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TECHNICAL SUPPORT DOCUMENT FOR

SECTION 194.23: REVIEW OF WIPP RECERTIFICATION

PERFORMANCE ASSESSMENT COMPUTER CODES

CRA Code Review

U. S. ENVIRONMENTAL PROTECTION AGENCY
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Note: This document is part of a series of PA code reviews done since the original CCA. This particular review was completed in September 2004 and is reported as part of our CRA decision. Issues noted in this report are finalized in the PABC Code Review, Docket A-98-49 Item II-B1-8 and in the EPA PABC Review TSD, Docket A-98-49 Item II-B1-16.

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EXECUTIVE SUMMARY

The U.S. Department of Energy (DOE) conducted a Performance Assessment (PA) to show compliance with U.S. Environmental Protection Agency's (EPA or the Agency) disposal regulations and compliance criteria at 40 CFR 194 as part of the Waste Isolation Pilot Plant F(WIPP) certification process. 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 and Section 194.22 - Quality Assurance. Since the Agency'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. The Agency reviewed the testing performed by DOE to demonstrate continued compliance with the addition of computer hardware and upgraded software. In 2003, two new hardware systems were added to the PA computational cluster, the Compaq ES45 and the Compaq Alpha 8400. This report presents the Agency's findings with respect to the qualification of the computer codes on the Compaq ES45 and the Compaq Alpha 8400. The Agency concludes that 36 (of the 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 with OpenVMS 7.3-1 are approved for use in compliance calculations for the WIPP performance assessment.

An earlier version of this report (dated March 31, 2004[REF1]) indicated that three codes (i.e., NUMBERS, SANTOS, DRSPALL) were insufficiently documented and tested and that additional reviews would be conducted as part of the Agency's review and evaluation of the CRA. Specifically, the Agency was to ensure that:

1. DRSPALL 1.0 is regression tested on the Compaq ES45 and 8400;

2. NUMBERS meets the QAP 19-1 requirements; and

3. SANTOS is properly evaluated for accuracy.

The DOE has subsequently provided additional information pertaining to the documentation and testing of DRSPALL and NUMBERS. After reviewing that information the Agency concludes that DRSPALL Version 1.0 is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1. The Agency also concludes that NUMBERS now meets the QAP 19-1 requirements. With respect to SANTOS, however, the DOE has not provided any additional information related to the accuracy of the SANTOS results.

1.0 INTRODUCTION

This report describes results of the U.S. Environmental Protection Agency (the Agency or EPA) review of performance assessment computer code development and testing activities performed by the U.S. Department of Energy (DOE) in support of their ongoing Performance Assessment 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 [REF3].

DOE conducted a Performance Assessment (PA) to show compliance with our disposal regulations as part of the WIPP certification process. DOE must demonstrate on a 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 original 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 OpenVMS 7.1 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 changes. 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. In 2003, two new hardware systems were added to the PA computational cluster, the Compaq ES45 and the Compaq Alpha 8400. For the Compliance Recertification Application (CRA) PA, DOE used Open VMS 7.3-1 as the operating system in conjunction with the Compaq ES40, ES45 and 8400. In June 2003[REF2], the Agency

presented their findings with respect to their review of 27 codes and three libraries that were migrated to the Compaq ES40. The Agency concluded that all of the 27 codes and three libraries that were migrated to the Compaq ES40 with OpenVMS 7.3-1 were approved for use in compliance calculations for the WIPP performance assessment.

With respect to the Compaq ES45 and 8400 hardware systems, most of the computer codes have undergone regression testing by DOE to ensure that each code will function correctly on the ES45 and 8400 platform running OpenVMS 7.3-1. In March 2004 [REF1], the Agency concluded that 36 (of the 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 with OpenVMS 7.3-1 were approved for use in compliance calculations for the WIPP performance assessment. As part of this most current technical review of the remaining three codes (e.g., NUMBERS, SANTOS, DRSPALL) the Agency is able to conclude that DRSPALL Version 1.0 is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1. The Agency also concludes that NUMBERS now meets the QAP 19-1 requirements. With respect to SANTOS, however, the DOE has not provided any additional information related to the accuracy of the SANTOS results.

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, the Agency's evaluation addresses whether these changes have materially affected the Agency's original determination that the computer codes were adequate to support the certification decision.

This 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 the Agency followed to review DOE's code migration activities. Section 5 summarizes each of the computer codes and libraries that were reviewed by the Agency. Section 6 provides the summary and conclusions. References are provided at the end of each section.

2.0 BACKGROUND

In §194.22, the Agency required that 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 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.

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.

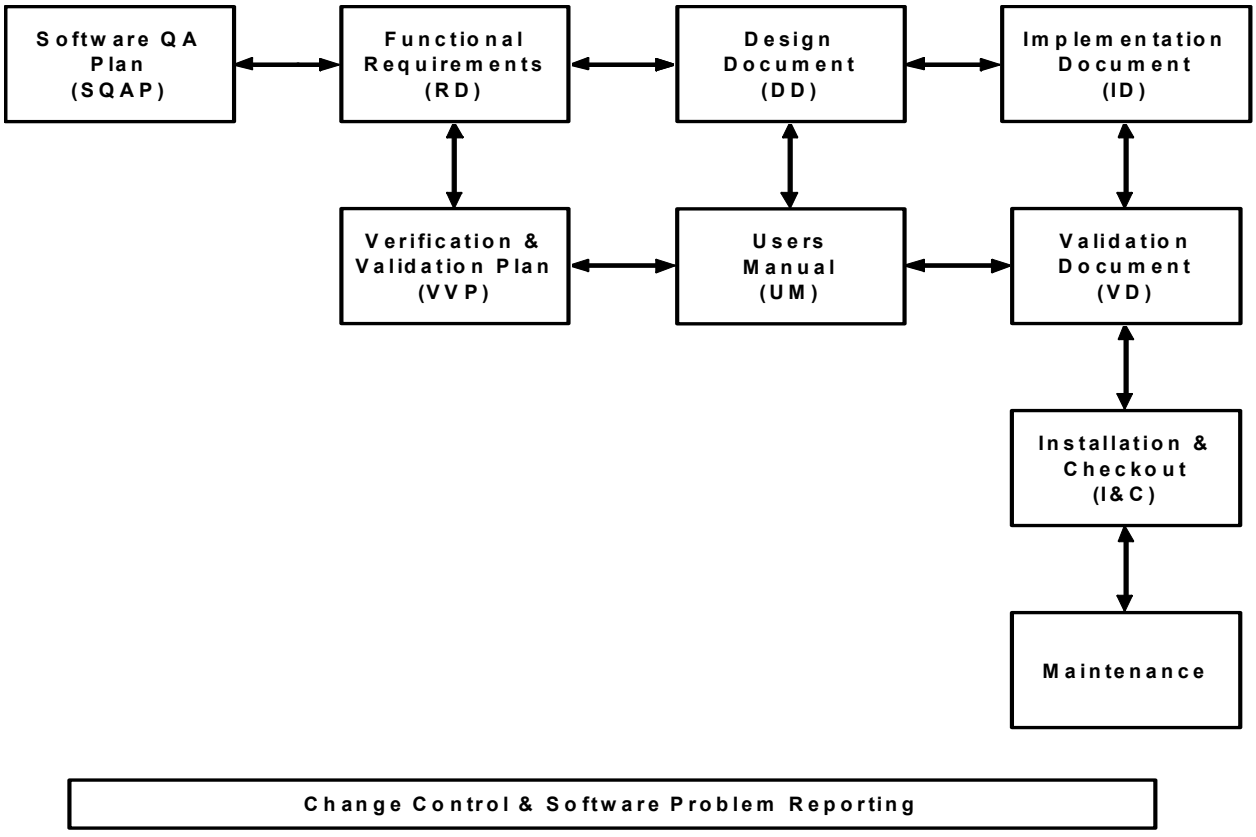
Planning Phase

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 and Verification and Validation Plan (RD/VVP)(Figure 1), which is a single document that identifies

Figure 1 Major Components of DOE's Software Development Process



the computational requirements of the code (e.g., MODFLOW2000 must be able to simulate ground-water 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)(Figure 1), 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 in 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 classifies 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, and the evaluation and resolution of the software problem is 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 makes 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 software, 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 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

- Analysis Report for the ES45 Regression Test

- Analysis Report for the 8400 Regression Test

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.

The Agency 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. In addition to the references cited above, the Agency reviewed User's Manuals, Validation Documents, Implementation Documents and Requirements Document & Verification and Validation Plans for each code. Since all 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 the Agency.

3.0 OVERVIEW OF DOE'S COMPUTER CODE MIGRATION ACTIVITIES

In August 2002 the operating system was upgraded to OpenVMS 7.3-1, and the DEC Alpha 2100s replaced by a Compaq ES40. In June 2003 [REF2], the Agency approved the qualification of the computer codes on the Compaq ES40 and the use of the PA computer codes on this computer. With the exception of NUMBERS, the Agency concluded that all of the remaining 38 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 (Table 3.1). In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 both running Open VMS 7.3-1. This configuration was used for the Compliance Recertification Application (CRA). Because of these changes, regression testing was conducted by DOE for the software codes and 3 libraries on the Compaq ES45 and 8400 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 ES45 and 8400) and comparing the code's output to the output from the code's previous approved validation tests (OpenVMS 7.3-1 running on the Compaq ES40). 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.

The test methodology and acceptance criteria described in AP-089 [REF4] 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 ES45 and 8400 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 previous validation of that code (i.e., Compaq ES40 with OpenVMS 7.3-1). The result was a comprehensive analysis of every test case and every acceptance criterion for each software code.

Table 3.1 Computer Codes Reviewed by the Agency

Code Name	Version	Code Name	Version
ALGEBRACDB	2.35	NUTS	2.05A
BLOTCDB	1.37	PANEL	4.02
BRAGFLO	5.0	PATTRN	1.0
CCDFGF	5.0A	PCCSRC	2.21
CCDFSUM	2.00	PEST	5.5
CUTTINGS_S	5.04A	POSTBRAG	4.00
DRSPALL	1.0	POSTLHS	4.07
DTRKMF	1.0	POSTSECOTP2D	1.04
EPAUNI	1.15A	PREBRAG	7.00
FMT	2.40	PRECCDFGF	1.00B
GENMESH	6.08	PRELHS	2.30
GROPECDB	2.12	PRESECOTP2D	1.22
ICSET	2.22	RELATE	1.43
LHS	2.41	SANTOS	2.17
LHS2STEP	1.04	SECOTP2D	1.41
MATSET	9.10	SGSIM	2.0
MODFLOW2000	1.6	SPLAT	1.02
NONLIN	2.0	STEPWISE	2.21
NUCPLOT	1.2	SUMMARIZE	2.20
NUMBERS	1.19		

In each case, 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.

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.

For several of the computer codes DOE ran the tests outlined in the Validation Plan and 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.

4.0 THE AGENCY'S REVIEW APPROACH

The Agency's review has been conducted by a team consisting of Agency and contractor personnel. The review was initiated 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 results obtained. The following preparatory activities were conducted before conducting on-site reviews:

- Tabulation of the Agency'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.

The following on-site review activities were conducted by the Agency:

- 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/hardware 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.

In addition to the on-site reviews, off-site activities were conducted that included review of relevant documents (e.g., Change Control and Error Reporting Forms, Code Tracking Sheets, Validation Documents), review of all DIFFERENCE files for all tests cases for each of the computer codes and 3 libraries that DOE tested. The results of these activities are summarized in Section 5, below.

References:

REF1. “Review of WIPP Performance Assessment Computer Code Migration Activities”, March 31, 2004. Environmental Protection Agency, EPA Docket: A-98-49, II-B3-70

REF2. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, Environmental Protection Agency, EPA Docket: A-98-49, II-B3-57

REF3. “Department of Energy’s Compliance Certification Application for the Waste Isolation Pilot Plant”, 1996, EPA Docket: A-93-02, II-G-1

REF4. “Analysis Plan for Upgrade of Operating System to OpenVMS 7.3-1 and Hardware to HP Alpha EM45", AP-089, Rev.0, (ERMS #523491), September 11, 2002 http://www.nwmp.sandia.gov/onlinedocuments/wipp-ap.htm

5.0 SUMMARY OF INDIVIDUAL COMPUTER CODE MIGRATION

The following section present the results of the Agency's computer code migration analysis for each individual code examined. Specific software and hardware configurations used in the CRA PA are reviewed, followed by the regression test methodology, the Agency's analysis of the testing, and the Agency'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]). In order to test new operating systems that were added in 2002-03 (Section 1), 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of ALGEBRACDB 2.35 [7] on those operating systems. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1 [8,9]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to ALGEBRACDB on the new hardware systems.

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]). In January 2003, regression test results from ALGEBRACDB 2.35 run on the ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of ALGEBRACDB 2.35 run on a Compaq ES40 with OpenVMS 7.3-1 [8,9].

CAMDAT database files (CDB) are produced in fourteen 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. In the previous ALGEBRACDB 2.35 validation, the CDB files were converted using GROPECDB 2.10. GROPECDB has since been revised to Version 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [5]. GROPECDB 2.12 has also been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Section 5.10, GROPECDB). For DOE's regression test, GROPECDB 2.12 is used to convert the CDB output files from ALGEBRACDB 2.35 in OpenVMS 7.3-1 to ASCII text files.

The regression test methodology uses the VMS DIFFERENCE command to compare output from ALGEBRACDB 2.35 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of ALGEBRACDB 2.35 on the Compaq ES40 with OpenVMS 7.3-1. 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 Test Results

The fifteen test cases for ALGEBRACDB 2.35 were executed on the on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of ALGEBRACDB 2.35 on the Compaq ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE believes that all differences found in the 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.

5.1.4 The Agency's Conclusions

The Agency 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 ES45 and 8400 with OpenVMS 7.3-1.

5.1.5 References

1. Analysis Report. 2003 "Analysis Report for the VMS 7.3-1 Regression Test" Sandia National Laboratories. WIPP:1.3.5.1.1: SFT: QA-L ERMS #525277.

2. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for ALGEBRACDB Version 2.35" (Document Version 1.00) Sandia National Laboratories. ERMS #228109.

3. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for ALGEBRACDB Version 2.35" (Document Version 1.01) Sandia National Laboratories. ERMS #241863.

4. WIPP PA (Performance Assessment). 1995. "Validation Document for ALGEBRACDB Version 2.35" (Document Version 1.00) Sandia National Laboratories. ERMS #228112.

5. WIPP PA (Performance Assessment). 1996. "Validation Document for ALGEBRACDB Version 2.35" (Document Version 1.01) Sandia National Laboratories. ERMS #241865.

6. WIPP PA – Validation(Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12, May 17, 1996" Sandia National Laboratories. ERMS #237497.

7. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.

8. WIPP PA – "Analysis Report for the ES45 Regression Test, March 6, 2003" Sandia National Laboratories. ERMS #530290.

9. WIPP PA – "Analysis Report for the 8400 Regression Test", Sandia National Laboratories. ERMS #527280.

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. In order to test new operating systems that were added in 2002-03 (Section 1), regression test results from BLOTCDB 1.37 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of BLOTCDB 1.37 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of BLOTCDB 1.37 [3]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[4,5]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to BLOTCDB 1.37 on the new hardware systems.

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 [3]. 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[3]. In January 2003, regression test results from BLOTCDB 1.37 run on the ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of BLOTCDB 1.37 run on a Compaq ES40 with OpenVMS 7.3-1 [4,5]. The regression test methodology uses the VMS DIFFERENCE command to compare output from BLOTCDB 1.37 on the Compaq ES40 running OpenVMS 7.3-1 to the output from ES45 and 8400 with OpenVMS 7.3-1.

5.2.3 Test Results

The six test cases for BLOTCDB 1.37 were executed on the Compaq ES45 and 8400 with 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 BLOT 1.37 by using the DIFFERENCE command. 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 The Agency's Conclusions

The Agency 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 BLOT 1.37. The Agency concludes that BLOT 1.37 meets the acceptance criteria in the RD/VVP and is validated for WIPP PA use on the ES45 and 8400 with OpenVMS 7.3-1.

5.2.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for BLOTCDB 1.37" Sandia National Laboratories. ERMS #237499.
2. WIPP PA (Performance Assessment). 1996. "Validation Document for BLOTCDB 1.37", Sandia National Laboratories. ERMS #237502.
3. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
4. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
5. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.3 BRAGFLO

This section presents the regression test results for the BRAGFLO Version 5.0 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]. Several changes were made to BRAGFLO 4.10 during its revision to BRAGFLO 5.0. This included removing a number of parameter assignments from embedded data to input data; moving the porosity surface from embedded data to input data; and changing the input-output format [16].

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.

In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of BRAGFLO 4.10 [13] on those operating systems. For the CCA, the DOE has modified BRAGFLO 4.10 to produce BRAGFLO 5.0 to allow the user to input information that was previously included in the BRAGFLO executable file [16]. Beginning with BRAGFLO 5.0, the user will provide various constants and molecular weights as well as information defining the porosity surface, which comes from the SANTOS software (Section 5.33). Changes from BRAGFLO 4.10 to BRAGFLO 5.0 involve input/output issues.

In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[14,15]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to BRAGFLO 4.10 and 5.0 on the new hardware systems.

