP CCA. PRELHS 2.10 was validated in
February 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of eight test cases met the acceptance criteria defined in the VVP/VD for PRELHS 2.10 [4, 5].

In August 1997 PRELHS was revised to Version 2.20 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of the eight test cases met the acceptance criteria defined in the VVP/VD [6, 7].

In August 2001, PRELHS was revised to Version 2.24 and was validated on a DEC Alpha 2100 with OpenVMS 7.2-1 [8, 9]. The validation test included three new test cases defined for Version 2.24. Previous versions of PRELHS accessed the old view-based Parameters Database. PRELHS 2.24 accesses the new procedure-based Parameters Database. The two databases are not compatible (i.e., PRELHS 2.24 cannot read a view-based Parameters Database), and the parameter entries that were created for testing the previous versions of PRELHS do not exist in the procedure-based Parameters Database. Therefore, the test cases used to test previous versions of PRELHS (Test Cases 1 through 8) were discarded, and three new test cases (Test Cases 9 through 11) were used to test PRELHS 2.24.

In November 2001, PRELHS was revised to Version 2.30 and was validated on a DEC Alpha 2100 with OpenVMS 7.2-1 [3]. PRELHS 2.30 accesses the new procedure-based Performance Assessment Parameter Database (PAPDB). It cannot read the databases accessed by previous versions of PRELHS. The primary difference between the PAPDB and the old database is the manner in which parameter entries are identified. In the old database, a parameter entry was uniquely identified by material and property, and its compliance type and its calculation. Each parameter entry in the PAPDB is uniquely identified by its material and property, and the associated analysis, computational code, and retrieval number. Therefore, Test Cases 9 through 11 were discarded by DOE and three new test cases (Test Cases 12 through 14) were designed to verify that PRELHS satisfies all of the requirements and additional functionality specified in the VVP/VD [3].

5.21.2 Test Methodology

The tests for this code comprised the three test cases described in the Verification and Validation Plan/ Validation Document for PRELHS Version 2.30 (VVP/VD) [3]. Regression test results from PRELHS 2.30 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PRELHS 2.30 run on a DEC Alpha 2100 with OpenVMS 7.2-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output
from PRELHS 2.30 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the previous validation of PRELHS 2.30. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

Since DOE did not regression test PRELHS 2.30 on the ES40 with OpenVMS 7.3-1 directly to the validation tests of PRELHS 2.30, run on a DEC Alpha 2100 with OpenVMS 6.1, it was necessary for EPA to further review the results of DOE’s earlier migration tests[1,2]. That review indicated that there were no numerical or other significant differences between PRELHS 2.30, run on a DEC Alpha 2100 with OpenVMS 7.2-1 and PRELHS 2.30, run with OpenVMS 6.1 on the same hardware. EPA therefore concludes, that DOE’s comparison approach is acceptable.

5.21.3 Test Results

The three test cases for PRELHS 2.30 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of PRELHS 2.30 on a DEC Alpha 2100 with OpenVMS 7.2-1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics.

5.21.4 EPA’s Conclusions

Since all differences between the results PRELHS 2.30, in OpenVMS 7.3-1, and PRELHS 2.30, in OpenVMS 7.2-1, are acceptable, EPA concludes that PRELHS 2.30 meets the acceptance criteria specified in the VVP/VD [3], and thus are considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.21.5 References


5.22 RELATE

This section presents the regression test results for the RELATE Version 1.43 code. RELATE 1.43 transfers information from one CAMDAT database file (the "Reference" database) to another CAMDAT database file (the "Object" database) using either the relative positions of the meshes defined on the reference and object databases or a symbolic mapping between the material and property names on the reference database and the material and property names on the object database. CAMDAT database files are also referred to as CDB files.

5.22.1 Introduction

RELATE version 1.42ZO was validated in October 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of three test cases met the acceptance criteria defined in the RD/VVP for RELATE 1.42ZO [1].

In March 1996, RELATE was revised to Version 1.43 and was validated on a DEC Alpha 2100 with OpenVMS 6.1. Test cases identical to the test cases for the validation of RELATE 1.42ZO
were run. The acceptance criteria for these test cases were satisfied by showing that the output from RELATE 1.43 was identical to the output of the RELATE 1.42Z0 validation tests. RELATE 1.43 was used in the WIPP Compliance Certification Application (CCA).

5.22.2 Test Methodology

The tests for this code comprised the three test cases described in the *Requirements Document & Verification and Validation Plan for RELATE Version 1.42Z0 (RD/VVP)* [1]. Regression test results from RELATE 1.43, run on the ES40 with OpenVMS 7.3-1, were compared to results from the validation tests of RELATE 1.43, run on a DEC Alpha 2100 with OpenVMS 6.1.