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]. Results of regression tests performed on BRAGFLO 4.10 run on the ES40 with OpenVMS 7.3-1 and on the DEC Alpha 2100 with OpenVMS 6.1 have been documented by the Agency [13]. In January 2003, regression test results from BRAGFLO 4.10 run on the ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of BRAGFLO 4.10 run on a Compaq ES40 with OpenVMS 7.3-1 [14,15]. In March 2003, BRAGFLO 5.0 was tested by performing all 12 test cases presented in the RD\VVP and comparing the results to the acceptance criteria [17].

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 from ES45 and 8400 with OpenVMS 7.3-1. Test Case 7 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 ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Sections 5.17, 5.27, and 5.25 for POSTBRAG, SUMMARIZE and SPLAT, respectively).

5.3.3 Test Results

The twelve test cases for BRAGFLO 4.10 were executed on the Compaq ES45 and 8400 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 Compaq ES40 with OpenVMS 7.3-1. DOE used the DIFFERENCE command to compare output files. 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. The Agency 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.

The twelve test cases for BRAGFLO 5.0 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1 [18]. Each test case generated output files, which were compared to the output files from the BRAGFLO 5.0 validation tests, executed on Compaq ES40 with OpenVMS 7.3-1. The differences are limited to code run date and time, file and platform names. 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. The Agency 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.

5.3.4 The Agency's Conclusions

Since all differences are acceptable, the Agency concludes that BRAGFLO 4.10 and BRAGFLO 5.0 meet the acceptance criteria specified in the VVP [1], and thus are validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.3.5 References

1. WIPP PA (Performance Assessment). 1997. "Requirements Document & Verification and Validation Plan for BRAGFLO Version 4.10" Sandia National Laboratories. ERMS #245227
2. WIPP PA (Performance Assessment). 1997. "Validation Document for BRAGFLO Version 4.10" Sandia National Laboratories. ERMS #245242
3. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for BRAGFLO Version 4.00" Sandia National Laboratories. ERMS #230702
4. WIPP PA (Performance Assessment). 1996. "Validation Document for BRAGFLO Version 4.00" Sandia National Laboratories. ERMS #230705
5. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for BRAGFLO Version 4.01" Sandia National Laboratories. ERMS #238122.
6. WIPP PA (Performance Assessment). 1996. "Validation Document for BRAGFLO Version 4.01" Sandia National Laboratories. ERMS #238135.
7. WIPP PA (Performance Assessment). 2001. "Change Control Form, Compaq/DEC Alpha FORTRAN 7.4A Compiler Upgrade" Sandia National Laboratories. ERMS #519716.
8. WIPP PA (Performance Assessment). 2001. "Software Problem Report 01-002 for PREBRAG 6.00 and BRAGFLO 4.10" Sandia National Laboratories. ERMS# 519714.
9. Digital Equipment Corporation. 1996. "OpenVMS 7.1 Release Notes, Section 5.8. Digital Equipment Corporation, Maynard Massachusetts, November 1996". Order number AA-QSBTA-TE.
10. WIPP PA (Performance Assessment). 1998. "WIPP PA Analysis Package for AP-042" Sandia National Laboratories. ERMS #249786.
11. WIPP PA (Performance Assessment). 2003. "BRAGFLO Test Case 7 Results for the OpenVMS 7.3-1 Regression Test" ERMS #525277.
12. Validation Report for BRAGFLO Version 4.10 Test Case 6 Using OpenVMS 7.3.1
13. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
14. WIPP PA – "Analysis Report for the ES45 Regression Test", March 6, 2003 Sandia National Laboratories. ERMS #530290.
15. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.
16. WIPP PA (Performance Assessment). 2003. "Change Control Form, BRAGFLO" Sandia National Laboratories. ERMS #525869.

17. WIPP PA (Performance Assessment). 2003. "Validation Document for BRAGFLO Version 5.00" Sandia National Laboratories. ERMS #525703.
18. WIPP PA (Performance Assessment). 2004. "Results of Regression Testing for BRAGFLO Version 5.00 Running on the Compaq ES45 and 8400 Platforms" Sandia National Laboratories.

5.4 CCDFGF

This section presents the regression test results for the CCDFGF 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.

5.4.1 Introduction

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]. 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 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.

In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of CCDFGF 3.01 [8] on those operating systems. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[9,10]. In August 2003, CCDFGF Version 3.01 was upgraded to Version 5.0. In March 2004, the format of the open statements were changed and the Version number of CCDFGF was upgraded from 5.0 to 5.0A[12]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to CCDFGF testing on the new hardware systems.

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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CCDFGF 3.01 run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from CCDFGF 3.01 on the Compaq ES45 and 8400 running OpenVMS 7.3-1 to the output from previous validation tests.

After CCDFGF was upgraded to Version 5.0, all of the tests described in the *Validation Plan for CCDFGF Version 5.00* (VP) [13]. Regression test results from CCDFGF 5.0A run on the ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CCDFGF 5.0 run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from CCDFGF 5.0A on the Compaq ES45 and 8400 running OpenVMS 7.3-1 to the output from previous validation tests.

5.4.3 Test Results

The five test cases for CCDFGF 3.01 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Each test case generated output files, which were compared to the output files from the CCDFGF 3.01 validation tests, executed on Compaq ES40 with OpenVMS 7.3-1. DOE used the DIFFERENCE command to compare output files. Output files from the test cases were compared to the corresponding output files from the validation of CCDFGF 3.01 by using the DIFFERENCE command. 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. The Agency also found that all other differences in output are acceptable; namely, that the differences are limited to code run dates and times.

The five test cases for CCDFGF 5.0A were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Each test case generated output files, which were compared to the output files from the CCDFGF 5.00 validation tests, executed on Compaq ES40 with OpenVMS 7.3-1. DOE used the DIFFERENCE command to compare output files. Output files from the test cases were

compared to the corresponding output files from the validation of CCDFGF 5.0A by using the DIFFERENCE command. 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. The Agency also found that all other differences in output are acceptable; namely, that the differences are limited to code run dates and times.

5.4.4 The Agency's Conclusions

Since all differences are acceptable, the Agency concludes that CCDFGF 3.01, 5.0 and 5.0A meet the acceptance criteria specified in the VVP [1, 2,13], and thus is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.4.5 References

1. WIPP PA (Performance Assessment). 1997. "Verification and Validation Plan for CCDFGF Version 3.00". Sandia National Laboratories. ERMS #245412.
2. WIPP PA (Performance Assessment). 1997. "Addendum to Verification and Validation Plan for CCDFGF Version 3.01". Sandia National Laboratories. ERMS #245412.
3. WIPP PA (Performance Assessment). 1996. "Validation Document for CCDFGF Version 1.01". Sandia National Laboratories. ERMS #242042.
4. WIPP PA (Performance Assessment). 1996. "Verification and Validation Plan for CCDFGF Version 1.01". Sandia National Laboratories. ERMS #242043.
5. WIPP PA (Performance Assessment). 1996. "Validation Document for CCDFGF Version 2.01". Sandia National Laboratories. ERMS #242772.
6. WIPP PA (Performance Assessment). 1996. "Verification and Validation Plan for CCDFGF Version 2.01". Sandia National Laboratories. ERMS #242768.
7. WIPP PA (Performance Assessment). 1997. "Validation Document for CCDFGF Version 3.00". Sandia National Laboratories. ERMS #245415.
8. WIPP PA (Performance Assessment). 1997. "Addendum to Validation Document for CCDFGF Version 3.01". Sandia National Laboratories. ERMS #245415.
9. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
10. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
11. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.
12. WIPP PA – "Analysis Report for CCDFGF Version 5.00A Regression Testing for the Compaq ES45 and 8400 Platforms " 2004 Sandia National Laboratories.
13. WIPP PA – "CCDFGF Change Control Form from 5.00 to 5.00A" 2003. Sandia National Laboratories. ERMS #531461.
14. WIPP PA (Performance Assessment). 2003. "Validation Document for CCDFGF Version 5.0". Sandia National Laboratories. ERMS #530042.

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].

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of CCDFSUM 2.00 [4] on those operating systems. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[5,6]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to CCDFSUM 2.00 on the new hardware systems.

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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CCDFSUM 2.00 run on the ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CCDFSUM 2.00 on the Compaq ES45 and 8400 running OpenVMS 7.3-1 to the output from the Compaq ES40 running OpenVMS 7.3-1. 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 the Agency 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 ES45 and 8400 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. The Agency also found that all differences in output are acceptable; namely, that the differences are limited to code run dates and time.

5.5.4 The Agency's Conclusions

The Agency 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. The Agency concludes that CCDFSUM 2.00 meets the acceptance criteria in the VVP and is validated for WIPP PA use on the ES45 and 8400 with OpenVMS 7.3-1.

5.5.5 References

1. WIPP PA (Performance Assessment). 1997. "Verification and Validation Plan for CCDFSUM Version 2.00". Sandia National Laboratories. ERMS #243920.
2. WIPP PA. 2001. "Nuclear Waste Management Program Procedure 9-1, Analyses" Sandia National Laboratories.
3. WIPP PA. 1997. "Validation Document for CCDFSUM Version 2.00". Sandia National Laboratories. ERMS #243925.
4. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
5. WIPP PA – "Analysis Report for the ES45 Regression Test, March 6, 2003" Sandia National Laboratories. ERMS #530290.
6. WIPP PA – "Analysis Report for the 8400 Regression Test", Sandia National Laboratories. ERMS #527280.

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_S 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]

In order to test new operating systems that were added in 2002-03 (Section 1), 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 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of CUTTINGS_S 5.04A [8]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[9,10]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to CUTTINGS_S 5.04A on the new hardware systems.

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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CUTTINGS_S 5.04A run on a ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CUTTINGS_S 5.04A on the Compaq ES45 and 8400 running OpenVMS 7.3-1 to the output from the Compaq ES40 running OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different between the two files.

5.6.3 Test Results

The nine test cases for CUTTINGS_S 5.04A were executed on the Compaq ES45 and 8400 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 Compaq ES45 with OpenVMS 7.3-1 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. The Agency 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 The Agency's Conclusions

There were no numerical differences between CUTTINGS_S 5.04A run on the Compaq ES45 and 8400 with OpenVMS 7.3-1 and CUTTINGS_S 5.04 run with ES40 with OpenVMS 7.3-1. Since all differences between the results of CUTTINGS_S 5.04A, are acceptable, the Agency concludes that CUTTINGS_S 5.04A meets the acceptance criteria specified in the RD/VVP [3], and thus is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.6.5 References

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2. Analysis Plan (AP-065). 2000 "Regression for the Upgrade to Open VMS Version 7.2 on the WIPP DEC Alpha Cluster" Sandia National Laboratories.
3. WIPP PA (Performance Assessment). 1997. "Requirements Document & Verification and Validation Plan for CUTTINGS_S Version 5.04". Sandia National Laboratories. ERMS #245971.
4. WIPP PA (Performance Assessment). 1996, "Requirements Document & Verification and Validation Plan for CUTTINGS_S Version 5.03" Sandia National Laboratories. ERMS #237763.
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7. WIPP PA (Performance Assessment). 1996. "Validation Document for GROPECDB Version 2.12", Sandia National Laboratories. ERMS #237497.
8. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
9. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
10. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.7 DRSPALL

This section presents the validation and verification results for the DRSPALL Version 1.0. DRSPALL calculates the volume of waste subjected to material failure and transport to the surface during an inadvertent drilling intrusion into WIPP repository. The code will use either text-formatted input and output files or CAMDAT database files [6] for I/O, and will calculate coupled repository and wellbore transient compressible fluid flow before, during, and after the drilling intrusion process. Mathematical models are included for bit penetration, multi-phase flow in the well, fluid expulsion at the surface, coupling of the well and the repository, repository spalling (tensile) failure associated with fluidized bed transport, and repository internal gas flow.

5.7.1 Introduction

DRSPALL calculates the spallings release, defined as the mass of waste subject to tensile failure and transport during an inadvertent drilling intrusion into a high-pressure WIPP repository. Cuttings removed by the direct action of the drill bit, and cavings removed by shear forces of the drilling mud against the drilled cavity wall are handled separately in the CUTTINGS code (Section 5.6). DRSPALL uses both text-formatted and CDB input and output files, and calculates coupled repository and wellbore transient compressible fluid flow before, during, and after the drilling intrusion process. Mathematical models include multi-phase flow in the well, fluid expulsion at the surface, coupling of the well and the repository, repository spalling (tensile) failure associated with fluidized bed transport, and repository internal gas flow. The wellbore model is one-dimensional linear, and the repository model is one-dimensional, either spherical or cylindrical.

DRSPALL is based on the theory of one-dimensional, time-dependent compressible isothermal fluid flow. Somewhat different forms of that theory are used, depending on whether the flow is in the wellbore or the repository, and whether the wellbore currently penetrates the repository. The wellbore and repository flows are coupled at a specified boundary. Flow in the well is treated as a compressible, viscous, multi-phase mixture of mud, gas, salt, and possibly waste solids. Flow in the repository is treated as viscous, compressible single-phase gas flow in a porous solid. At the cavity forming the repository-wellbore boundary (following penetration), waste solids freed by drilling, tensile failure, and associated fluidization may enter the wellbore flow stream. Between the well and the repository, flow is treated according to the state of penetration. The wellbore calculations use time-marching finite differences. These are part of a single computational loop. The numerical method is Eulerian in that zone boundaries are fixed, and fluid moves through the interfaces by convection. Quantities are zone-centered and integration is explicit in time. The repository calculations also use time-marching finite differences that are part of a single computational loop. The method is implicit with spatial derivatives determined after the time increment.

Software Requirements (NP 19-1) requires that seven primary documents be developed, reviewed and maintained for the DRSPALL software: the Software QA plan, a Requirements Document (RD), Verification and Validation Plan (WP), User's Manual (UM), Design Document (DD), Implementation Document (ID), and the Validation Document (VD). Configuration control is maintained through completion of Installation & Checkout (I&C) documentation for all changes made to DRSPALL , and system software and/or system hardware. In addition, Change Control (CC) and Software Problem Report (SPR) documents are completed, as appropriate.

DRSPALL was originally developed in Digital Visual FORTRAN Version 6 and was designed to run under Microsoft WindowsTM. However, for implementation in WIPP and other similar performance assessments (PA) the code has been ported to the WIPP Alpha-Cluster running Open VMS. DRSPALL Version 1.00 was built in September 2003; the validation of DRSPALL Version 1.00 was conducted on a COMPAQ ES40 platform and documented in the Verification and Validation Plan and Validation Document for DRSPALL Version 1.00 [4]. In January

2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to DRSPALL 1.0 on the new hardware systems.

5.7.2 Test Methodology

The test set for DRSPALL consists of four test cases that are designed to address the requirements established in Section 2 of the VVP\VD [4]. The test cases are numbered #1, #2, #4, and #5 (i.e., there is no Test Case #3). Functional testing was performed by running the test cases with the production executable for DRSPALL. (The production executable is used to perform the CRA calculations.) The production executable is generated as described in the DRSPALL Implementation Document [3]. All files used in functional testing will be stored in class QE0l00 of the DRS library of the Software Configuration Management System (SCMS) accessible from the WIPP Alpha Cluster. The files include the DRSPALL input and output files, all procedure files to execute DRSPALL, and output files from other numerical solutions used for comparisons. A single test case requires that DRSPALL be executed one or more times. Each execution is referred to by DOE as a "case" or "subcase" or "run". For example, Test Case #5 has six subcases, labeled case 5.1 through 5.7 (5.4 is not defined), and the files for the test case are distinguished by "TC51 " through "TC57" in their names.

The entire test suite for DRSPALL Version 1.0 was executed on the COMPAQ ES45 and 8400 platforms with Open VMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from DRSPALL 1.0 on the Compaq ES45 and 8400 running OpenVMS 7.3-1 to the output from the Compaq ES40 running OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different between the two files.

5.7.3 Test Results

DRSPALL reads its run parameters from an input control file (file extension ".DRS"). The DRSPALL User's Manual [5] provides instructions on constructing and interpreting the input control file. Each subcase of the four test cases has its own input control file. The input control file contains the test subcase number (as "Validation Test Case"). DRSPALL responds to the test case number by creating special output files that contain information used for validation, by initializing conditions (e.g., boundary conditions) specific to the test case, and by limiting the processing to that necessary for validation. The Design Document for DRSPALL [2] describes any non-standard processing that is dependent on the test case. Each execution of DRSPALL generates an output CAMDAT file (".CDB") and an output diagnostics file (".DBG"). The DRSPALL User's Manual [5] describes the variables output on the CAMDAT file. Variables on a CAMDAT file may be extracted in tabular form using the GROPECDB utility (Section 5.12) or plotted using the BLOTCDB utility (Section 5.2). In addition to the standard output files, a particular test case may generate additional files to be used for validation only. These validation files are described under the relevant test case section.
Most test cases compare the results of the DRSPALL execution with those generated by analytical and other numerical solutions. These solutions are described in detail in the relevant test case section in the VVP\VD [4].

The DRSPALL test cases are run with a set of procedure files. Each test case has its own procedure file, and each subcase has a procedure file. The procedure file for the test case (e.g., DRS_TC5.COM) executes all subcases. It creates a subdirectory for the subcase, fetches the subcase procedure file from the SCMS, and executes the subcase procedure file, usually by submitting a job to a batch queue. The procedure file for the subcase (e.g., DRS TC5l.COM) fetches the DRSPALL input file(s), and executes DRSPALL with the appropriate input and output file designations. The subcase procedure file may also do some simple postprocessing on the CAMDAT file, but most post-processing will be done manually by the tester. The test cases are designed to meet the requirements coverage presented in Section 6 of the VVP\VD. these test cases. All subcases of the four test cases for DRSPALL were executed on the COMPAQ ES45 and 8400 platforms with Open VMS 7.3-1. Output from the test cases were compared to the corresponding output files from the validation of DRSPALL on a COMPAQ ES40 with Open VMS 7.3-1. The comparison found that the differences in the output files were limited to code run dates and time, file and directory names, platform names and execution statistics.

5.7.4 The Agency's Conclusions

There were no numerical differences between DRSPALL Version 1.0 run on the Compaq ES45 and 8400 with OpenVMS 7.3-1 and DRSPALL Version 1.0 run with ES40 with OpenVMS 7.3-1. Since all differences between the results of DRSPALL Version 1.0 , are acceptable, the Agency concludes that DRSPALL Version 1.0 meets the acceptance criteria specified in the RD/VVP, and thus is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.7.5 References

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2. WIPP PA (Performance Assessment). 2003. "Design Document for DRSPALL Version 1.00 (document version 1.10)" Sandia National Laboratories. ERMS #529878.
3. WIPP PA (Performance Assessment). 2003. "Implementation Document for DRSPALL Version 1.00 (document version 1.20)" Sandia National Laboratories. ERMS #524781.
4. WIPP PA (Performance Assessment). 2003. "Verification and Valedation Plan and Validation Document for DRSPALL Version 1.00 (document version 1.10)" Sandia National Laboratories. ERMS #524782.
5. WIPP PA (Performance Assessment). 2003. "User's Manual for DRSPALL Version 1.00 (document version 1.10)" Sandia National Laboratories. ERMS #524780.
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5.8 DTRKMF

This section presents the validation and verification results for the DTRKMF Version 1.0. This document describes the working design of the software DTRKMF (Double precision TRacKing with MODFLOW 2000 [1] file input) that was developed to visualize the flow fields computed as part of the PA process. This visualization is accomplished by abstracting the two-dimensional (2-D) or three-dimensional (3-D) flow fields into one dimensional (1-D) particle tracks and then mapping simplified transport solutions onto these tracks. This mapping approach greatly reduces the cost of computing transport solutions and also produces solutions with considerably less numerical dispersion.

5.8.1 Introduction

DTRKMF is used for estimating the migration paths of neutrally buoyant particles through a known porous media fluid velocity field. As output, the program provides the spatial location of the particle over time until the particle reaches a user-defined boundary. The flow field that is input to DTRKMF is a discretized velocity field - values of velocities for discrete locations within a computational domain. The DTRKMF software will use linear assumptions to develop a semi-analytical technique to solve a system of ordinary differential equations (ODEs) representing fluid flow in a porous media. DTRKMF was developed using the Lahey/Fujitsu Fortran 95 Compiler on an i686 PC running the Red Hat Linux release 7.2 Operating System. The DTRKMF code is documented as specified in NQA-2a-1990 in the Design Document, User's Manual, the Requirements Document & Verification and Validation Plan, the Validation Document, and the Implementation Document [2-7].

5.8.2 Test Methodology

The validation of DTRKMF involved two test cases that were designed to test and verify that the DTRKMF code correctly tracks particle motion under the following specific conditions:

1) A two-dimensional, discretized steady state velocity field in which the flow directions vary from point to point, and in which, over the domain of interest, the magnitudes vary in a non-linear fashion.
2) The positions of the origins of each velocity vector correspond to a finite-difference grid that has nonuniform spacing of columns and rows.

5.8.3 Test Results

For the two test cases, the domain of interest is a square that is 1000 x 1000 m. The grid contains 400 cells - twenty rows and twenty columns. The cell widths and heights vary from 100 x 100 m at the lower left hand corner to 20 x 20 m at the upper right hand corner. Three particles were released at coordinates (600,950), (650,950) and (8.5,17.5). The coordinates for the third particle were specified by *i-j* index indicating the center of cell located in the 8th row and the 17th column. This corresponds to *x-y* coordinates equal to (621.8181, 946.1717). The functional requirements were verified by a series of hand calculations, visual inspections of the data, and spread sheets.

5.8.4 The Agency's Conclusions

The Agency has determined that the information required to be submitted to the Agency pertaining to DTRKMF provides an adequate description of the code used in the calculations, a description of the limits of applicability of the code, detailed instructions for executing the computer code, hardware and software requirements to run the code, input and output formats with explanations of each input and output variable and parameter, listings of input and output files from sample computer runs, and reports on code verification, benchmarking, validation and quality assurance procedures that are adequate for use in CRA PA. Therefore, the Agency finds that DOE is in compliance with §194.23(c)(2).

5.8.5 References

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4. WIPP PA, 2002b. *WIPP PA Verification & Validation Plan For DTRKMF Version 1.00;* Document Version 1.00; ERMS #523243, Sandia National Laboratories, Albuquerque, NM.WIPP PA, 2002c. *WIPP PA User's Manual For DTRKMF (Version 1.00);* Document Version 1.00;ERMS #523246, Sandia National Laboratories, Albuquerque, NM.
5. WIPP PA, 2000, *WIPP PA Requirements Document For DTRKCDB (Version 1.00), Document Version 1.00*; EMRS #515806, Sandia National Laboratories, Albuquerque, NM.`WIPP PA, 2002a, *WIPP PA Requirements Document For DTRKMF Version 1.00, Document*
6. WIPP PA, 2002b, *WIPP PA User's Manual For DTRKMF Version 1.00, Document Version 1.00*; EMRS #523246, Sandia National Laboratories, Albuquerque, NM.
7. WIPP PA, 2002c, *WIPP PA Verification and Validation Plan For DTRKCDB (Version 1.00), Document Version 1.00*; EMRS #515089, Sandia National Laboratories, Albuquerque, NM.

5.9 EPAUNI

This section presents the regression test results for Versions 1.14, 1.15 and 1.15A of the EPAUNI 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.

5.9.1 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]. In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of EPAUNI 1.14 on those operating systems [2]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[3,4]. In

March 2003, the code underwent further regression testing to verify its operation on the ES45 platform [8]. The code version changed to version 1.15 in May 2003 to allow more user control on input and to create logical output names. In July of 2003, EPAUNI was updated to version 1.15A. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to EPAUNI 1.14, 1.15, and 1.15A on the new hardware systems.

5.9.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of EPAUNI 1.14 run on a ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from various versions of the codes. Results of the five test cases run with EPAUNI 1.15 on the ES45 and 8400 with OpenVMS 7.3-1 were subsequently compared against the output from the previous validation of EPAUNI 1.14. Most recently test results from EPAUNI 1.15A run on the ES45 and 8400 platforms with OpenVMS 7.3-1 were compared to results from the validations tests of EPAUNI 1.15 run on the ES40 with OpenVMS 7.3-1 [9].

5.9.3 Test Results

The results of the test described above are that only very minor differences (e.g., spacing, version number) were found for the five test cases.

5.9.4 The Agency's Conclusions

Since there are only minor differences between the results of EPAUNI 1.14, in OpenVMS 7.3-1, and EPAUNI 1.14, in OpenVMS 6.1, the Agency concludes that EPAUNI 1.14 meets the acceptance criteria specified in the VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Furthermore, since there are only minor differences between the results of EPAUNI 1.15, in OpenVMS 7.3-1, and EPAUNI 1.14, in OpenVMS 6.1, the Agency concludes that EPAUNI 1.15 meets the acceptance criteria specified in the RD and VVP [1, 2], and thus is considered as validated on the COMPAQ ES40 with OpenVMS 7.3-1. Finally, the Agency also concludes that EPAUNI 1.15A meets the acceptance criteria specified in the VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.9.5 References

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2. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
3. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
4. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.
5. WIPP PA (Performance Assessment). 2003. “Design Document for EPAUNI Version 1.15” Sandia National Laboratories. ERMS #529567.
6. WIPP PA (Performance Assessment). 2003. “User’s Manual for EPAUNI Version 1.15” Sandia National Laboratories. ERMS #529570.
7. WIPP PA (Performance Assessment). 2003. “Validation Document for EPAUNI Version 1.15” Sandia National Laboratories. ERMS #529568.
8. WIPP PA (Performance Assessment). 2003. “Addenda to Validation Document for EPAUNI Version 1.15” Sandia National Laboratories. ERMS #530204
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5.10 FMT

This section presents the regression test results for the FMT Version 2.40 code. FMT 2.40 calculates the chemical equilibrium in high-ionic-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].

5.10.1 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 created. 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].

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of FMT 2.40 on those operating systems [11]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[12,13]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to FMT 2.40 on the new hardware systems.

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 FMT Version 2.40 RD/VVP) [1]. Regression test results from FMT 2.40, run on the ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of FMT 2.40, run on the ES40 with OpenVMS 7.3-1 [11].

The regression test methodology uses the VMS DIFFERENCE command to compare output from FMT 2.40 on the Compaq ES45 and 8400 with OpenVMS7.3-1 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.

5.10.3 Test Results

The eight test cases for FMT 2.40 were executed on the Compaq ES45 and 8400 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 Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.10.4 The Agency's Conclusions

Since all differences in the regression results are acceptable, the Agency concludes that FMT 2.40 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS Version 7.3-1.

5.10.5 References

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7. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for FMT Version 2.20" Sandia National Laboratories. ERMS #242044.
8. WIPP PA (Performance Assessment). 1997. "Validation Document for FMT Version 2.30" Sandia National Laboratories. ERMS #243038.
9. WIPP PA (Performance Assessment). 1997. "Requirements Document & Verification and Validation Plan for FMT Version 2.30" Sandia National Laboratories. ERMS #243035.
10. Memorandum dated February 4, 2003. "Additional Evaluation of FMT Test Case 1" Sandia National Laboratories. ERMS #525279.
11. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
12. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.

13. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.11 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.

5.11.1 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). In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of GENMESH 6.08 on those operating systems [6]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[7,8]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to GENMESH 6.08 on the new hardware systems.

5.11.2 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 ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of GENMESH 6.08, run on the ES40 with OpenVMS 7.3-1.

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 GROPECDB 2.10. GROPECDB 2.12 has been validated on a Compaq ES40 with OpenVMS 7.3-1 as part of the OpenVMS 7.3-1 Regression Test [6]. It has also been validated on the ES45 and 8400 with OpenVMS 7.3-1 (see Section 5.10). For this regression test, GROPECDB 2.12 is used to convert the CDB output files from GENMESH 6.08 in OpenVMS 7.3-1.

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 ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware testing 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 hardware regression test, DOE only compares the "GROPE" output files. This approach is considered acceptable by the Agency.

5.11.3 Test Results

The nine test cases for GENMESH 6.08 were executed on the Compaq ES45 and 8400 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 Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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

5.11.4 The Agency's Conclusions

Since all differences in the regression test results of GENMESH 6.08 are acceptable, the Agency concludes that GENMESH 6.08 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.11.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for GENMESH Version 6.08" Sandia National Laboratories. ERMS #240688.
2. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for GENMESH Version 6.07ZO" Sandia National Laboratories. ERMS #223334

3. WIPP PA (Performance Assessment). 1996. “GENMESH Version 6.08, Software Installation and Checkout Form” Sandia National Laboratories. ERMS #230696.
4. WIPP PA (Performance Assessment). 1997. “Inspection of GENMESH, Version 6.08", [(w/att) Attachment 1 & 2] Sandia National Laboratories. ERMS #245466.
5. WIPP PA (Performance Assessment) 1996. “Validation Document for GROPECDB Version 2.12” Sandia National Laboratories. ERMS #237497.
6. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
7. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
8. WIPP PA – “Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.12 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).

5.12.1 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).

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency’s approval with respect to the migration and verification of GROPECDB 2.12 on those operating systems [4]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[5,6]. The discussion below documents the test methodology, regression test results, and the Agency’s conclusions with respect to GROPECDB 2.12 on the new hardware systems.

5.12.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of GROPECDB 2.12 run on the ES40 with OpenVMS 7.3-1

The regression test methodology uses the VMS DIFFERENCE command to compare output from GROPECDB 2.12 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of GROPECDB 2.12 running on ES40 with OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.12.3 Test Results

The eight test cases for GROPECDB 2.12 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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

5.12.4 The Agency's Conclusions

Since all differences in the regression test results of GROPEC.12 are acceptable, the Agency concludes that GROPECDB 2.12 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.12.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for GROPECDB Version 2.12". Sandia National Laboratories. ERMS #237494.
2. WIPP PA (Performance Assessment). 1996. "Validation Document for GROPECDB Version 2.12", Sandia National Laboratories. ERMS #237497
3. CMS Inspection of GROPECDB, Version 2.12, ERMS #246352, July 8, 1997.
4. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.

5. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
6. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.13 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.

5.13.1 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.

In order to test new operating systems that were added in 2002-03 (Section 1), 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 2.22 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of ICSET 2.22 on those operating systems [5]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[6,7]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to ICSET 2.22 on the new hardware systems.

5.13.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of ICSET Version 2.21ZO run on the ES40 with OpenVMS 7.3-1.

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 GROPECDB 2.10. GROPECDB has since been revised to Version 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4]. GROPECDB 2.12 has been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Section 5.10). For this regression test, GROPECDB 2.12 was used to convert the CDB output files from RELATE 1.43 in OpenVMS 7.3-1.

5.13.3 Test Results

The six cases for ICSET 2.22 were executed on the Compaq ES45 and 8400 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 the ES40 with OpenVMS 7.3-1 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. The Agency also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time, and file names.

5.13.4 The Agency's Conclusions

Since all differences between the results of the ICSET regression test, are acceptable, the Agency concludes that ICSET 2.22 meets the acceptance criteria specified in the RD/VVP [1], and thus is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.13.5 References

1. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for ICSET version 2.21ZO". Sandia National Laboratories. ERMS #223623.
2. WIPP PA (Performance Assessment). 1995. "Validation Document for ICSET version 2.21ZO", Sandia National Laboratories. ERMS #223620.
3. WIPP PA (Performance Assessment). 1995. "Change Control Form" for ICSET 2.22, Sandia National Laboratories. ERMS #236482.
4. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12" Sandia National Laboratories. ERMS #237497.
5. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
6. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
7. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.14 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. The LHS program 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. LHS sampling is generally used for the WIPP PA.

5.14.1 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).

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of LHS 2.41 on those operating systems [6]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[7,8]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to LHS 2.41 on the new hardware systems.

5.14.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of LHS 2.41 run on the ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from LHS 2.41 on the Compaq ES45 and 8400 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.

5.14.3 Test Results

The ten test cases for LHS 2.41 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. No differences were found.

5.14.4 The Agency's Conclusions

Since no differences were found, the Agency concludes that LHS 2.41 meets the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.14.5 References

1. WIPP PA (Performance Assessment). 1996 "Requirements Document & Verification and Validation Plan for LHS Version 2.41" Sandia National Laboratories. ERMS #230731.
2. WIPP PA (Performance Assessment). 1995 "Requirements Document & Verification and Validation Plan for LHS Version 2.32ZO" Sandia National Laboratories. ERMS #223533.
3. WIPP PA (Performance Assessment). 1995. "Validation Document for LHS Version 2.32ZO" Sandia National Laboratories. ERMS #223536.
4. WIPP PA (Performance Assessment). 1996. "Validation Document for LHS Version 2.41" Sandia National Laboratories. ERMS #230734.
5. OpenVMS 7.1 Release Notes, Section 5.8. Digital Equipment Corporation, Maynard Massachusetts, November 1996. Order number AA-QSBTB-TE.
6. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
7. WIPP PA – "Analysis Report for the ES45 Regression Test, March 6, 2003" Sandia National Laboratories. ERMS #530290.
8. WIPP PA – "Analysis Report for the 8400 Regression Test " Sandia National Laboratories. ERMS #527280.

* 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" ERMS #238837. This discrepancy had been previously identified and documented and will be corrected during the next revision to the code documentation.

5.15 LHS2STEP

This section presents the regression test results for the LHS2STEP Version 1.04 code. The purpose of LHS2STEP is to read an LHS sampled output file containing the independent variables, and write an output file for either the STEPWISE (Section 5.37) or PCCSRC (Section 5.24) codes.

5.15.1 Introduction

LHS2STEP Version 1.04 was validated in November 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4, 5] by demonstrating that the results of three Test Cases (1 through 3) met the acceptance criteria defined in the RD/VVP for LHS2STEP 1.04 [2, 3].

The tests selected used in this regression testing of this code are the three test cases described in the *Requirements Document & Verification and Validation Plan for LHS2STEP Version 1.03 and Addendum Version 1.04* (RD/VVP) [2, 3]. Three sets of regression tests were executed and the results evaluated.