CAMDAT database files (CDB) are produced in each of the three RELATE test cases. The output CDB files are converted from a binary, CDB, file to an ASCII, PRT, file for comparison during the validation process. In the previous RELATE 1.43 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [2]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see Section 5.10). For this regression test, GROPE 2.12 is used to convert the CDB output files from RELATE 1.43 in OpenVMS 7.3-1, as well as RELATE 1.43 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

The regression test methodology uses the VMS DIFFERENCE command to compare output from RELATE 1.43 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the previous validation of RELATE 1.43.

5.22.3 Test Results

The three test cases for RELATE 1.43 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of RELATE 1.43 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers. EPA found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers.

5.22.4 EPA's Conclusions
Since all differences between the results of RELATE 1.43, in OpenVMS 7.3-1, and RELATE 1.43, in OpenVMS 6.1, are acceptable, EPA concludes that RELATE 1.43 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS Version 7.3-1.

5.22.5 References

5.23 PRESECOTP2D
This section presents the regression test results for the PRESECOTP2D Version 1.22 code. The purpose of PRESECOTP2D 1.22 is to create all the input files required to run the code SECOTP2D. Material properties, grid information, and source term information are obtained from CAMDAT databases. The velocity field is obtained from a transfer file written by PRESECOFL2D. Since the Compliance Certification Application (CCA) the PRESECOTP2D code has undergone a series of revisions. PRESECOTP2D Version 1.11ZO was used in the WIPP CCA. PRESECOTP2D 1.11ZO was validated in September 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by regression testing to a validated primitive package [3] that demonstrated that the results of two test cases (2 and 3) met the acceptance criteria defined in the RD/VVP for PRESECOTP2D 1.11ZO [4].

5.23.1 Introduction
In August 1996 PRESECOTP2D was revised to Version 1.20 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [5, 6]. Test Case 1 for the validation of PRESECOTP2D 1.20 was identical to test case for the validation of PRESECOTP2D 1.11ZO. The acceptance criteria for this test case was satisfied by showing that the output from PRESECOTP2D 1.20 was identical to the output of the PRESECOTP2D 1.11ZO validation tests. Test Cases 2 and 3 were modified to test code functionality that changes from version 1.11ZO to version 1.20. In these test cases, the acceptance criteria were satisfied by analysis of the output of PRESECOTP2D 2.20.

In June 1997, PRESECOTP2D was revised to version 1.22 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [1, 2]. The validation test included the three test cases defined for version 1.20, and an additional Test Case 4. Test Case 4 was added to verify the variable time
step functionality by showing the time increments produced by the code match those produced by the algorithm in the user’s manual [7]. Acceptance criteria for Test Cases 1-3 were satisfied by comparing output of PRESECOTP2D 1.22 to the output of PRESECOTP2D 1.20, while the acceptance criteria for Test Case 4 were satisfied by analysis of the output of PRESECOTP2D 1.22.

6.23.2 Test Methodology
The tests for this code comprised the four test cases described in the Requirements Document & Verification and Validation Plan for PRESECOTP2D Version 1.22 (RD/VVP) [1]. Regression test results from PRESECOTP2D 1.22 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PRESECOTP2D 1.22 run on a DEC Alpha 2100 with OpenVMS 6.1 [2].

The regression test methodology uses the VMS DIFFERENCE command to compare output from PRESECOTP2D 1.22 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of PRESECOTP2D 1.22. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.23.3 Test Results
The four test cases for PRESECOTP2D 1.22 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of PRESECOTP2D 1.22 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names, system version numbers and execution statistics.

5.23.4 EPA’s Conclusions
Since all differences between the results of PRESECOTP2D 1.22 in OpenVMS 7.3-1, and PRESECOTP2D 1.22 in OpenVMS 6.1 are acceptable, EPA concludes that PRESECOTP2D 1.22 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.
5.23.5 References


5.24 SECOTP2D

This section presents the regression test results for the SECOTP2D Version 1.41 code. SECOTP2D performs single or multiple component radionuclide transport in fractured or granular aquifers. Fractured porous media are represented using a dual porosity model. The code uses total variation diminishing (TVD) schemes to model the advection part of the transport equation.

5.24.1 Introduction

Since the Compliance Certification Application (CCA) the SECOTP2D code has undergone a series of revisions. SECOTP2D Version 1.30 was used in the WIPP CCA. SECOTP2D 1.30 was validated in April 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of three test cases met the acceptance criteria defined in the RD/VVP for SECOTP2D 1.30 [3,4].
In July 1997, SECOTP2D was revised to Version 1.41 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of six new test cases met the acceptance criteria defined in the RD/VVP for SECOTP2D 1.41 [1, 2].

5.24.2 Test Methodology
The tests for this code comprised the four test cases described in the *Requirements Document & Verification and Validation Plan for SECOTP2D Version 1.41* (RD/VVP) [1]. Regression test results from SECOTP2D 1.41 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of SECOTP2D 1.41 run on a DEC Alpha 2100 with OpenVMS 6.1 [2].

Regression testing of binary output from SECOTP2D 1.41 required the use of other WIPP PA codes to convert the information into a format that could be compared, using the VMS DIFFERENCE command, to corresponding post-processor files from the previous validation. Test Cases 1, 2, and 6 required the software modules, POSTSECOTP2D 1.04 and GROPECDB 2.12; and Test Cases 4 & 5 required POSTSECOTP2D 1.04 and SUMMARIZE 2.20. These are the same codes that were used in the previous validation of SECOTP2D 1.41 running on a DEC Alpha 2100 with OpenVMS 6.1, and they have now been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the VMS 7.3-1 Regression Test (see sections pertaining to POSTBRAG, GROPECDB, and SUMMARIZE, respectively).

The regression test methodology uses the VMS DIFFERENCE command to compare post-processed output from SECOTP2D 1.41 on the Compaq ES40 with OpenVMS 7.3-1 to the corresponding output from the previous validation of SECOTP2D 1.41 running on a DEC Alpha 2100 with OpenVMS 6.1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.24.3 Test Results
The test set for SECOTP2D consists of six cases. The test cases for SECOTP2D 1.41 were executed on the Compaq ES40 with OpenVMS 7.3-1, and output files were compared to the corresponding output files from the validation of SECOTP2D 1.41 on a DEC Alpha 2100 with OpenVMS 6.1 by using the DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names, platform names and system version numbers. No numerical differences were found. EPA also found that all differences in output are acceptable; namely, that the differences are limited to code run dates and times, file and directory names, platform names and system version numbers. EPA also concluded that there were no numerical differences.
5.24.4   EPA’s Conclusions
Since all differences between the results of SECOTP2D 1.41 in OpenVMS 7.3-1 and
SECOTP2D 1.41 in OpenVMS 6.1 are acceptable, EPA concludes that SECOTP2D 1.41 meets
the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the
Compaq ES40 with OpenVMS 7.3-1.

5.24.5   References
   and Validation Plan for SECOTP2D Version 1.41.” Sandia National Laboratories. Sandia
   WIPP Central Files WPO # 45732.
   Version 1.41.” Sandia National Laboratories. Sandia WIPP Central Files WPO # 45735.
   and Validation Plan for SECOTP2D Version 1.30.” Sandia National Laboratories. Sandia
   WIPP Central Files WPO # 36693.
4.   WIPP PA (Performance Assessment). 1996. ‘Validation Document for SECOTP2D
   Version 1.30.” Sandia National Laboratories. Sandia WIPP Central Files WPO # 36694.

5.25   SPLAT
This section presents the regression test results for the SPLAT Version 1.02 code. SPLAT is a
generic plotting code that allows the user to plot data extracted from an input data file. The plot
can be tailored with user commands.

5.25.1   Introduction
SPLAT Version 1.01 was validated in May of 1996 on a DEC Alpha 2100 with OpenVMS 6.1
by demonstrating that the results of six test cases met the acceptance criteria defined in the
RD/VVP for version 1.01 [2]. The validation for the test set used to perform functional testing
for SPLAT 1.01 consisted of six test cases (VD for SPLAT 1.01 [3]).

In October of 1996, SPLAT was revised to Version 1.02, which was validated with OpenVMS 6.1
on a DEC Alpha 2100 using seven test cases [1,2]. Test cases 1 through 4 were validated through
regression testing while tests five and six underwent acceptance testing (described in more detail
below). The regression testing was accomplished by comparing the results from Version 1.02 to the
results of Version 1.01 using the VMS DIFFERENCE utility. In section 10.0 of the RD/VVP
associated with version 1.01 [2] it is stated that all six of these test cases are suitable for regression testing. The regression test methodology uses the VMS DIFFERENCE command to compare output from SPLAT 1.02 on the DEC Alpha 2100 with OpenVMS6.1 to the output from the previous validation of SPLAT 1.01.

However, as a result of changes that were made in the code to correct errors in Version 1.01, the results of test cases five and six (Version 1.02) were not the same results as those observed in testing of Version 1.01. These changes were related to Version 1.02’s ability to change the minor tick interval using the AXIS SCALE USER and REPLOT commands. The parameters associated with the minor tick intervals were ignored in Version 1.01, but were not in Version 1.02. Therefore the plots associated with test cases five and six were not regression tested, but evaluated “by hand” as described in the RD/VVP for SPLAT 1.02 [3] and documented in the associated VD [4]. The seventh test case was created to verify that the changes made for Version 1.02 were implemented correctly. It was validated by comparing output results to the defined set of acceptance criteria in the RD/VVP for SPLAT 1.02 [1].

5.25.2 Test Methodology
The tests for this code comprised the seven test cases described in the Requirements Document & Verification and Validation Plan for SPLAT Version 1.02 (RD/VVP) [1]. Regression test results from SPLAT 1.02 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of SPLAT 1.02 run on a DEC Alpha 2100 with OpenVMS 6.1.