1.) Regression test results from LHS2STEP 1.04 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of LHS2STEP 1.04 run on a DEC Alpha 2100 with OpenVMS 6.1.
2.) Regression test results from LHS2STEP 1.04 run on the ES45 with OpenVMS 7.3-1 were compared to results from the validation tests of LHS2STEP 1.04 run on the ES40 with OpenVMS 7.3-1.
3.) Regression test results from LHS2STEP 1.04 run on the 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of LHS2STEP 1.04 run on the ES40 with OpenVMS 7.3-1.

5.15.2 Test Methodology

As described in the AP-089 [6], the regression test methodology uses the VMS DIFFERENCE command to compare output from LHS2STEP 1.04 on the COMPAQ ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of LHS2STEP Version 1.04 with OpenVMS 6.1 for the ES40 and OpenVMS 7.3-1 for the ES45 and 8400. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files. Comparing each pair of output files results in a list of differences. Differences that are limited to code run date and time, platform names, system version numbers, directory and file names, user names, and execution statistics are acceptable. Differences involving numerical output require additional analysis by DOE to determine the origin of the differences and whether the differences affect the code's performance. Numerical differences may be determined to be acceptable based on the analysis of each difference.

5.15.3 Test Results

The three test cases for LHS2STEP 1.04 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 LHS2STEP 1.04 on a DEC Alpha 2100 with OpenVMS 6.1 by using the VMS DIFFERENCE command. The comparison found that all differences in output are limited to code run date and time, platform names, system version numbers, and directory and file names. The three test cases for LHS2STEP 1.04 were executed on the COMPAQ ES45 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of LHS2STEP 1.04 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. The comparison found that all differences in output are limited to code run date and time, platform names, system version numbers, and directory and file names.

The three test cases for LHS2STEP 1.04 were executed on the COMPAQ 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of LHS2STEP 1.04 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. The comparison found that all differences in output are limited to code run date and time, platform names, system version numbers, and directory and file names.

5.15.4 The Agency's Conclusions

Since the differences between the results of LHS2STEP 1.04, in OpenVMS 7.3-1, and LHS2STEP 1.04, in OpenVMS 6.1 are acceptable, the Agency concludes that LHS2STEP 1.04 meets the acceptance criteria specified in the RD/VVP [2, 3], and thus is considered as validated on the COMPAQ ES40 with OpenVMS 7.3-1.

Since there were no differences between the results of LHS2STEP 1.04, on the COMPAQ ES45 with OpenVMS 7.3-1, and LHS2STEP 1.04, on the ES40 with OpenVMS 7.3-1, the Agency concludes that LHS2STEP 1.04 meets the acceptance criteria specified in the RD/VVP [2, 3], and thus is considered as validated on the COMPAQ ES45 with OpenVMS 7.3-1.

Since there were no differences between the results of LHS2STEP 1.04, on the COMPAQ 8400 with OpenVMS 7.3-1, and LHS2STEP 1.04, on the ES40 with OpenVMS 7.3-1, the Agency concludes that LHS2STEP 1.04 meets the acceptance criteria specified in the RD/VVP [2, 3], and thus is considered as validated on the COMPAQ 8400 with OpenVMS 7.3-1.

5.15.5 References

1. U.S. DOE (U.S. Department of Energy). 1996. "Title 40 CFR 191 Compliance Certification Application for the Waste Isolation Pilot Plant" DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.

2. WIPP PA (Performance Assessment). 1995. “Requirements Document & Verification and Validation Plan for LHS2STEP Version 1.03” (Document Version 1.00) Sandia National Laboratories. ERMS #227932.
3. WIPP PA (Performance Assessment). 1996. “Requirements Document & Verification and Validation Plan for LHS2STEP Version 1.03 and Addendum Version 1.04” (Document Version 1.00) Sandia National Laboratories. ERMS #227932.
4. WIPP PA (Performance Assessment). 1995. “Validation Document for LHS2STEP Version 1.03” (Document Version 1.00) Sandia National Laboratories. ERMS #227933.
5. WIPP PA (Performance Assessment). 1996. “Validation Document for LHS2STEP Version 1.03 and Addendum Version 1.04” (Document Version 1.00) Sandia National Laboratories. ERMS #227933.
6. Analysis Plan (AP-089). 2002 “Upgrade of Operating System to OpenVMS 7.3-1 and Hardware to HP Alpha ES45” Sandia National Laboratories. ERMS #523491.

5.16 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 using 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.

5.16.1 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.

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency’s approval with respect to the migration and verification of MATSET 9.10 on those operating systems [5]. In January

2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[6,7]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to MATSET 9.10 on the new hardware systems.

5.16.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of MATSET 9.10 run on ES40 with OpenVMS 7.3-1.

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 GROPECDB 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4]. GROPECDB 2.12 has also been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression testing (see Section 5.10). For this regression test, GROPECDB 2.12 was used to convert the CDB output files from MATSET 9.10 in OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from MATSET 9.10 on the Compaq ES45 and 8400 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.

5.16.3 Test Results

The three test cases for MATSET 9.10 were executed on the Compaq ES45 and 8400 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 the ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.16.4 The Agency's Conclusions

Since all differences between the results of the ICSET regression test are acceptable, the Agency concludes that MATSET 9.10 meets the acceptance criterion specified in the VVP/VD [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.16.5 References

1. WIPP PA (Performance Assessment) 1995. “Verification and Validation Plan/ Validation Document for MATSET Version 9.10” Sandia National Laboratories. ERMS #519734.
2. WIPP PA (Performance Assessment). 1996. “Validation Document for MATSET Version 9.0” Sandia National Laboratories. ERMS #230690.
3. WIPP PA (Performance Assessment). 1996. “Requirements Document & Verification and Validation Plan for MATSET Version 9.0” Sandia National Laboratories. ERMS #230687.
4. WIPP PA (Performance Assessment) 1996. “Validation Document for GROPECDB Version 2.12” Sandia National Laboratories. ERMS #237497.
5. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
6. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
7. WIPP PA – “Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.17 MODFLOW2000

This section presents DOE’s verification and validation of MODFLOW2000. The MODFLOW2000 code, Version 1.6, is an acquired code that solves both steady state and transient groundwater flow problems. The MODFLOW groundwater software was developed by the US Geological Survey and has been continually upgraded since the first version, MODFLOW88, was released in 1988.

5.17.1 Introduction

MODFLOW is a computer program that numerically solves the three-dimensional ground-water flow equation for a porous medium by using a finite-difference method. MODFLOW is designed to be modular in that different functionalities such as wells, rivers, evapotranspiration, etc. can be added as modules to the basic groundwater flow solutions. Although MODFLOW was designed to be easily enhanced, the design was oriented toward additions to the ground-water flow equation. Frequently there is a need to solve additional equations; for example, transport equations and equations for estimating parameter values that produce the closest match between model-calculated heads and flows and measured values. The version of MODFLOW used by DOE, MODFLOW2000 (MF2K) is designed to accommodate the solution of equations in addition to the ground-water flow equation. The user's manual for MODFLOW 2000 [4] contains an overview of the old and added design concepts, documents one new package, and contains input instructions for using the model to solve the ground-water flow equation. For transient and steady state, single-phase, ground water flow problems, the MODFLOW2000 software is executed with the prescribed boundary and initial conditions, running under the Linux operating system.

Software Requirements (NP 19-1) requires that seven primary documents be developed, reviewed and maintained for the MODFLOW software: the Software QA plan, a Requirements Document (RD), Verification and Validation Plan (VVP), User's Manual (UM), Design Document (DD), Implementation Document (ID), and the Validation Document (VD). DOE reviewed the preexisting documentation available for MODFLOW2000 from the US Geological Survey and found it to provide the necessary information that is usually within the RD, DD, UM and VVP. Therefore, the only additional documents that were produced by DOE are the Software QA Plan, the ID, VD and the Installation and Check Out forms. DOE notes that documentation for version 1.6 will remain as the base documents for any future versions of the software with addenda for each of the documents defining the additional scope of the revised software. Configuration control is maintained through completion of Installation & Checkout (I&C) documentation for all changes made to MODFLOW2000, and system software and/or system hardware. In addition, Change Control (CC) and Software Problem Report (SPR) documents are completed, as appropriate.

5.17.2 Test Methodology

The DOE designed 8 test cases to verify the functional requirements necessary for the verification/validation of the computer code for the WIPP PA. The input files and corresponding output files are provided with the installation package. Listings of these files are included in Appendix A to the VD corresponding to the test number and test name. Validation testing consisted of running all test cases and checking resulting output for consistency with documented results. The test cases were run with the production executable for MF2K. The production executable was created on the target platform by the code sponsor and stored using CVS version control on the target platform (CVSROOT - /h/WIPPcvs, repository - src/mf2k). The executable, source code and test problems were also stored in SCMS on the WIPP Compaq Alpha cluster (Library- MF2K, class- VER_0160). DOE believes that by using the production executable for functional testing it will not be necessary to rerun the test set when an executable is required for a Performance Assessment calculations. The MF2K production executable and input and output test files were obtained from configuration management and placed in the test directories on the target platform. All of the input files were used unmodified from the source code package, except for the **.nam* file, where the file pathnames were modified to reflect the different syntax between the Windows and Linux operating systems. The MF2K output listing files, **.lst*, created during testing were compared to the output listing files obtained from the MF2K installation package and differences were noted and addressed. The listing file is the primary ASCII text file created by MF2K and contains an input echo, solver performance information, calculated head and a budget summary. This same procedure was used for all the tests, with the exception of Test Case #8, the algebraic multi-grid (AMG) test. The intent of Test Case 8 is to verify the Linked algebraic Multi-Grid solver (LMG) package which was not included in the MODFLOW2000 test suite. A test identical to Test Case #1, BCF2SS, was chosen except that the solver has been switched from the Strongly Implicit Procedure (SIP) to the LMG or linked algebraic Multi-Grid solver. The results of Test Case #8 were compared to the results of Test Case #1.

The test was considered successful if the MODFLOW2000 output listing file was the same as the documented listing file, within reasonable accuracy and accounting for date and filename changes. Reasonable accuracy was defined as numerically equal, except in the last printed digit for numbers printed with 6 or less digits or in the digits greater than the 6th for numbers printed with greater than 6 digits. Original output files are listed in the Appendix H of the Validation Document while the output files generated during testing were stored in CVS on the target platform and in SCMS accessible from the WIPP VMS Alpha cluster and. The same criteria were used for all the test cases.

5.17.3 Test Results

The differences for all of the tests are due to addition of the build date to the listing header and path name syntax differences between Windows and Linux. There were not numerical differences except for the (IN -OUT) variable which was calculated as the difference between two large numbers (>7 digits). The discrepancy was in the insignificant digits of the original two numbers. The differences are due to addition of the build date to the listing header and path name syntax differences between Windows and Linux. Numerical differences are in the 6th digit or greater, except for the (IN - OUT) variables which were calculated as the difference between two large numbers (>7 digits). The discrepancies were in the insignificant digits of the original two numbers.

5.17.4 The Agency's Conclusions

All test results met the acceptance criteria specified in Section 5.2 of the VD. Those differences that were present were character differences due to the addition of the build date to the listing header; and in syntax differences between Windows and Linux path names; or were floating-point differences in insignificant digits. The AMG/LMG test produced very different output listings due to solver specific output, but the head results and groundwater budgets were the same as the PCG (Test Case#1, BCF2SS) results to within the acceptance criteria. Therefore, the Agency concludes that MODFLOW-2000 Version 1.6 can be considered verified on the specified Linux platform.

5.17.5 References

1. WIPP PA, 2002. Code Classification and Review of Pre-Existing Documentation for MODFLOW. Memo from Sean McKenna to Mario Chavez, Sept. 30, 2002, Sandia National Laboratories, Albuquerque, NM ERMS #523942
2. Donald, M.G., Harbaugh, A.W., 1988, *A Modular Three-Dimensional Finite-Difference Ground-water Flow Model*, TWI 6-A1, 588 p. U.S. Geologic Survey, Reston, Va ERMS #522202
3. Harbaugh, A.W., Banta, E.R., Hill, M.C., and McDonald, M.G., 2000, *MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model -- User Guide To ModularizationConcepts And The Ground-Water Flow Process*: U.S. Geological Survey Open-File Report 00-92 ERMS #522197
4. *MODFLOW-2000, MODFLOW-2000, The U.S. Geological Survey Modular Ground-Water Model -- User Guide to the LINK-AMG (LMG) Package for Solving MATRIX Equations Using an Algebraic Multigrid Solver*: U.S. Geological Survey Open-File Report 00-92 ERMS #522220
5. http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html ERMS #522195 Documentation of a computer program to simulate horizontal flow barriers using the U.S. Geological Survey Modular three-dimensional finite-difference groundwater flow model: USGS Open-File Report 92-477 ERMS #525469.

5.18 NONLIN

This section presents the regression test results for the NONLIN Version 2.0 code. The purpose of NONLIN is to compute Pitzer parameters and standard chemical potentials for chemical species in concentrated electrolyte systems (brines).

5.18.1 Introduction

NONLIN Version 2.0 was validated in January 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [4, 5] by demonstrating that the results of nine Test Cases (1 through 9) met the acceptance criteria defined in the RD/VVP for NONLIN 2.0 [2, 3]. The tests selected for use in the regression testing of this code are the nine test cases described in the *Requirements Document & Verification and Validation Plan for NONLIN Version 2.0 and Addendum* (RD/VVP) [2, 3].
Three sets of regression tests were executed and the results evaluated.

1.) Regression test results from NONLIN 2.0 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of NONLIN 2.0 run on a DEC Alpha 2100 with OpenVMS 6.1.

2.) Regression test results from NONLIN 2.0 run on the ES45 with OpenVMS 7.3-1 were compared to results from the validation tests of NONLIN 2.0 run on the ES40 with OpenVMS 7.3-1.

3.) Regression test results from NONLIN 2.0 run on the 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of NONLIN 2.0 run on the ES40 with OpenVMS 7.3-1.

5.18.2 Test Methodology

As described in the AP-089 [6], the regression test methodology uses the VMS DIFFERENCE command to compare output from NONLIN 2.0 on the COMPAQ ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of NONLIN Version 2.0 with OpenVMS 6.1 for the ES40 and OpenVMS 7.3-1 for the ES45 and 8400. Differences that are limited to code run date and time, platform names, system version numbers, directory and file names, user names, and execution statistics are considered by the Agency to be acceptable. Differences involving numerical output require additional analysis by DOE to determine the origin of the differences and whether the differences affect the code's performance. Numerical differences may be determined to be acceptable based on the analysis of each difference.

5.18.3 Test Results

The nine test cases for NONLIN 2.0 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 NONLIN 2.0 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 directory and file names.

The nine test cases for NONLIN 2.0 were executed on the COMPAQ 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of NONLIN 2.0 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to directory and file names.

The nine test cases for NONLIN 2.0 were executed on the COMPAQ ES45 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of NONLIN 2.0 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to directory and file names. All nine test cases are identical, including the names of input and output files, to the VMS 7.3-1 regression tests explained above.

5.18.4 The Agency's Conclusions

Since the differences between the results of NONLIN 2.0, in OpenVMS 7.3-1, and NONLIN 2.0, in OpenVMS 6.1 are acceptable, the Agency concludes that NONLIN 2.0 meets the acceptance criteria specified in the RD/VVP [2, 3], and thus is considered as validated on the COMPAQ ES40 with OpenVMS 7.3-1. Furthermore, Since the differences between the results of NONLIN 2.0, on the COMPAQ 8400 with OpenVMS 7.3-1, and NONLIN 2.0, on the ES40 with OpenVMS 7.3-1 are all acceptable, the Agency concludes that NONLIN 2.0 meets the acceptance criteria specified in the RD/VVP [2, 3], and thus is considered as validated on the COMPAQ 8400 with OpenVMS 7.3-1. Finally, since the differences between the results of NONLIN 2.0, on the COMPAQ ES45 with OpenVMS 7.3-1, and NONLIN 2.0, on the ES40 with OpenVMS 7.3-1 are acceptable, the Agency concludes that NONLIN 2.0 meets the acceptance criteria specified in the RD/VVP [2, 3], and thus is considered as validated on the COMPAQ ES45 with OpenVMS 7.3-1.

5.18.5 References

1. U.S. DOE (U.S. Department of Energy). 1996. "Title 40 CFR 191 Compliance Certification Application for the Waste Isolation Pilot Plant" DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.
2. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for NONLIN Version 2.0" (Document Version 1.00) Sandia National Laboratories. ERMS #230738.

3. WIPP PA (Performance Assessment). 1997. “Requirements Document & Verification and Validation Plan for NONLIN Version 2.0 and Addendum” (Document Version 1.00) Sandia National Laboratories. ERMS #230738
4. WIPP PA (Performance Assessment). 1996. “Validation Document for NONLIN Version 2.0” (Document Version 1.00) Sandia National Laboratories. ERMS #230743.
5. WIPP PA (Performance Assessment). 1996. “Validation Document for NONLIN Version 2.0 and Addendum” (Document Version 1.00) Sandia National Laboratories. ERMS #230743.
6. Analysis Plan (AP-089). 2002 “Upgrade of Operating System to OpenVMS 7.3-1 and Hardware to HP Alpha ES45” Sandia National Laboratories. ERMS #523491.

5.19 NUCPLOT

This section presents the regression test results for the NUCPLOT version 1.20 code. The purpose of NUCPLOT is to produce Tukey box plots of variable data. An important advantage of NUCPLOT is that it provides a way, in a small format, to compactly display variability in a large range of data. NUCPLOT can be used as a sensitivity and uncertainty analysis tool anywhere in the WIPP PA code sequence. It is commonly used to examine the output of the BRAGFLO and SECOTP2D code sequences.

5.19.1 Introduction

NUCPLOT Version 1.20 was validated in March 2002 on DEC Alpha with OpenVMS 7.2-1 [2] by demonstrating that the results of nine Test Cases (1 through 6) met the acceptance criteria defined in the VVP/VD for NUCPLOT 1.20 [2]. The tests selected for use in the regression testing of this code are the nine test cases described in the *Verification and Validation Plan and Validation Document for NUCPLOT Version 1.20* (VVP/VD) [2].

1) Regression test results from NUCPLOT 1.20 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of NUCPLOT 1.20 run on DEC Alpha with OpenVMS 7.2-1.
2) Regression test results from NUCPLOT 1.20 run on the ES45 with OpenVMS 7.3-1 were compared to results from the validation tests of NUCPLOT 1.20 run on the ES40 with OpenVMS 7.3-1.
3) Regression test results from NUCPLOT 1.20 run on the 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of NUCPLOT 1.20 run on the ES40 withOpenVMS 7.3-1.

5.19.2 Test Methodology

As described in the AP-089 [3], the regression test methodology uses the VMS DIFFERENCE command and in some cases a visual comparison to compare output from NUCPLOT 1.20 on the

COMPAQ ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of NUCPLOT Version 1.20 with OpenVMS 7.2-1 for the ES40 and OpenVMS 7.3-1 for the ES45 and 8400.

The initial version of NUCPLOT 1.20 qualified was on the DEC Alpha running OpenVMS7.2-1. This validated version of NUCPLOT was the basis for regression testing. Comparing each pair of output files results in a list of differences. Differences that are limited to code run date and time, platform names, system version numbers, directory and file names, user names, and execution statistics are acceptable. Differences involving numerical output require DOE to conduct additional analysis to determine the origin of the differences and whether the differences affect the code's performance. Numerical differences may be determined to be acceptable based on the analysis of each difference.

5.19.3 Test Results

The nine test cases for NUCPLOT 1.20 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 NUCPLOT 1.20 on DEC Alpha with OpenVMS 7.2-1 by using the VMS DIFFERENCE command and visual comparison. DOE believes that all differences found in the output are acceptable; namely, that the differences are limited to code run date and time, platform names, system version numbers, user names, and directory and file names.

The nine test cases for NUCPLOT 1.20 were executed on the COMPAQ ES45 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of NUCPLOT 1.20 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE believes that all differences found in the output are acceptable; namely, that the differences are limited to code run date and time, platform names, system version numbers, user names, and directory and file names. Because the length of the files names were the same as the ones being compared to, a visual comparison was not needed for the PST file in Test Case 8 of the ES45 testing. All nine test cases are identical, including the names of input and output files, to the VMS 7.3-1 regression tests explained above.

The nine test cases for NUCPLOT 1.20 were executed on the COMPAQ 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of NUCPLOT 1.20 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE believes that all differences in output are acceptable; namely, that the differences are limited to code run date and time, platform names, system version numbers, user names, and directory and file names. Because the length of the files names were the same as the ones being compared to, a visual comparison was not needed for the PST file in Test Case 8 of the ES45 testing. All nine test cases are identical, including the names of input and output files, to the VMS 7.3-1 regression tests explained above.

5.19.4 The Agency's Conclusions

Since the differences between the results of NUCPLOT 1.20, in OpenVMS 7.3-1, and NUCPLOT 1.20, in OpenVMS 7.2-1 are acceptable, the Agency concludes that NUCPLOT 1.20 meets the acceptance criteria specified in the VVP/VD [2], and thus is considered as validated on the COMPAQ ES40 with OpenVMS 7.3-1.

Since the differences between the results of NUCPLOT 1.20, on the COMPAQ ES45 with OpenVMS 7.3-1, and NUCPLOT 1.20, on the ES40 with OpenVMS 7.3-1 were acceptable, the Agency concludes that NUCPLOT 1.20 meets the acceptance criteria specified in the VVP/VD [2], and thus is considered as validated on the COMPAQ ES45 with OpenVMS 7.3-1.

Since the differences between the results of NUCPLOT 1.20, on the COMPAQ 8400 with OpenVMS 7.3-1, and NUCPLOT 1.20, on the ES40 with OpenVMS 7.3-1 were all acceptable, the Agency concludes that NUCPLOT 1.20 meets the acceptance criteria specified in the VVP/VD [2], and thus is considered as validated on the COMPAQ 8400 with OpenVMS 7.3-1.

5.19.5 References

1. U.S. DOE (U.S. Department of Energy). 1996. "Title 40 CFR 191 Compliance Certification Application for the Waste Isolation Pilot Plant." DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.
2. WIPP PA (Performance Assessment). 2002. "Verification and Validation Plan and Validation Document for NUCPLOT Version 1.20" (Document Version 1.20) Sandia National Laboratories. ERMS# 520492
3. Analysis Plan (AP-089). 2002 "Upgrade of Operating System to OpenVMS 7.3-1 and Hardware to HP Alpha ES45" Sandia National Laboratories. ERMS #523491.

5.20 NUMBERS

This section presents the verification and validation tests for NUMBERS. NUMBERS is a shell program which reads and stores data from a finite element model described in the EXODUS database format. Within this shell program are several utility routines which calculate information about the finite element model. The utilities currently implemented in NUMBERS allow the analyst to determine information such as (1) the volume and coordinate limits of each of the materials in the model; (2) the mass properties of the model; (3) the minimum, maximum, and average element volumes for each material; (4) the volume and change in volume of a cavity; (5) the nodes or elements that are within a specified distance from a user-defined point, line, or plane; (6) an estimate of the explicit central-difference timestep for each material; (7) the validity of

contact surfaces or slide lines, that is, whether two surfaces overlap at any point; and (8) the distance between two surfaces.

5.20.1 Introduction

The NUMBERS program is a shell program which reads and stores data from a finite element model [SANTOS, Section 5.34]. Within this shell program are several utility routines which calculate information about the finite element model. The utilities currently implemented in NUMBERS allow the analyst to determine:

- the volume and coordinate limits of each of the materials in the model;
- the mass properties of the model;
- the minimum, maximum, and average element volumes for each material;
- the volume and change in volume of a cavity;
- the nodes or elements that are within a specified distance from a user-defined point, line, or plane;
- an estimate of the explicit central-difference timestep for each material;
- the validity of contact surfaces or slidelines, that is, whether two surfaces overlap at any point; and
- the distance between two surfaces.

These utilities have been developed to automate and simplify some of the tasks normally performed during an analysis. The NUMBERS program reads the finite element model and results from a file written in binary file format. Originally, NUMBERS was written solely to calculate the mass properties of a body. However, once the basic function of reading and storing as a database was in place, several tasks were implemented. Tasks such as determining node and element numbers, verifying contact surfaces, and others, are now performed more efficiently and, hopefully, more accurately since the code performs the repetitive calculations automatically. Although the original reason for developing NUMBERS was to simply calculate mass properties, the code now functions as a shell that can be easily extended by analysts who require specific calculations or need to create information not currently available. The analyst can simply write a subroutine to perform their function, and insert it into NUMBERS. For most cases, adding a function to NUMBERS requires only writing the function subroutine, adding the command name to the table of valid commands, and adding a few statements to call the routine.

DOE's original position with respect to the documentation and testing of NUMBERS was that it was not subject to the specific software requirements of WIPP QAP 19-1 for the following three reasons[2]: (1) it is used in conjunction with WIPP but was not specifically developed for WIPP; (2) is used in conjunction with a number of other codes applied to other projects; and (3) it is not executed on any WIPP computer system. The Agency, however, maintains a position that the software requirements associated with the documentation and testing of NUMBERS must be consistent with with QAP 19-1. Since the issuance of the March 2004 version of this report, the

DOE has provided the following documentation related to the fulfillment of QAP 19-1 requirements for NUMBERS Version 1.19:

- Users Manual,
- Quality Assurance Project Plan,
- Implementation Document,
- Software Installation and Checkout Forms
- Verification and Validation Plan
- A 1989 Sandia Report describing NUMBERS

5.20.2 Test Methodology

The test set for NUMBERS consists of two test cases. Both test cases verify the Functional Requirement that the cavity volume and change in cavity volume are correctly calculated. Test Case 1 tests the cavity volume on both a planar (1A) and axisymmetric (1B) case with a simplified mesh that yields an analytic solution, Test Case 2 tests the cavity volume with an actual SANTOS [Section 5.34] output file used in WIPP calculations.

The computational mesh for the first test case was defined so that there is a simple analytic solution to the area and volume within the cavity at each time step. As the mesh deforms, two triangular areas arc removed from the initial cavity, then a third triangular area is added to the cavity. Two points of each triangular region are fixed at the corners of the initial rectangular cavity. Thus, the base of each triangle is known and the height is determined by the deformation of the third point. The area and volume of the three triangular regions are calculated in an EXCEL spreadsheet. The volumes predicted with NUMBERS are subsequently compared against the analytic solution. The acceptance criteria require the cavity volume calculated by NUMBERS must be within 0.5% of the hand-calculated cavity volume.

Test Case 2 verifies NUMBERS capability to calculate time-dependent cavity volume using a mesh output by SANTOS from an actual WIPP calculation. Test Case 2 verifies the volume on planar geometry with 20 quadrilateral elements. Note that for planar 2D geometry the volume is equivalent to the area.

The Agency has requested that DOE provide a comparison between NUMBERS output and that explicitly derived from the SANTOS calculations. This comparison will be performed by summing the void space calculated by SANTOS on an element by element basis and comparing this total volume with the equivalent output in NUMBERS. This comparison will provide insight into whether the NUMBERS code provides reliable output when the solid matrix is highly deformed.

5.20.3 Test Results

The NUMBERS output for the planar Test Case (1A) indicates that the cavity volume calculated by NUMBERS differs by at most 0.02% from the analytic solution over all time steps. This is within the 0.5% acceptance criteria. Alternatively, the NUMBERS output for the axisymetric Test Case (1B) indicates that the cavity volume calculated by NUMBERS differs by at most 0.05% from the analytic solution over all time steps. This is within the 0.5% acceptance criteria. Therefore, the acceptance criteria for Test Case 1 have been successfully met.

For the second test case, the NUMBERS output is compared to that obtained independently from SANTOS. The SANTOS calculated area at the final time step is 3.9661794 which matches the volumes predicted by NUMBERS (3.966) to all significant digits, so the acceptance criteria is met for the deformed cavity at the final time step.

5.20.4 The Agency's Conclusions

Since NUMBERS has now been documented in accordance with QAP-1 and all differences in the test case results of NUMBERS 1.19 are acceptable, the Agency concludes that NUMBERS 1.19 meets the acceptance criteria specified in the RD/VVP [6], and thus is considered as validated on the Compaq 8400 with TRU 64, UNIX V.5.1B.

5.20.5 References

1. SNL 1989. *A Collection of Utilities for Pre- and Postprocessing Two- and Three-Dimensional EXODUS Finite Element Models* . Sandia National Laboratories, Albuquerque, New Mexico. SAND88-0737.
2. Chavez M. 2003. Correspondence to P. Shoemaker titled SANTOS Exemptions ERMS #533933. Sandia National Laboratories, Albuquerque, New Mexico.
3. WIPP PA (Performance Assessment). 2004. "User's Manual Criteria Addenda to Sandia Report SAND88-0737" Sandia National Laboratories. ERMS #535648.
4. WIPP PA (Performance Assessment). 2004. "Implementation Document for NUMBERS Version 1.19" Sandia National Laboratories. ERMS# 535647.
5. WIPP PA (Performance Assessment). 2004. "Software Quality Assurance Plan for NUMBERS Version 1.19" Sandia National Laboratories. ERMS# 534712.
6. WIPP PA (Performance Assessment). 2004. "Verification and Validation Plan/Validation Document for NUMBERS Version 1.19" Sandia National Laboratories. ERMS# 535646.

5.21 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.

5.21.1 Introduction

DOE used NUTS for isothermal transport in the rock matrix for WIPP PA. 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.

In order to test new operating systems that were added in 2002-03 (Section 1), regression test results from NUTS 2.05A run on the ES40 with OpenVMS 7.3-1 were compared to results from

the validation tests of NUTS 2.05A run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of NUTS 2.05A on those operating systems [19]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[20,21]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to NUTS 2.05A on the new hardware systems.

5.21.2 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 ES45 and 8400 running OpenVMS 7.3-1 were compared to results from the installation and checkout tests of NUTS 2.05A executed on the ES40 running OpenVMS 7.3-1. The regression test methodology uses the OpenVMS DIFFERENCE command to compare output from NUTS 2.05A on the Compaq ES45 and 8400 running OpenVMS 7.3-1 to the output from the validation of NUTS 2.05A on the ES40 running OpenVMS 7.2-1. Test Case 7 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 ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Sections 5.17, 5.27, and 5.25 for POSTBRAG, SUMMARIZE and SPLAT, respectively.)

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 the Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression tests (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.

5.21.3 Test Results

Each test case generated output files, which were compared to the output files from the NUTS 2.05A validation tests, done on the ES40 with OpenVMS 7.3-1. 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 ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware 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. The Agency 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.

5.21.4 The Agency's Conclusions

Since all differences in the regression test results of NUTS 2.05A are acceptable, the Agency concludes that NUTS 2.05A meets the acceptance criteria specified in the RD/VVP [3], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.21.5 References

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2. Analysis Plan (AP-065). 2000 "Regression for the Upgrade to Open VMS Version 7.2 on the WIPP DEC Alpha Cluster." Sandia National Laboratories.
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5. WIPP PA (Performance Assessment). 1996. "User's Manual for NUTS Version 2.02" Sandia National Laboratories. ERMS #237927.
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7. WIPP PA (Performance Assessment). 1997. " Change Control Form for NUTS, Version 2.05" Memorandum to Distribution, J. J. Loukota, Sandia National Laboratories. ERMS #246624.
8. WIPP PA (Performance Assessment). 2001. "Change Control Form for NUTS, Version 2.05A" Memorandum to Distribution, P. Painter, Sandia National Laboratories. ERMS #515790.
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14. WIPP PA (Performance Assessment). 1996. "Validation Document for NUTS Version 2.02" Sandia National Laboratories. ERMS #237929.
15. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for NUTS Version 2.03" Sandia National Laboratories. ERMS #242618.
16. WIPP PA (Performance Assessment). 1996. "Software Problem Report 96-012 for NUTS Version 2.02" Memorandum to Distribution, J. J. Loukota, Sandia National Laboratories. ERMS #241769.
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21. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.22 PANEL

This section presents the regression and validation test results for Versions 4.00 and 4.02 of the PANEL 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.

5.22.1 Introduction

PANEL 3.50ZO was initially 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). 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].

In order to test new operating systems that were added in 2002-03 (Section 1), 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 6.1. In March of 2003, several modifications were made to Panel and the version number was changed from 4.00 to 4.02 [13]. The test set used for PANEL 4.02 consists of all nine of the test cases presented in Sections 9 of the RD/VVP[14].

In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of PANEL 4.00 on those operating systems [10]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[11,12]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to PANEL 4.00 and 4.02 on the new hardware systems.

5.22.2 Test Methodology

The tests for this code comprised the nine test cases described in the *requirements Document and Verification and Validation Plan for PANEL Version 4.00* (RD/VVP) [3]. Testing of PANEL was conducted in the following manner:

1) 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 6.1.
2) Regression test results from PANEL 4.00, run on the ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of PANEL 4.00, run on the ES40 with OpenVMS 7.3-1.
3) Regression test results from PANEL 4.02, run on the ES40 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of PANEL 4.00, run on the ES40 with OpenVMS 7.3-1.
4) Regression test results from PANEL 4.02, run on the ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of PANEL 4.02, run on the ES40 with OpenVMS 7.3-1.

CAMDAT database files (CDB) are produced in each of the nine PANEL test cases. The output CDB files are converted from a binary, CDB, file to an ASCII text file for comparison during the validation process. In the previous PANEL 4.00 validation, the CDB files were converted using GROPECDB 2.10. GROPECDB has since been revised to Version 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [9]. GROPECDB 2.12 has also been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware

regression test (see Section 5.10). For the most recent regression tests, GROPECDB 2.12 is used to convert the CDB output files from PANEL 4.02 in OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from previous verification exercises.

5.22.3 Test Results

The nine test cases for PANEL 4.00 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

The nine test cases for PANEL 4.02 were executed on the Compaq ES40 and 8400 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 the Compaq ES40 and 8400with OpenVMS 7.3-1 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. The Agency 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.