Validation of SPLAT 1.02 running on a Compaq ES40 with OpenVMS 7.3-1 was accomplished by visually comparing output plot files to the same output plot files from the previous validation of SPLAT 1.02 running on a DEC Alpha 2100 using OpenVMS 6.1. These files were identified in the SPLAT 1.02 RD/VVP as necessary to determine that the test case met its acceptance criteria [1].

5.25.3 Test Results
The seven test cases for SPLAT 1.02 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output plot files from the test cases were visually compared to the corresponding output files from the validation of SPLAT 1.02 on a DEC Alpha 2100 with OpenVMS 6.1. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names. After conducting an independent visual comparison, EPA also found that all differences in output are acceptable; namely, that the differences are
limited to code run date and time, file and directory names.

5.25.4 EPA’s Conclusions
Since all differences between the results of SPLAT 1.02 in OpenVMS 7.3-1 and SPLAT 1.02 in OpenVMS 6.1 are acceptable, EPA concludes that SPLAT 1.02 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.25.5 References


5.26 STEPWISE
This section presents the regression test results for the STEPWISE Version 2.21 code.
STEPWISE is a statistical code that evaluates variable importance by developing regression models between the observed response and input variables using either a forward, backward, or stepwise regression procedure on the raw or ranked data. STEPWISE 2.20 was validated in November 1995 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of three test cases met the acceptance criteria defined in the RD/VVP for STEPWISE 2.20 [2]. STEPWISE 2.20 was used in the WIPP Compliance Certification Application (CCA).

5.26.1 Introduction
In November of 1996, STEPWISE was revised to version 2.21. Version 2.21 was validated on the DEC Alpha 2100 with OpenVMS 6.1 by a combination of acceptance and regression testing. Test Cases 1-3 were validated through regression testing while Test Cases four and five underwent acceptance testing. Test Cases four and five were created to illustrate the correction of
errors found in Version 2.20 and were validated by comparing output results to the acceptance criteria defined in the RD/VVP for STEPWISE 2.21 [1].

5.26.2 Test Methodology
The tests for this code comprised the five test cases described in the Requirements Document & Verification and Validation Plan for STEPWISE Version 2.21 RD/VVP) [1]. Regression test results from STEPWISE 2.21, run on the ES40 with OpenVMS 7.3-1, were compared to results from the validation tests of STEPWISE 2.21, run on a DEC Alpha 2100 with OpenVMS 6.1. The regression test methodology uses the VMS DIFFERENCE command to compare output from STEPWISE 2.21 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the previous validation of STEPWISE 2.21. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.26.3 Test Results
The five test cases for STEPWISE 2.21 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of STEPWISE 2.21 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, user names, platform names, system version numbers and execution statistics. EPA found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, user names, platform names, system version numbers and execution statistics.

5.26.4 EPA’s Conclusions
Since all differences between the results of STEPWISE 2.21, in OpenVMS 7.3-1, and STEPWISE 2.21, in OpenVMS 6.1, are acceptable, EPA concludes that STEPWISE 2.21 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS Version 7.3-1.

5.26.5 References
and Validation Plan for STEPWISE Version 2.20.” Sandia National Laboratories. Sandia WIPP Central Files WPO # 27767.

5.27 SUMMARIZE
This section presents the regression test results for the SUMMARIZE Version 2.20 code. SUMMARIZE 2.20 is a data integration and conversion utility code for the analysis of binary input data. SUMMARIZE reads data from CAMDAT binary data (CDB) files and generates one or more tabular ASCII output files.

5.27.1 Introduction
Since the Compliance Certification Application (CCA) the SUMMARIZE code has undergone a series of revisions. SUMMARIZE Version 2.10 was used in the WIPP CCA. SUMMARIZE 2.10 was validated in May 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of seven test cases met the acceptance criteria defined in the RD/VVP for SUMMARIZE 2.10. [2, 3]

In August 1996 SUMMARIZE was revised to Version 2.15 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [5, 6]. Test Cases 2, 3, 5, 6 and 7 for the validation of SUMMARIZE 2.15 were identical to test cases for the validation of SUMMARIZE 2.10. The acceptance criteria for these test cases were satisfied by DOE in which they demonstrated that the output from SUMMARIZE 2.15 was identical to the output of the SUMMARIZE 2.10 validation tests. Test Cases 1 and 4 were modified to test code functionality that changes from Version 2.10 to Version 2.15. In these test cases, the acceptance criteria were satisfied by analysis of the output of SUMMARIZE 2.15.

In July 1997, SUMMARIZE was revised to Version 2.20 and was validated on a DEC Alpha 2100 with OpenVMS 6.1 [1, 2]. The validation test included the seven test cases defined for Version 2.15, and an additional Test Case 8. Test Case 8 was added to verify the correction of an error found in Version 2.15. Acceptance criteria for Test Cases 1-7 were satisfied by comparing output of SUMMARIZE 2.20 to the output of SUMMARIZE 2.15, while the acceptance criteria for Test Case 8 were satisfied by analysis of the output of SUMMARIZE 2.20.