The nine test cases for PANEL 4.02 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of PANEL 4.02 on the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.22.4 The Agency's Conclusions

Since all differences in the regression test results of PANEL 4.02 are acceptable, the Agency concludes that PANEL 4.02 meets the acceptance criteria specified in the RD/VVP [3], and thus are considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.22.5 References

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12. WIPP PA – “Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.
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14. WIPP PA (Performance Assessment). 2003. “Requirements Document and Verification and Validation Plan for PANEL Version 4.02” Sandia National Laboratories. ERMS #526649.
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5.23 PATTRN

This section presents the regression test results for the PATTRN Version 1.0 code. The purpose of PATTRN is to detect PATTRNs in scatterplots of independent variables versus dependent variables. A PATTRN in a scatterplot may be an indication of a relationship between the independent variable and dependent variable on the scatterplot.

5.23.1 Introduction

PATTRN Version 1.00 was validated in March 1999 on a DEC Alpha 2100 with OpenVMS 7.1[3] by demonstrating that the results of seventeen Test Cases (1 through 17) met the acceptance criteria defined in the RD/VVP for PATTRN 1.00 [2]. The tests selected for use in the regression testing of PATTRN Version 1.00 are the seventeen test cases described in the *Requirements Document & Verification and Validation Plan for PATTRN Version 1.00* (RD/VVP) [2]. DOE performed three sets of regression tests that included:

1) Regression test results from PATTRN 1.00 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PATTRN 1.00 run on a DEC Alpha 2100 with OpenVMS 7.1.

2) Regression test results from PATTRN 1.00 run on the ES45 with OpenVMS 7.3-1 were compared to results from the validation tests of PATTRN 1.00 run on the ES40 with OpenVMS 7.3-1.

3) Regression test results from PATTRN 1.00 run on the 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of PATTRN 1.00 run on the ES40 with OpenVMS 7.3-1.

5.23.2 Test Methodology

As described in the AP-089 [4], the regression test methodology uses the VMS DIFFERENCE command to compare output from PATTRN 1.00 on the COMPAQ ES40, ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of PATTRN Version 1.00 with OpenVMS 7.1 for the ES40 and OpenVMS 7.3-1 for the ES45 and 8400.

The initial version of PATTRN Version 1.00 qualified was on the DEC Alpha running OpenVMS 7.1. This validated version of PATTRN was the basis for regression testing. Comparing each pair of output files results in a list of differences. Differences that are limited to code run date and time, platform names, system version numbers, directory and file names, user names, and execution statistics are considered acceptable by the Agency. Differences involving numerical output require DOE to perform additional analysis to determine the origin of the differences and whether the differences affect the code's performance. Numerical differences may be determined to be acceptable based on the analysis of each difference.

5.23.3 Test Results

The seventeen test cases for PATTRN 1.00 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 PATTRN 1.00 on a DEC Alpha 2100 with OpenVMS 7.1 by using the VMS DIFFERENCE command. The comparison found that there were no differences in output. Since there were no differences between the results of PATTRN 1.00, in OpenVMS 7.3-1, and PATTRN 1.00, in OpenVMS 7.1, DOE concluded that PATTRN 1.00 meets the acceptance criteria specified in the RD/VVP [2], and thus is considered by DOE as validated on the COMPAQ ES40 with OpenVMS 7.3-1.

The seventeen test cases for PATTRN 1.00 were executed on the COMPAQ ES45 with OpenVMS 7.3-1. DOE compared the output files from the test cases to the corresponding output files from the validation of PATTRN 1.00 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE concluded that there were no differences in output. All seventeen test cases are identical, including the names of input and output files, to the VMS 7.3-1 regression tests explained above. Since there were no differences between the results of PATTRN 1.00, on the COMPAQ ES45 with OpenVMS 7.3-1, and PATTRN 1.00, on the ES40 with OpenVMS 7.3-1, DOE concluded that PATTRN 1.00 meets the acceptance criteria specified in the RD/VVP [2], and thus is considered as validated on the COMPAQ ES45 with OpenVMS 7.3-1.

The seventeen test cases for PATTRN 1.00 were executed on the COMPAQ 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of PATTRN 1.00 on the COMPAQ ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. The comparison found that there were no differences in output. Since there were no differences between the results of PATTRN 1.00, on the COMPAQ 8400 with OpenVMS 7.3-1, and PATTRN 1.00, on the ES40 with OpenVMS 7.3-1, DOE concluded that PATTRN 1.00 meets the acceptance criteria specified in the RD/VVP [2], and thus is considered as validated on the COMPAQ 8400 with OpenVMS 7.3-1.

5.23.4 The Agency's Conclusions

Since all differences in the regression test results of PATTRN 1.00 are acceptable, the Agency concludes that PATTRN 1.00 meets the acceptance criteria specified in the RD/VVP [2], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.23.5 References

1. U.S. DOE (U.S. Department of Energy). 1996. "Title 40 CFR 191 Compliance Certification Application for the Waste Isolation Pilot Plant" DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.
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5.24 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.

5.24.1 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].

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of PCCSRC 2.21 on those operating systems [3]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[4,5]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to PCCSRC 2.21 on the new hardware systems.

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 PCCSRC version 2.21* RD/VVP) [1]. Regression test results from PCCSRC 2.21 run on the ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of PCCSRC 2.21 run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from PCCSRC 2.21 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the original validation of PCCSRC 2.21.

5.24.3 Test Results

The four test cases for PCCSRC 2.21 were executed on the Compaq ES45 and 8400 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 the Compaq ES45 and 8400 with OpenVMS 7.3-1 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. The Agency 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.

5.24.4 The Agency's Conclusions

Since all differences in the regression test results of PCCSRC 2.21 are acceptable, the Agency concludes that PCCSRC 2.21 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.24.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document and Verification and Validation Plan for PCCSRC" Version 2.21 Sandia National Laboratories. ERMS #227772.
2. WIPP PA (Performance Assessment). 1995. "Validation Document for PCCSRC version 2.21" Sandia National Laboratories. ERMS #227775.
3. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
4. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
5. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.25 PEST

This section presents the verification and validation of the PEST Version 5.5 code. The PEST code, version 5.5, is an acquired system to solve the problem of parameter estimation for any mathematical model, but with specific application to WIPP PA for optimizing T-fields using pilot points in conjunction with the MODFLOW2000 groundwater flow model. In the context of the Culebra T-fields, PEST is used to iteratively optimize a spatially correlated residual field that is then added to the original mean T-field to produce the final T-field. PEST is freely available on the web at: http://www.sspa.com/PEST/ For the optimization of the residual fields, the PEST software is used console executable on a PC running the Linux operating system.

5.25.1 Introduction

PEST is a parameter estimation program that can be used with other models to calibrate parameters quickly using a set of known observations. Models produce numbers and if there are field or laboratory measurements corresponding to some of these numbers, PEST can adjust model parameter and/or excitation data so that the discrepancies between the pertinent model-generated numbers and the corresponding measurements are reduced to a minimum. It does this by taking control of the model execution and running it as many times as is necessary in order to determine this optimal set of parameters and/or excitations. The modeler must inform PEST of where the adjustable parameters and excitations are to be found in the model input files. Once PEST is provided this information, it can rewrite these model input files using whatever parameters and excitations are appropriate at any stage of the optimization process. Files are constructed so that PEST can identify those numbers on the model output files that correspond to the actual observations that have been made. Thus, each time PEST runs the model, it is able to read those model outcomes which must be matched to field or laboratory observations. After calculating the mismatch between the two sets of numbers, and evaluating how best to correct that mismatch, it adjusts model input data and runs the model again.

Software Requirements (NP 19-1) requires that seven primary documents be developed, reviewed and maintained for the PEST software. the Software QA plan, a Requirements Document (RD), Verification and Validation Plan (WP), User's Manual (UM), Design Document (DD), Implementation Document (ID), and the Validation Document (VD). Documentation for Version 5.5 will remain the base documents with addenda for each of the documents defining the additional scope of the software for any newer versions of the software. Configuration control will be maintained through completion of Installation & Checkout (I&C) documentation for all changes made to PEST, and system software and/or system hardware. In addition, Change Control (CC) and Software Problem Report (SPR) documents will be defined, as appropriate. As defined in NP 19-1, an installation & checkout, software problem reporting, change control, software configuration control, and appropriate revisions to the quality assurance documents will be prepared, reviewed, and maintained for each change step during the software life cycle.

5.25.2 Test Methodology

The testing consists of six separate tests using the pilot point method. The test cases used for the functional testing of PEST are:

1) An aquifer model with four homogeneous zones bounded by a river, two groundwater flow lines and a ground water divide. There are 21 boreholes for head measurements and 1 pumping well. There are 29, 4, 1 and 1 pilot points in the four zones, respectively. This test is run in steady-state mode without using regularization.
2) Test case 2 is the same as test case 1 except that the test is run under transient mode. Similar to test case 1, this test case is run without using regularization.
3) Test Case 3 is the same as test case 1 except that the regularization mode is used.
4) Test Case 4 is the same as test case 2 except that the regularization mode is used.

5) Test Case 5 is a problem based on a geophysical inversion model with software commonly used in geophysical data analysis for the interpretation of "Vertical Electrical Sounding" (VES) measurements. This test problem has been adapted here for testing user intervention using the parameter hold file.
6) Test Case 6 is the same test case as 5 except that the test case has been adapted for parameter setting - Log-transform, bounds and tied.

Input and output files for all of the test cases have been stored in SCMS accessible from the WIPP Alpha cluster (Library - PEST, Class- VER_0551) and in CVS on the target platform (Repository - */h/WIPPcvs/src/pest55*.)

5.25.3 Test Results

The acceptance criteria for the pilot point test cases 1 to 4 are that PEST should produce a transmissivity field that would generate the correct head observations to within the significant digits of the given observations, which is 3. Given that the head measurements are in 10's of meters, this acceptance criteria results in PEST needing to match the heads to within 0.10 meters of the true value.

The acceptance criteria for Test Case 5 are that the expected results are met. These expected results are described in the VP[3]. For Test Case 5, the expected results are that during each optimization iteration PEST should record the fact that it has detected the presence of the parameter hold file and has held parameter *h2* at its current value in accordance with the instructions found in that file. An inspection of file *ves3.rec* should reveal, however, that parameter *h2* is simply fixed at its initial value. In the latter case PEST does not even compute a column of its Jacobian matrix pertaining to the fixed parameter *h2*. Where a parameter is held through the parameter hold file, however, PEST computes sensitivities of observations with respect to this parameter, for it only knows that it must hold this parameter after completion of the filling of the Jacobian matrix, and prior to testing parameter upgrades. Also for Test Case 5, the files *ves2.par* and *ves3.par* need to be compared. These are the "parameter value files" recording optimized parameter values resulting from the *ves2* and *ves3* PEST runs. Parameter values should be "numerically identical" (i.e. identical except, perhaps, in all but the last 1 or 2 significant figures) between the two files; furthermore, parameter *h2* should be retained at its initial value, viz. 4.0. Confirmation of the identity of parameter values verifies proper operation of PEST's user- intervention functionality.

The acceptance criteria for Test Case 6 are that the expected results are met. These expected results are described in CRWMS M&O, 2002 and are repeated here. The acceptance criteria for Test Case 6, involves a comparison of the run record files *ves5.rec* and *ves1.rec.kp* and should reveal that PEST calculates an almost identical set of parameter values for the two cases (optimized parameter values are listed near the ends of those files). However, depending on the computer platform, more optimization iterations will normally be required for completion of the *ves5* case than for that of the *ves1* case. After PEST has run to completion, optimized parameter

values will be listed in the run record file *ves6.rec* and in the parameter value file *ves6.par*. Compare *ves6.par* with *ves3.par*; recall that parameter *h2* was fixed at 4.0 for the *ves3* case. Because its "natural value" is 10.0, the fixing of *h2* at 4.0, and the placing of an upper bound on *h2* of 4.0, have the same effect. Hence optimized parameter values listed in files *ves3.par* and *ves6.par* should be nearly identical. Note that, in spite of the limitations placed on the movement of parameter *h2*, the objective function calculated at the end of the optimization process should still be quite low due to operation of the "principal of equivalence" described earlier; an inspection of file *ves6.rec* will reveal a final "phi" value of about 2.6´10-2. An inspection of the run record file *ves7.rec* should reveal that parameters *ro1* and *ro3* maintain the same value throughout the optimization process. It will also show that optimized parameter values for this case are nearly identical to those of the *ves1* case (compare *ves7.par* with ves1.par.kp). This is because, even with no constraints, the optimized values for *ro3* and *ro1* are equal.

All the test results were within the expected limits of accuracy and uniqueness and met all specified criteria. PEST does not generate unique results, which is why it is used to calibrate models that have many unknowns. The results show that PEST performed as expected on the Linux system.

5.25.4 The Agency's Conclusions

All test results met the acceptance criteria specified in section 5.3 of the VD. Therefore, the Agency considers PEST verified on the Linux system.

5.25.5 References

1. CRWMS M&O, 2002, "Validation Test Plan (VTP) for PEST" Version 5.5 (to be published.) CRWMS M&O, Las Vegas, NV. Prepared by John Doherty for Los Alamos National Laboratory, 64 pp ERMS #523969
2. CRWMS M&O, 2002, "Design Document (DD) for PEST" Version 5.5 (to be published), CRWMS M&O, Las Vegas, NV, Prepared by John Doherty for Los Alamos National Laboratory, 87 pp ERMS #523970
3. CRWMS M&O, 2002, "Requirements Document (RD) for PEST" Version 5.5, CRWMS M&O, Las Vegas, NV, Prepared by John Doherty for Los Alamos National Laboratory, 40 pp ERMS #523971
4. Doherty, J., 2002, "PEST: Model Independent Parameter Estimation", Fourth Edition, Watermark Numerical Computing, 279 pp ERMS #523967
5. Doherty, J., 2000, "Using Pilot Points to Calibrate Steady State and Transient Ground Water Models", unpublished notes, 35 pp
6. WIPP PA, 2002, "Code Classification and Review of Pre-Existing Documentation for PEST" Version 5.5 (Memorandum revision 3.0). Memorandum from Jianjun Lin to Rodger Coman, September 16, 2002 ERMS #523871

5.26 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.

5.26.1 Introduction

For WIPP PA, POSTBRAG is used to create CAMDAT files from BRAGFLO output 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.

In order to test new operating systems that were added in 2002-03 (Section 1), regression test results from POSTBRAG 4.00 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of POSTBRAG 4.00 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of POSTBRAG 4.00 on those operating systems [6]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[7,8]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to POSTBRAG 4.00 on the new hardware systems.

5.26.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared by DOE to results from the validation tests of POSTBRAG 4.00 run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from POSTBRAG 4.00 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the original validation of POSTBRAG 4.00.

5.26.3 Test Results

The two test cases for POSTBRAG 4.00 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1, and compared to results from the validation tests of POSTBRAG 4.00 run on the ES40 with OpenVMS 7.3-1. 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, platform names, system version numbers and execution statistics. The Agency 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.

5.26.4 The Agency's Conclusions

Since all differences in the regression test results of POSTBRAG 4.00 are acceptable, the Agency concludes that POSTBRAG 4.00 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.26.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for POSTBRAG Version 4.00". Sandia National Laboratories. ERMS #230681.
2. WIPP PA (Performance Assessment). 1996. "Validation Document for POSTBRAG Version 4.00", Sandia National Laboratories. ERMS #230685.
3. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for POSTBRAG Version 3.05ZO". Sandia National Laboratories. ERMS #223603.
4. WIPP PA (Performance Assessment). 1995. "Validation Document for POSTBRAG Version 3.05ZO", Sandia National Laboratories. ERMS #223604.
5. WIPP PA (Performance Assessment). 2002. "Software Problem Report" (SPR) for BLOTCDB Version 1.37. SPR # 02-004, Sandia National Laboratories. ERMS #525354.
7. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
8. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
9. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.27 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.

5.27.1 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, POSLHS 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).

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of POSTLHS 4.07 on those operating systems [4]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[5,6]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to POSTLHS 4.07 on the new hardware systems.

5.27.2 Test Methodology

The tests for this code comprised the two test cases described in the *Requirements Document & Verification and Validation Plan for POSTLHS 4.06Z0* RD/VVP) [1]. Regression test results from POSTLHS 4.07, run on the ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of POSTLHS 4.07, run on the ES40 with OpenVMS 7.3-1.

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 text file for comparison during the validation process. In the previous POSTLHS 4.07 validation, the CDB files were converted using GROPECDB 2.10. GROPECDB has since been revised to Version 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [3]. GROPECDB 2.12 has been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Section 5.10). The regression test methodology uses the VMS DIFFERENCE command to compare output from POSTLHS 4.07 on the Compaq ES45 and 8400 with OpenVMS7.3-1 to the output from the previous validation of POSTLHS 4.07.

5.27.3 Test Results

The two test cases for POSTLHS 4.07 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.27.4 The Agency's Conclusions

Since all differences in the regression test results of POSTLHS 4.07 are acceptable, the Agency concludes that POSTLHS 4.07 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.27.5 References

1. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for POSTLHS Version 4.06ZO" Sandia National Laboratories. ERMS #223552.
2. WIPP PA (Performance Assessment). 1996. "Software Installation and Checkout Form, POSTLHS Version 4.07" Sandia National Laboratories. ERMS #230717.
3. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12" Sandia National Laboratories. ERMS #237497.
4. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
5. WIPP PA – "Analysis Report for the ES45 Regression Test, March 6, 2003" Sandia National Laboratories. ERMS #530290.
6. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.28 POSTSECOTP2D

This section presents the regression test results for the POSTSECOTP2D Version 1.04 code. POSTSECOTP2D creates a CAMDAT file (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).