SUMMARIZE 2.20 has one current Software Problem Report [6]. The subroutine SURFER_PRINT_TWO_D_GRID prints data to a file that can be read by the SURFER plotting program. This subroutine contains an error that causes the data to be printed incorrectly. The error was determined by DOE (and checked by EPA) to be of no consequence since the SURFER
output capability is not used by WIPP PA. SUMMARIZE has not been revised to correct the error. Test Case 3 produces SURFER-formatted output as part of the test case. Hence, DOE expected to find numerical differences in the output of Test Case 3.

5.27.2 Test Methodology
The tests for this code comprised the eight test cases described in the Requirements Document & Verification and Validation Plan for SUMMARIZE Version 2.20 (RD/VVP) [1]. Regression test results from SUMMARIZE 2.20 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of SUMMARIZE 2.20 run on a DEC Alpha 2100 with OpenVMS 6.1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from SUMMARIZE 2.20 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of SUMMARIZE 2.20. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.27.3 Test Results
The eight test cases for SUMMARIZE 2.20 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of SUMMARIZE 2.20 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. With the exception of Test Case 3, DOE and EPA conclude that all differences in output are acceptable; namely, that the differences are limited to code run date and time, file and directory names, platform names and system version numbers.

The only difference in numerical output was found in Test Case 3. As described in Section 5.27.1, SUMMARIZE 2.20 contains an error that causes the subroutine SURFER_PRINT_TWO_D_GRID to print incorrect data. Test Case 3 includes the SURFER output functionality and generates the SURFER output file. As a consequence of the error, the numerical output of Test Case 3 differs from the output of the validation test. Since the SURFER functionality is not used in WIPP PA and the error is documented in the Software Problem Report, EPA considers this difference acceptable.

5.27.4 EPA’s Conclusions
Since all differences between the results of SUMMARIZE 2.20, in OpenVMS 7.3-1, and SUMMARIZE 2.20, in OpenVMS 6.1, are acceptable, EPA concludes that SUMMARIZE 2.20 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated.
on the Compaq ES40 with OpenVMS Version 7.3-1.

5.27.5 References


5.28 CAM LIBRARIES

This section presents the regression testing for the CAM libraries, specifically the CAMCON_LIB Version 2.20 and CAMDAT_LIB Version 1.25 software libraries

5.28.1 CAMCON_LIB

This section presents the regression test results for the CAMCON_LIB Version 2.20 software library. CAMCON_LIB is a collection of routines that perform Quality Assurance, File processing, Free-Field Input processing, String processing, and Finite Element Index processing. The data manipulations to be performed are expressed as algebraic equations involving the existing and/or newly created data.

5.28.1.1 Introduction

As a consequence of the upgrade to OpenVMS 7.3-1, CAMCON_LIB was re-compiled on the
ES40 to create version 2.20. No changes were made to the CAMCON_LIB source code. The *Implementation Document for CAMCON_LIB 2.20* [6] documents the build of CAMCON_LIB 2.20. CAMCON_LIB 2.16 was used in the WIPP Compliance Certification Application (CCA) [1]. CAMCON_LIB 2.16 was validated in January 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of seven Test Cases (1 through 7) met the acceptance criteria defined in the RD/VVP for CAMCON_LIB 2.16 (document Version 1.00) [3].

In January 1999 source code changes were made to CAMCON_LIB and the code was revised to Version 2.18. CAMCON_LIB 2.18 was validated on a DEC Alpha 2100 with OpenVMS 7.1 [4,5]. Test Cases 1-7 for the validation of CAMCON_LIB 2.18 were identical to test cases for the validation of CAMCON_LIB 2.16. The acceptance criteria for these test cases were satisfied by showing that the output from CAMCON_LIB 2.18 was identical to the output of the CAMCON_LIB 2.16 validation tests.

5.28.1.2 Test Methodology
The tests for this library comprised the seven test cases described in the *Requirements Document & Verification and Validation Plan for CAMCON_LIB Version 2.16* (RD/VVP) [3]. Regression test results from CAMCON_LIB 2.20 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CAMCON_LIB Version 2.18 run on a DEC Alpha 2100 with OpenVMS 7.1, as documented in the Change Control Form for CAMCON_LIB, Version 2.18 [4] and the memo Regression testing of CAMCON_LIB Version 2.18 [5].

Since DOE did not regression test CAMCON_LIB Version 2.18 on the ES40 with OpenVMS 7.3-1 directly to the validation tests of CAMCON_LIB Version 2.18, run on a DEC Alpha 2100 with OpenVMS 6.1, it was necessary for EPA to further review the results of DOE’s earlier migration tests[1,2]. That review indicated that there were no numerical or other significant differences between CAMCON_LIB Version 2.18, run on a DEC Alpha 2100 with OpenVMS 7.2-1 and CAMCON_LIB Version 2.18, run with OpenVMS 6.1 on the same hardware. EPA therefore concludes, that DOE’s comparison approach is acceptable.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CAMCON_LIB 2.20 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of CAMCON_LIB 2.18 with OpenVMS 7.1. The VMS DIFFERENCE command
compares two files and identifies records that are different in the two files.

5.28.1.3 Test Results
The seven test cases for CAMCON_LIB 2.20 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of CAMCON_LIB 2.18 on a DEC Alpha 2100 with OpenVMS 7.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to library run date and time, platform names, system version numbers, execution statistics, the directory and file names. EPA found that all differences in output are acceptable; namely, that the differences are limited to library run date and time, platform names, system version numbers, execution statistics, the directory and file names.

5.28.1.4 EPA’s Conclusions
Since all differences between the results of CAMCON_LIB 2.20, in OpenVMS 7.3-1, and CAMCON_LIB 2.18, in OpenVMS 7.1, are acceptable, EPA concludes that CAMCON_LIB 2.20 meets the acceptance criteria specified in the RD/VVP [3], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.28.1.5 References

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5.28.2 CAMDAT_LIB
This section presents the regression test results for the CAMDAT_LIB Version 1.25 software library. CAMDAT_LIB is a collection of routines that read from and write to a computational database (CAMDAT) file for use by WIPP PA computer codes. The data manipulations to be performed are expressed as algebraic equations involving the existing and/or newly created data.

5.28.2.1 Introduction
As a consequence of the upgrade to OpenVMS 7.3-1, CAMDAT_LIB was re-compiled on the ES40 to create version 1.25. No changes were made to the CAMDAT_LIB source code. The Implementation Document for CAMDAT_LIB 1.25 [3] documents the build of CAMDAT_LIB 1.25. CAMDAT_LIB 1.22 was used in the WIPP Compliance Certification Application (CCA). CAMDAT_LIB 1.22 was validated in January 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of seven Test Cases (1 through 7) met the acceptance criteria defined in the RD/VVP for CAMDAT_LIB 1.22 (document Version 1.00) [1].

5.28.2.2 Test Methodology
The tests for this library comprised the seven test cases described in the Requirements Document & Verification and Validation Plan for CAMDAT_LIB Version 1.22 (RD/VVP) [1]. Regression test results from CAMDAT_LIB 1.25 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CAMDAT_LIB 1.22 run on a DEC Alpha 2100 with OpenVMS 6.1, as documented in the Validation Document for CAMDAT_LIB Version 1.22 (VD) [2].

CAMDAT database files (CDB) are produced in CAMDAT_LIB Test Case 7. The output CDB files are converted from a binary, CDB, file to an ASCII file for comparison during the validation process. In the previous CAMDAT_LIB 1.22 validation, the CDB files were converted using GROPE 2.10. GROPE has since been revised to Version 2.12. GROPE 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4]. GROPE 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the Analysis Report for the OpenVMS 7.3-1 Regression Test (see Section 5.10, GROPECDB) [5]. For this regression test,
GROPE 2.12 is used to convert the CDB output files from CAMDAT_LIB 1.25 in OpenVMS 7.3-1, as well as CAMDAT_LIB 1.22 in OpenVMS 6.1, thereby eliminating the potential for differences because of different GROPE versions.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CAMDAT_LIB 1.25 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of CAMDAT_LIB 1.22 with OpenVMS 6.1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.28.2.3 Test Results
The seven test cases for CAMDAT_LIB 1.25 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of CAMDAT_LIB 1.22 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to library run date and time, execution statistics, and the directory and file names. EPA found that all differences in output are acceptable; namely, that the differences are limited to library run date and time, execution statistics, and the directory and file names.

5.28.2.4 EPA’s Conclusions
Since all differences between the results of CAMDAT_LIB 1.25, in OpenVMS 7.3-1, and CAMDAT_LIB 1.22, in OpenVMS 6.1, are acceptable, EPA concludes that CAMDAT_LIB 1.25 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.28.2.5 References

5.28.2 CAMSUPES_LIB
This section presents the regression test results for the CAMSUPES_LIB Version 2.22 software library. The CAMSUPES_LIB library is a collection of routines that perform system-dependent functions and allocate memory for arrays at run time for FORTRAN-77 programs. The system dependent functions provide a uniform interface to necessary operating system functions that are not included in the ANSI FORTRAN-77 standard. The purpose of the memory management routines is to allow an applications programmer to write standard, readable FORTRAN-77 code making efficient use of memory resources.

5.28.2.1 Introduction
As a consequence of the upgrade to OpenVMS 7.3-1, CAMSUPES_LIB was re-compiled on the ES40 to create version 2.22. No changes were made to the CAMSUPES_LIB source code. The Implementation Document for CAMSUPES_LIB 2.22 (document Version 1.04) (ID) [5] documents the build of CAMSUPES_LIB 2.22. CAMSUPES_LIB 2.18 was used in the WIPP Compliance Certification Application (CCA) [1]. CAMSUPES_LIB 2.18 was validated in January 1996 on a DEC Alpha 2100 with OpenVMS 6.1 by demonstrating that the results of two Test Cases (1 and 2) met the acceptance criteria defined in the RD/VVP for CAMSUPES_LIB 2.18 (document Version 1.00) [6].