5.28.1 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.

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of POSTSECOTP2D 1.04 on those operating systems [6]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[7,8]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to POSTSECOTP2D 1.04 on the new hardware systems.

5.28.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of POSTSECOTP2D 1.04 run on the ES40 with OpenVMS 7.3-1.

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 text file for comparison during the validation process. In the previous POSTSECOTP2D 1.04 validation, the CDB files were converted using GROPECDB 2.10. GROPECDB has since been revised to Version 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [5]. GROPECDB 2.12 has been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part

of the hardware regression test (see Section 5.10). For this regression test, GROPECDB 2.12 is used to convert the CDB output files from POSTSECOTP2D 1.04 in OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from POSTSECOTP2D 1.04 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the previous validation of POSTSECOTP2D 1.04 running on the Compaq ES40 with OpenVMS 7.3-1.

5.28.3 Test Results

Two test cases for POSTSECOTP2D 1.04 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1, and the output files were compared to the corresponding output files from the validation of POSTSECOTP2D 1.04 on the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.28.4 The Agency's Conclusions

Since all differences in the regression test results of POSTSECOTP2D 1.04 are acceptable, the Agency concludes that POSTSECOTP2D 1.04 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.28.5 References

1. WIPP PA (Performance Assessment). 1997. "Requirements Document and Verification and Validation Plan for POSTSECOTP2D Version 1.04". Sandia National Laboratories. ERMS #245696.
2. WIPP PA (Performance Assessment). 1997. "Validation Document for POSTSECOTP2D Version 1.04". Sandia National Laboratories. ERMS #245699.
3. WIPP PA (Performance Assessment). 1995. "Requirements Document and Verification and Validation Plan for POSTSECOTP2D Version 1.02". Sandia National Laboratories. ERMS #237304.
4. WIPP PA (Performance Assessment). 1996. "Validation Document for POSTSECOTP2D Version 1.02". Sandia National Laboratories. ERMS #237370.
5. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12" Sandia National Laboratories. ERMS #237497.
6. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.

7. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
8. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.29 PREBRAG

This section presents the regression test results for the PREBRAG Version 6.00 code, and verification and validation tests for Version 7.0 . 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.

5.29.1 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. In March 2003, several modifications were made to PREBRAG 6.0 primarily remove the "hardwiring of parameter values" and the code was updated to PREBRAG 7.0 [11].

In order to test new operating systems that were added in 2002-03 (Section 1), regression test results from PREBRAG 6.0 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PREBRAG 6.0 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of PREBRAG 6.0 on those operating systems[6]. In January 2003, two

new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[7,8]. Testing of PREBRAG 7.0 consisted of conducting the three functional test cases described in Section 6 of the VD[9]. These test were conducted on the Compaq ES45 and 8400 platforms with Open VMS 7.3-1. Output files from these test cases were compared to the corresponding output files from the validation of PREBRAG 7.0 on the Compaq ES45 with Open VMS 7.3-1. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to PREBRAG 6.0 and 7.0 on the new hardware systems.

5.29.2 Test Methodology

The tests for this code comprised the three test cases described in the R*equirements Document & Verification and Validation Plan for PREBRAG Version 6.00* RD/VVP) [1]. Regression test results from PREBRAG 6.00 run on the ES45 and 4500 with OpenVMS 7.3-1 were compared to results from the validation tests of PREBRAG 6.00 run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from PREBRAG 6.00 on the Compaq ES45 and 4500 with OpenVMS 7.3-1 to the output from the previous validation of PREBRAG 6.00.
The approach used to validate PREBRAG Version 7.00 involves 3 test cases to satisfy the Functional Requirements presented in Section 9 of the RD\VVP [10]. Testing of PREBRAG 7.0 consisted of conducting the three functional test cases described in Section 6 of the VD[9]. These test were conducted on the Compaq ES45 and 8400 platforms with Open VMS 7.3-1. Output files from these test cases were compared to the corresponding output files from the validation of PREBRAG 7.0 on the Compaq ES45 with Open VMS 7.3-1.

5.29.3 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 DIFFERENCE command was used to compare corresponding output files from the validation of PREBRAG. DOE concluded that all differences in output are acceptable; namely, that the differences are limited to code run date and time. The Agency also found that all differences in output are acceptable; namely, that the differences are limited to code run date and time.

5.29.4 The Agency's Conclusions

Since all differences in the regression test results of PREBRAG 6.00 and 7.00 are acceptable, the Agency concludes that PREBRAG 6.00 and 7.00 meet the acceptance criteria specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS Version 7.3-1.

5.29.5 References

1. WIPP PA (Performance Assessment). 1996. “Requirements Document & Verification and Validation Plan for PREBRAG Version 6.00”. Sandia National Laboratories. ERMS #230676.
2. WIPP PA (Performance Assessment). 1996. “Validation Document for PREBRAG Version 6.00”, Sandia National Laboratories. ERMS #230679.
3. WIPP PA (Performance Assessment). 1995. “Validation Document for PREBRAG Version 5.05ZO”, Sandia National Laboratories. ERMS #223596.
4. WIPP PA (Performance Assessment). 1995. “Requirements Document & Verification and Validation Plan for PREBRAG Version 5.05ZO”. Sandia National Laboratories. ERMS #223594.
5. WIPP PA (Performance Assessment). 2001. “Software Problem Report 01-002 for PREBRAG 6.00 and BRAGFLO 4.10" Sandia National Laboratories. ERMS# 519714.
6. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
7. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
8. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.
9. WIPP PA (Performance Assessment). 2003. “Validation Document for PREBRAG Version 7.00”, Sandia National Laboratories. ERMS #526627
10. WIPP PA (Performance Assessment). 2003. “Requirements Document & Verification and Validation Plan for PREBRAG Version 7.0”. Sandia National Laboratories. ERMS #526625.
11. WIPP PA (Performance Assessment). 2003. “Change Control Form Version 7.0”. Sandia National Laboratories. ERMS #526257.
12. WIPP PA (Performance Assessment). 2004. “Analysis Report for PREBRAG Version 7.00 Regression Testing for the Compaq ES45 and 8400 Platforms”. Sandia National Laboratories

5.30 PRECCDFGF

This section presents the regression test results for the PRECCDFGF Version 1.00B, and verification and validation tests for Version 1.00A. PRECCDFGF collates output from all other WIPP PA codes and formats this output into the RELTAB input file for CCDFGF.

5.30.1 Introduction

Version 1.0 of PRECCDFGF was used to support calculations during the CCA. In 2003, Version 1.0 was upgraded to Version 1.0A and this new version of the code was tested by following the procedures outlined by the single test included in the Validation Plan on the COMPAQ ES40 and 8400 with Open VMS 7.3-1 [1]. In September of 2003, minor changes were made in the codes

output reporting and the Version number was changed from 1.0A to 1.0B. To ensure that this version was working properly the DOE regression tested Version 1.0B against Version 1.0A on the COMPAQ ES40 and 8400 with Open VMS 7.3-1[2].

5.30.2 Test Methodology

The regression test methodology uses the VMS DIFFERENCE command to compare output from PRECCDFGF 1.00B on the COMPAQ ES45 and 8400 platforms with Open VMS 7.3-1 to the output from the validation of PRECCDFGF 1.00B on the COMPAQ ES40 with Open VMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files. At the end of the DIFFERENCE output, the utility reports the number of sections and the number of records in which differences were found.

5.30.3 Test Results

The single test case for PRECCDFGF 1.00B was executed by DOE on the COMPAQ ES45 and 8400 platforms with Open VMS 7.3-1. The output files from the test were compared to the corresponding output file from the validation of PRECCDFGF 1.00B on a COMPAQ ES40 with Open VMS 7.3-1 by using the VMS DIFFERENCE command [3]. Comparing each pair of output files results in a list of differences. Differences that are limited to code run dates and time, file and directory names, user names, platform names and execution statistics. There were no differences involving numerical output.

5.30.4 The Agency's Conclusions

Because there are no differences between the results of PRECCDFGF 1.00B executed on the COMPAQ ES45 and 8400 platforms in Open VMS 7.3-1, and PRECCDFGF 1.00B executed on the COMPAQ ES40 platform in Open VMS 7.3., 1, the Agency concludes that PRECCDFGF 1.00B meets the acceptance criteria specified in the VVP [1], and thus is considered as validated on the COMPAQ ES45 and 8400 platforms with Open VMS 7.3-1.

5.30.5 References

1. WIPP PA (Performance Assessment). 2003. "Verification and Validation Plan for PRECCDFGF Version 1.00A Document Version 1.02" Sandia National Laboratories. ERMS #530467.
2. WIPP PA (Performance Assessment). 2003. "Regression testing of PRECCDFGF 1.00B (Addendum to Validation Document for PRECCDFGF 1.00A)" Sandia National Laboratories. ERMS #531450.
3. WIPP PA (Performance Assessment). 2004. "Analysis Report for PRECCDFGF Version 1.00B Regression Testing for the ES45 and 8400 Platforms" Sandia National Laboratories

5.31 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.

5.31.1 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].

In order to test new operating systems that were added in 2002-03 (Section 1), regression test results from PRELHS 2.3 run on the ES40 with OpenVMS 7.3-1 were compared to results from the validation tests of PRELHS 2.3 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003,

the Agency completed a report documenting the Agency's approval with respect to the migration and verification of PRELHS 2.3 on those operating systems [11]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[12,13]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to PRELHS 2.3 on the new hardware systems.

5.31.2 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]. With the exception of Test Case 12, regression test results from PRELHS 2.30 run on the ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of PRELHS 2.30 run on the ES40 with OpenVMS 7.3-1. Subsequent to the upgrade to Open VMS 7.3-1, Test Case 12 for PHRLHS 2.30 was modified to correct a minor inconsistency in the input file [14]. PRELHS 2.30 was validated with the revised input file [14]. In this analysis, DOE compared the output of PRELHS 2.3 from the 8400 to the output of PRELHS 2.3 validation tests. The Agency has reviewed DOE's verification activities with respect to this matter and finds DOE approach acceptable.

The regression test methodology uses the VMS DIFFERENCE command to compare output from PRELHS 2.30 on the Compaq ES45 and 8400 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.

5.31.3 Test Results

The three test cases for PRELHS 2.30 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. As mentioned above, with the exception of Test Case 12, output files from the test cases were compared to the corresponding output files from the validation of PRELHS 2.30 on the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.31.4 The Agency's Conclusions

Since all differences in the regression test results of PRELHS 2.30 are acceptable, the Agency concludes that PRELHS 2.30 meets the acceptance criteria specified in the VVP/VD [3], and thus are considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.31.5 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.
2. Analysis Plan (AP-065). 2000 “Regression for the Upgrade to Open VMS Version 7.2 on the WIPP DEC Alpha Cluster” Sandia National Laboratories.
3. WIPP PA (Performance Assessment). 2001. “Requirements Document & Verification and Validation Plan for PRELHS Version 2.30" Sandia National Laboratories. ERMS #519721.
4. WIPP PA (Performance Assessment). 1996. “Requirements Document & Verification and Validation Plan for PRELHS Version 2.10" Sandia National Laboratories. ERMS #230712.
5. WIPP PA (Performance Assessment). 1996. “Validation Document for PRELHS Version 2.10" Sandia National Laboratories. ERMS #230716
6. WIPP PA (Performance Assessment). 1997. “Requirements Document & Verification and Validation Plan for PRELHS Version 2.20" Sandia National Laboratories. ERMS #243935.
7. WIPP PA (Performance Assessment). 1997. “Validation Document for PRELHS Version 2.20" Sandia National Laboratories. ERMS #243938.
8. WIPP PA (Performance Assessment). 2001. “Verification and Validation Plan for PRELHS Version 2.24" Sandia National Laboratories. ERMS #513612.
9. WIPP PA (Performance Assessment). 2001. “Validation Document for PRELHS Version 2.24" Sandia National Laboratories. ERMS #518675.
10. WIPP PA (Performance Assessment). 2002. “Verification and Validation Plan, Validation Document and Criteria Forms for PRELHS, Version 2.30" Sandia National Laboratories. ERMS #519722.
11. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
12. WIPP PA – “Analysis Report for the ES45 Regression Test, March 6, 2003" Sandia National Laboratories. ERMS #530290.
13. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.
14. WIPP PA (Performance Assessment). 2003. “Addenda to Verification and Validation Plan/Validation Document for PREHLHS version 2.30" Sandia National Laboratories. ERMS #525224.

5.32 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].

5.32.1 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.

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of PRESECOTP2D 1.22 on those operating systems [8]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[9,10]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to PRESECOTP2D 1.22 on the new hardware systems.

5.32.2 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 ES45 with OpenVMS 7.3-1 were compared to results from the validation tests of PRESECOTP2D 1.22 run on the ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from PRESECOTP2D 1.22 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the previous validation of PRESECOTP2D 1.22. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.32.3 Test Results

The four test cases for PRESECOTP2D 1.22 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.32.4 The Agency's Conclusions

Since all differences in the regression test results of PRESECOTP2D 1.22 are acceptable, the Agency concludes that PRESECOTP2D 1.22 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.32.5 References

1. WIPP PA (Performance Assessment). 1997. "Requirements Document & Verification and Validation Plan for PRESECOTP2D Version 1.22" Sandia National Laboratories. ERMS #245957.
2. WIPP PA (Performance Assessment). 1997. "Validation Document for PRESECOTP2D Version 1.22" Sandia National Laboratories. ERMS #245965.
3. "Primitive Data Package" for PRESECOTP2D, Version 1.11ZO, Version date 8/16/93, Binder with the following information: Abstract User Manual, On-Line Help, Verification, Review, Driver, and Source. Sandia National Laboratories. Record ERMS #220278.
4. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for PRESECOTP2D Version 1.11ZO" Sandia National Laboratories. ERMS #223324.
5. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for PRESECOTP2D Version 1.20" Sandia National Laboratories. Sandia WIPP Central Files ERMS #237295.
6. WIPP PA (Performance Assessment). 1996. "Validation Document for PRESECOTP2D Version 1.20" Sandia National Laboratories. ERMS #240254.

7. WIPP PA (Performance Assessment). 1997. “User’s Manual for PRESECOTP2D Version 1.22" Sandia National Laboratories. Sandia Central Files ERMS #245963.
8. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
9. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
10. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.

5.33 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.

5.33.1 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 1.42ZO validation tests. RELATE 1.43 was used in the WIPP Compliance Certification Application (CCA).

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency’s approval with respect to the migration and verification of RELATE 1.43 on those operating systems [3]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[4,5]. The discussion below documents the test methodology, regression test results, and the Agency’s conclusions with respect to RELATE 1.43 on the new hardware systems.

5.33.2 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 ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of RELATE 1.43, run on the ES40 with OpenVMS 7.3-1.

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, text file for comparison during the validation process. In the previous RELATE 1.43 validation, the CDB files were converted using GROPECDB 2.10. GROPECDB has since been revised to Version 2.12. GROPECDB 2.12 was validated in June 1996 on a DEC Alpha 2100 with OpenVMS 6.1 [2]. GROPECDB 2.12 has also been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Section 5.10). For this regression test, GROPECDB 2.12 is used to convert the CDB output files from RELATE 1.43 in OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from RELATE 1.43 on the Compaq ES45 and 8400 with OpenVMS7.3-1 to the output from the previous validation of RELATE 1.43.

5.33.3 Test Results

The three test cases for RELATE 1.43 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.33.4 The Agency's Conclusions

Since all differences in the regression test results of RELATE 1.43 are acceptable, the Agency concludes that RELATE 1.43 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS Version 7.3-1.

5.33.5 References

1. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for RELATE Version 1.42ZO" Sandia National Laboratories. ERMS #224184.
2. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12" Sandia National Laboratories. ERMS #237497.

3. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
4. WIPP PA – “Analysis Report for the ES45 Regression Test, March 6, 2003" Sandia National Laboratories. ERMS #530290.
5. WIPP PA – “Analysis Report for the 8400 Regression Test “ Sandia National Laboratories. ERMS #527280.

5.34 SANTOS

This section presents the verification and validation test results for SANTOS code. The SANTOS computer code consists of mathematical model equations that predict the mechanical deformation of the repository through salt creep closure of the Salado. These equations are used to predict void space porosities based on the ambient pressure in the repository. This relationship of pressure versus porosity is then used in the BRAGFLO computer code to calculate the impact of Salado salt creep closure on fluid flow.

5.34.1 Introduction

SANTOS Version 2.0 was originally validated for the CCA on the Cray platform. In April 2002, SANTOS was migrated to the Linux platform running on a PC and the Version number was changed to 2.17. The Department re-evaluated the code using the same acceptance criteria defined in the SANTOS Verification and Qualification Document [3]. Since the CCA, the Department has made unspecified changes to the code. The Department, however, has not tested the new functionalities associated with the changes in the code because it does not plan to use them to support the recertification performance assessment. The Department also intends to use SANTOS calculations that have been performed on the Compaq Alpha 8400 running a True 64 Unix Operating System. Therefore, the Department also validated SANTOS on this system by using the same acceptance criteria defined in the SANTOS Verification and Qualification Document identified above.