5.28.2.2 Test Methodology
The tests for this software library comprised the two test cases described in the Verification and Validation Plan for CAMSUPES_LIB Version 2.20 (document Version 1.01) (VVP) [3]. Regression test results from CAMSUPES_LIB 2.22 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of CAMSUPES_LIB Version 2.20 run on a DEC Alpha 2100 with OpenVMS 7.1, as documented in the Validation Document for
CAMSUPES_LIB Version 2.20 (document Version 1.02) (VD) [4].

Since DOE did not regression test CAMSUPES_LIB Version 2.18 on the ES40 with OpenVMS 7.3-1 directly to the validation tests of CAMSUPES_LIB Version 2.18, run on a DEC Alpha 2100 with OpenVMS 6.1, it was necessary for EPA to further review the results of DOE’s earlier migration tests[1,2]. That review indicated that there were no numerical or other significant differences between CAMSUPES_LIB Version 2.18, run on a DEC Alpha 2100 with OpenVMS 7.2-1 and CAMSUPES_LIB Version 2.18, run with OpenVMS 6.1 on the same hardware. EPA therefore concludes, that DOE’s comparison approach is acceptable.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CAMSUPES_LIB 2.22 on the Compaq ES40 with OpenVMS 7.3-1 to the output from the validation of CAMSUPES_LIB 2.20 with OpenVMS 7.1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.28.2.3 Test Results
The two test cases for CAMSUPES_LIB 2.22 were executed on the Compaq ES40 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of CAMSUPES_LIB 2.20 on a DEC Alpha 2100 with OpenVMS 7.1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to execution statistics, library run date and time, the directory and file names. EPA found that all differences in output are acceptable; namely, that the differences are limited to execution statistics, library run date and time, the directory and file names.

5.28.2.4 EPA's Conclusions
Since all differences between the results of CAMSUPES_LIB 2.22, in OpenVMS 7.3-1, and CAMSUPES_LIB 2.20, in OpenVMS 7.1, are acceptable, EPA concludes that CAMSUPES_LIB 2.22 meets the acceptance criteria specified in the VVP [3], and thus is considered as validated on the Compaq ES40 with OpenVMS 7.3-1.

5.28.2.5 References
1. Analysis Plan (AP-042). 1998 “Regression for the Upgrade to Open VMS Version 7.1 on
the WIPP COMPAC Alpha Cluster.” Sandia National Laboratories.


6.0 SUMMARY AND CONCLUSIONS

EPA reviewed the code migration for each of the 27 computer codes and three libraries migrated to the Compaq ES40 with Open VMS 7.301. Our initial concerns developed during the course of the review are presented with related issue resolution, as well as our final conclusions.

6.1 EPA’s INITIAL CONCERNS

After the Agency’s initially completed a review of the computer code migration a number of issues were identified that are related to whether the computer codes meet the requirements specified in §194.22 and §194.23 of the Rule. These issues and resolutions are described below.

**Issue 1: Incremental Regression Testing**

Regression testing of the computer codes has been conducted in a series of incremental steps in which the results of the regression tests on the Alpha Open VMS 7.1 platform were compared against the results obtained during the CCA with the Open VMS 6.1 platform. Results of this
comparison were used as the baseline for the regression testing of the VMS 7.2 testing. Subsequent regression tests are being compared against results obtained during the latest hardware and/or software change. This approach raises concerns that small changes observed among the sequential regression tests may not be indicative of the true cumulative change from the OpenVMS operating system, version 6.1.

Resolution: For most of the computer codes, the DOE compared regression test results from the ES40 with OpenVMS 7.3-1 to results from the validation tests run on a DEC Alpha 2100 with OpenVMS 6.1. For those cases where the DOE was unable to compare the ES40 with OpenVMS 7.3-1 results to the validation tests run on a DEC Alpha 2100 with OpenVMS 6.1, the Agency traced through DOE's regression tests results from OpenVMS 7.3-1, to 7.2 and 7.1, and ultimately back to 6.1 to ensure that the cumulative effect of the incremental differences was acceptable.

**Issue 2: Acceptance Criteria of Regression Tests**

The acceptance criteria for the regression tests are currently very subjective and it is left to the judgement of the reviewer as to whether the differences in the regression tests are significant. An illustration of why this approach becomes problematic are the regression test results obtained for the computer code BRAGFLO. The regression test comparison for the Open VMS 6.1 and VMS 7.2. operating systems are presented in Appendix A3 of Analysis Package AP-042 (dated May 27, 1999). The discussion indicates that considerable differences (on the order of 10% gas saturations) were observed between the Open VMS 6.1 and VMS 7.2 regression tests. The resolution proposed by the reviewers is as follows From WIPP performance assessment (PA) point of view, brine saturation (and not gas saturation) is used in calculations beyond BRAGFLO. This conclusion fails to consider the interrelationships between gas and brine saturations with respect to relative permeabilities which ultimately translates to the mobility of gas and brine predicted by BRAGFLO. It may be that 10% percent differences in the brine saturations are insignificant in the overall PA results, but this insensitivity needs to be demonstrated.

Resolution: The DOE evaluated the impact under PA-like conditions of potentially significant differences observed in the regression test results. Furthermore, the DOE made comparisons and evaluations as to whether the observed differences would still allow the computer codes to meet the acceptance criteria outlined in the Requirements Document & Verification and Validation Plan (RD/VVP).
**Issue 3: Testing of Existing Functionality**

In a number of instances, not all of the original functional tests have been completed when changing the hardware or software. This approach leaves open the possibility that untested code functions no longer work properly.

**Resolution:** The DOE conducted difference comparisons for all of the test cases outlined in the Requirements Document & Verification and Validation Plan (RD/VVP).

**Issue 4: Testing of New Functionality**

The testing of any new functionality added to the computer codes raises two issues. First, the new functionality must be tested, and second the new functionality may require that a new base case be developed for the other functional tests. For instance, the molecular weight of cellulosics has been changed from the version of BRAGFLO used in the CA/PAVT. This change has increased the gas generation rate which will lead to higher repository pressures. These changes may impact the results from the base case simulations for the other functional tests.

**Resolution:** DOE developed functional tests for new code functionalities, and the effects of the new functions were evaluated against the base case functional tests.

**Issue 5: Traceability of Computer Codes/ Libraries**

In several instances, particularly with respect to the code libraries, it is currently very difficult to trace the regression testing of the code(s)/libraries to a specific operating system or hardware change.

**Resolution:** In AP-089, the DOE provided descriptions for the computer codes and libraries that allowed the sequence of the regression testing to be traced and evaluated.

**Issue 6: Traceability within CMS Framework**

The post CCA/PAVT regression testing has not been completely conducted within the CMS
framework which makes the retrievability of files difficult in terms of reproducing the tests. The versions of the codes and resultant output files that are to be used for the recertification determination must be regression tested within the CMS framework.

Resolution: DOE performed their regression test results from the ES40 with OpenVMS 7.3-1 to results from the validation tests run on a DEC Alpha 2100 with OpenVMS 6.1 within the CMS framework. As part of EPA’s review, the Agency retrieved selected DIFFERENCE files from the CMS framework for evaluation.

**Issue 7: Adequacy of Functional Tests**

In several instances, errors have been discovered subsequent to code qualification in the computer codes even though the code passed all of the functional tests.

Resolution: DOE reviewed all of the functional tests to determine if more rigorous tests should be devised. DOE is currently performing additional test on CCDFGF.

**6.2 EPA’s FINAL CONCLUSIONS**

The Agency has reviewed DOE’s code migration activities associated with 27 computer codes and three libraries that DOE has migrated to the Compaq ES40 with OpenVMS 7.3-1. EPA relied on the following reports as primary sources of information:

- Summary of Performance Assessment System Upgrades Since the Compliance Certification Application
- Analysis Package for AP-042 (documents the upgrade from Open VMS operating software from Version 6.1 to Version 7.1)
- Analysis Package for Regression Testing the Upgrade to OpenVMS Version 7.2 on the WIPP DEC Alpha Cluster
- Analysis Package for Regression Testing for the Compaq Alpha ES40 Hardware Upgrade
on the WIPP DEC Alpha Cluster

- Analysis Package for Regression Testing for the upgrade of Operating System to Open VMS 7.3-1 and Hardware to HP Alpha ES45

In addition to the references cited above, the EPA reviewed User’s Manuals, Validation Documents, Implementation Documents and Requirements Document & Verification and Validation Plans for each code. Since all of the of the code modifications that have been made since certification are documented on Change Control, Software Installation and Checkout Forms, these forms have also been reviewed by EPA.

During EPA’s initial review the Agency found seven concerns that DOE needed to resolve before the agency could approve the migration of the computer codes. The initial concerns are listed below:

1) Incremental Regression Testing
2) Acceptance Criteria of Regression Tests
3) Testing of Existing Functionality
4) Testing of New Functionality
5) Traceability of Computer Code/Libraries
6) Traceability within CMS Framework
7) Adequacy of Functional Tests

After completing the Agency’s review the EPA has concluded that the DOE’s modifications to their code migration activities have satisfactorily solved the concerns identified above, and that the 27 computer codes and three libraries migrated to the Compaq ES40 with OpenVMS 7.3-1 are approved for use in compliance calculations for the WIPP performance assessment. Changes to the operating system, to computer codes, and new hardware - such as the Compaq ES45 - will be reviewed for the recertification. EPA expects that the required future documentation would include the DIFFERENCE files presented in a format similar to that presented for the Compaq ES40 tests.