SANTOS is designed to simulate salt creep that results in a time-dependent reduction of disposal room volume. Creep is attributed to differences in principal stresses in the salt induced by room excavation. The pre-excavation stress state is hydrostatic, characterized by the equality of principal stresses. After excavation, the salt flows like a viscous fluid until the stress state becomes hydrostatic once again. Volumetric strain of the salt is considered elastic, similar to fluids that lack volumetric viscosity.

Total room volume is composed of two parts: a solid part equal to the volume of solid waste placed in a room, and a void part equal to the room volume less the solid volume. Fluid pressure in the room void space and resistance of solid waste to compression impede room volume reduction. The room solid volume is considered constant, although decomposition of the solid waste by chemical and biological processes occurs in time. These processes generate gas pressure in addition to the pressure increase caused by compression of air trapped within a sealed room.

Pressure generation caused by waste decomposition is governed by the ideal gas law and waste decomposition rate, which varies in time.

Gas pressure within the room may be generated in excess of the weight of the overlying strata and cause room volume reduction to cease and, indeed, to begin a relative expansion. This creates the possibility that fracturing of less ductile anhydrite beds near repository rooms will occur, providing additional volume for pressure relief.

The importance of salt creep and related room void volume and gas pressure variation is in their effect on direct brine and spall release volumes. Void volume relates to gas and brine storage, while gas pressure directly influences fluid flow rates within the repository and the volume of waste released to the surface during a human intrusion event. The room closure rate is slow enough to not affect the active life of the repository (about 25 years), but is much faster than waste decomposition. During the CCA it was assumed that closure is essentially complete within about one hundred years, while gas pressure build-up is maintained over hundreds of years.

5.34.2 Test Methodology

The SANTOS Verification and Qualification Document [3,4] defines 21 test cases. These cases are designed to ensure that all requirements identified in the Requirements Document section of the SANTOS Quality Assurance Document [2] are satisfied. All of the tests were rerun using the same 21 cases and the results were compared with the analytic solution or solutions from other codes presented in the Verification and Qualification Document.

The 21 test cases systematically exercise various aspects of SANTOS including the large displacement, large strain capability needed for creep closure analysis. Problem 20 is of particular interest because of the benchmark comparisons of SANTOS with the SANCHO, SPECTRUM and ANSALT codes. The comparison problem (Problem 20) is the isothermal strip model of a half-room and half-pillar geometry that contains various strata (salt, anhydrite and clay seams) represented by slide lines. SANTOS met the benchmark criteria. This same problem (Problem 20) was rerun by the Agency during a technical qualification study at Sandia National Laboratories with identical results.

The SANTOS Verification and Qualification Document [3,4] also contains a number of example problems that demonstrate that the computer model successfully implements the numerical equations. Theoretically, there can be no guarantee that a computer code is free of coding errors or conflicts. However, numerous example problems and a long history of successful code application indicate that SANTOS is reliable. This inference means that the code functions as intended. Given physically realistic input data, the output data from an adequately discretized grid and a well-converged program run can be viewed with confidence.

Requirements are outlined in Sections 2.0 and 3.0 of the Quality Assurance Document for SANTOS [2]. The 21 functional requirements described in Section 2.0 are those necessary for

code usage in WIPP performance assessments. These include handling the two-dimensional, large displacement, finite strain, time-dependent response of salt and the inelastic response of other geologic media such as anhydrite. Modeling of contact surfaces is also a requirement, as is the consolidation of porous materials. The latter differs from a conventional soil mechanics (porous geologic medium) consolidation process, which requires a genuinely coupled material model. Compaction is a more apt description of this material model requirement that is intended for waste behavior.

5.34.3 Test Results

The description of test cases, input files, and acceptance criteria exercise all portions of the code required in the list of Section 2.0 of the Quality Assurance Document for SANTOS [2]. However, specific acceptance criteria are replaced by comparisons with known solutions or with solutions obtained independently using other computer codes. The Agency considers this approach to be acceptable in that it provides a conventional way of validating computer codes through a series of comparisons with known analytical and numerical results that test various combinations of code options. There are no performance or attribute requirements for SANTOS relative to WIPP.

5.34.4 The Agency's Conclusions

It appears that SANTOS test cases may appropriately verify that the code produces adequate results for the tests conducted. However, based on results of our recent Advanced Mixed Waste Treatment Facility review we question implementation and ability of the Department's SANTOS code or its secondary codes, such as NUMBERS, to adequately model creep closure of a waste room and determine the waste porosity and room volume as a function of time. We believe that SANTOS or its secondary post processing codes appear to underestimate the stress applied to the waste as well as the waste room volume as a results of creep closure. The overall accuracy of SANTOS model predictions are currently being reviewed by the Agency and SNL and will be completed during the CRA review.

5.34.5 References

1. Stone, C.M. 1997. *SANTOS-A Two-dimensional Finite-Element Program for the Quasi-Static, Large Deformation, Inelastic Response of Solids*. SAND90-0543. Sandia National Laboratories, Albuquerque, New Mexico. 1997.
2. WIPP PA (Performance Assessment) *Quality Assurance Document, Version 1.0 for SANTOS* ERMS #237673. Sandia National Laboratories, Albuquerque, New Mexico.1997.
3. WIPP PA (Performance Assessment). *Verification and Qualification Document for SANTOS* ERMS #235675. Sandia National Laboratories, Albuquerque, New Mexico. 1997.

4. WIPP PA (Performance Assessment). *Verification and Qualification Document for SANTOS* ERMS #530091. Sandia National Laboratories, Albuquerque, New Mexico. 2003.

5.35 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.

5.35.1 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].

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of SECOTP2D 1.41 on those operating systems [5]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[6,7]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to SECOTP2D 1.41 on the new hardware systems.

5.35.2 Test Methodology

The tests for this code comprised the six 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of SECOTP2D 1.41 run on the ES40 with OpenVMS 7.3-1.

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[5], and they have now been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware 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 ES45 and 8400 with OpenVMS 7.3-1 to the corresponding output from the previous validation of SECOTP2D 1.41 running on the Compaq ES40 with OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.35.3 Test Results

The test set for SECOTP2D consists of six cases. The test cases for SECOTP2D 1.41 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1, and output files were compared to the corresponding output files from the previous validation of SECOTP2D 1.41 on the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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. The Agency also concluded that there were no numerical differences.

5.35.4 The Agency's Conclusions

Since all differences in the regression test results of SECOTP2D 1.41 are acceptable, the Agency concludes that SECOTP2D 1.41 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.35.5 References

1. WIPP PA (Performance Assessment). 1997. "Requirements Document and Verification and Validation Plan for SECOTP2D Version 1.41" Sandia National Laboratories. ERMS #245732.
2. WIPP PA (Performance Assessment). 1997. "Validation Document for SECOTP2D Version 1.41" Sandia National Laboratories. ERMS #245735.
3. WIPP PA (Performance Assessment). 1996. "Requirements Document and Verification and Validation Plan for SECOTP2D Version 1.30" Sandia National Laboratories. ERMS #236693.

4. WIPP PA (Performance Assessment). 1996. “Validation Document for SECOTP2D Version 1.30" Sandia National Laboratories. ERMS #236694.
1. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
2. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
3. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.

5.36 SGSIM

This section presents the validation and verification testing for the SGSIM Version 2.0 code. SGSIM generates multiple realizations of the values of a parameter at locations defined on a two dimensional grid using the geostatistical Gaussian sequential simulation algorithm. The output is in the form of two ASCII text files – a diagnostic file and a file containing the SGSIM output.

5.36.1 Introduction

The SGSIM, Version 2.0 code is an acquired code designed to solve the problem of simulating partially correlated values in one, two and three-dimensional domains conditional to measured values at random locations within the domain. In the context of the Culebra flow field calculations, SGSIM will be used to create the initial conditional residual fields that will then be updated by PEST (Section 5.25). Residual fields are necessary as the estimated mean transmissivity values (as estimated from the multiple regression tests) do not honor the transmissivity values at the measurement locations. SGSIM software is used on a PC running the Linux operating system. The SGSIM code is documented as specified in NQA-2a-1990 in the User’s Manual, the Requirements Document & Verification and Validation Plan, the Validation Document, and the Implementation Document [1-6]. A design document (DD) is not needed for acquired software under NP-19-1.

5.36.2 Test Methodology

The validation of SGSIM consists of reproduction of both a univariate and bivariate distribution, as well as, checking the accuracy and precision of SGSIM output. Three test cases are used to qualify the code and have been structured such that a single shell script must be executed (*test_sgsim.sh*). This shell script is presented in Appendix 4 of the VVP [5]. The shell script, *test_sgsim.sh* generates the 100 SGSIM realizations and runs all of the postprocessing codes necessary to evaluate the ability of SGSIM to meet the criteria specified in the three test cases. This shell generates two sets of output files named *qatest.#.out* and *gam_qa.#.out.* The # sign is replaced with numbers from 1 to 100 for each realization.

The base input file to SGSIM, *sgsim_org.par*, the source for the *modgeom.c* code, the *addcoord.par* file, and the source for the *addcoord.f* code are all listed in Appendix 1 of the VVP

[5]. The test data set used for SGSIM was obtained in the Sandia National Laboratories Flow and Transport Visualization Laboratory. The data were collected by a gas permeameter on a 36x36 sampling grid on a large, flat piece of rock. The log permeability values were then transformed into the current values used in the test data set and are saved in the file "exhaust.dat". These data allow SGSIM to be tested on a data set that exhibits spatial correlation. A total of 214 samples were obtained at random locations from the data set. The random draws were done by generating two random numbers from 1 to 36 and using these random numbers as the coordinates for the sample point. The random draw was done such that the same point could not be chosen twice. The 214 sample data are saved in the file rand_214.dat. In the testing described below, the subset of 214 points is used in test case 1 and 2, and the results obtained from using this subset are compared to results obtained from the full data set in test case 3.

The objective of Test Case #1 is to demonstrate that SGSIM can reproduce a univariate distribution. Test Case #1 starts with the 214 point sample set, termed the known values. SGSIM generates 100 realizations of parameter values at all grid points, conditioning each realization to the 214 known values. The parameter values in each realization are binned in a histogram with 80 intervals, each interval being 0.15 units wide. The histograms for each realization are then combined to produce a distribution of frequencies for each histogram bin. These distributions of frequencies are compared to the histogram of the known values.

The objective of Test Case #2 is to demonstrate that SGSIM can reproduce a bivariate distribution. Test Case #2 starts with the 214 point sample set, termed the known values. The variogram for the known values is computed and a model is fit to this variogram. This variogram model is then used as input to SGSIM. SGSIM generates 100 realizations of parameter values at all grid points, conditioning each realization to the 214 known values. The variogram for each realization is computed and the set of 100 variograms are combined to produce a range of variogram, or gamma, values as a function of lag distance. These simulated values are then compared to the original input model variogram. This comparison shows if SGSIM can accurately reproduce a bivariate distribution in the form of a variogram.

The original input data set comprises 1,296 data values from which a random selection of 214 data values was made for Test Cases 1 and 2. Test Case #3 uses the remaining 1,082 data points to check the precision and accuracy of the realizations produced by SGSIM from the 214 point data set used in Test Cases 1 and 2.

5.36.3 Test Results

For test case #1, the results of the univariate distribution reproduction show that for 8 of the 80 bins the known frequency value is outside of the simulated maximum and minimum. In other words, for 72 of the 80 bins (90 percent) the known value falls within the simulated minimum and maximum values. Based upon the Verification and Validation Plan (VVP), [5] Section 4.1.3, and the Requirements Document (RD) [4], Section 2.0, DOE believes that the results of Test Case #1 satisfy the acceptance criteria.

The criterion for test case #2 is that the simulated variograms bracket the input variogram model at least 90 percent of the lag spacings evaluated (WIPP PA, 2003, Verification and Validation Plan For SGSIM Version 2.00, Sandia National Laboratories, Albuquerque, New Mexico, [5]). This criterion is checked by determining whether or not the input model variogram value at each lag lies between the minimum and maximum simulated variogram values.

The values of the input model variogram, as well as the mean, minimum and maximum simulated variogram values show that of the 32 lag spacings that were evaluated, only one of them, 3 percent of the total, did the simulated values fail to bracket the input model. Therefore, DOE believes that SGSIM meets the criterion stated for test case #2.

For test case #3, the accuracy and precision are checked by comparing the simulated values at sampled locations. The criterion for test case #3 is that the absolute difference between the target and simulated proportions be less than 0.05. The results of the test show that the maximum difference is 0.0315 and occurs for the bin covering 39 to 61 percent of the distribution. This maximum difference is less than 0.05 and thus DOE concludes that SGSIM passes test case #3.

5.36.4 The Agency's Conclusions

The Agency has determined that the information required to be submitted to the Agency pertaining to SGSIM provides an adequate description of the code used in the calculations, a description of the limits of applicability of the code, detailed instructions for executing the computer code, hardware and software requirements to run the code, input and output formats with explanations of each input and output variable and parameter, listings of input and output files from sample computer runs, and reports on code verification, benchmarking, validation and quality assurance procedures that are adequate for use in CRA PA. Therefore, the Agency finds that DOE is in compliance with §194.23(c)(2).

5.36.5 References

1. Deutsch, C. V., and A.G. Journel, A.G., 1998. *GSLIB: Geostatistical Software Library and User's Guide: Second Edition ,* Oxford University Press, New York, 369 pp.
2. Deutsch, C.V., 1996, Direct Assessment of Local Accuracy and Precision, *Geostatistics*
3. WIPP PA, 2003, Software Quality Assurance Plan For SGSIM Version 2.00, Sandia National Laboratories, Albuquerque, New Mexico, ERMS #523914
4. WIPP PA, 2003, Requirements Document For SGSIM Version 2.00, Sandia National Laboratories, Albuquerque, New Mexico, ERMS #523913
5. WIPP PA, 2003, Verification and Validation Plan For SGSIM Version 2.00, Sandia National Laboratories, Albuquerque, New Mexico, ERMS #523914

5.37 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.

5.37.1 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 seven 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 seven 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 OpenVMS 6.1 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].

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of SPLAT 1.02 on those operating systems [5]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[6,7]. The discussion

below documents the test methodology, regression test results, and the Agency's conclusions with respect to SPLAT 1.02 on the new hardware systems.

5.37.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of SPLAT 1.02 run on the ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from SPLAT 1.02 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the previous validation of SPLAT 1.02. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.37.3 Test Results

The seven test cases for SPLAT 1.02 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1 and output files were compared to the corresponding output files from the previous validation of SPLAT 1.02 on the Compaq ES40 with OpenVMS 7.3-1 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. After conducting an independent visual comparison, the Agency 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.

5.37.4 The Agency's Conclusions

Since all differences in the regression test results of SPLAT 1.02 are acceptable, the Agency concludes that SPLAT 1.02 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.37.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for SPLAT Version 1.02" Sandia National Laboratories. ERMS #241866.
2. WIPP (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for SPLAT Version 1.01" Sandia National Laboratories. ERMS #237482.

3. WIPP PA (Performance Assessment). 1996. “Validation Document for SPLAT Version 1.01" Sandia National Laboratories. ERMS #237485.
4. WIPP PA (Performance Assessment). 1996. “Validation Document for SPLAT Version 1.02" Sandia National Laboratories. ERMS #241867.
5. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
6. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
7. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.

5.38 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).

5.38.1 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 new 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].

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency’s approval with respect to the migration and verification of STEPWISE 2.21 on those operating systems [3]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[4,5]. The discussion below documents the test methodology, regression test results, and the Agency’s conclusions with respect to STEPWISE 2.21 on the new hardware systems.

5.38.2 Test Methodology

The tests for this code comprised 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 ES45 and 8400 with OpenVMS 7.3-1, were compared to results from the validation tests of STEPWISE 2.21, run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from STEPWISE 2.21on the Compaq ES45 and 8400 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.

5.38.3 Test Results

The five test cases for STEPWISE 2.21were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of STEPWISE 2.21on the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.38.4 The Agency's Conclusions

Since all differences in the regression test results of STEPWISE 2.21 are acceptable, the Agency concludes that STEPWISE 2.21 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS Version 7.3-1.

5.38.5 References

1. WIPP PA (Performance Assessment). 1996. "Requirements Document & Verification and Validation Plan for STEPWISE Version 2.21" Sandia National Laboratories. ERMS #242250.
2. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for STEPWISE Version 2.20" Sandia National Laboratories. ERMS #227767.
3. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
4. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.

5. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.39 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 text output files.

5.39.1 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 changed 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 the Agency) 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.

In order to test new operating systems that were added in 2002-03 (Section 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. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of SUMMARIZE 2.20 on those operating systems [7]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[8,9]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to SUMMARIZE 2.20 on the new hardware systems.

5.39.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of SUMMARIZE 2.20 run on the ES40 with OpenVMS 7.3-1. The regression test methodology uses the VMS DIFFERENCE command to compare output from SUMMARIZE 2.20 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the previous validation of SUMMARIZE 2.20. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.39.3 Test Results

The eight test cases for SUMMARIZE 2.20 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 by using the VMS DIFFERENCE command. DOE and the Agency 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.

5.39.4 The Agency's Conclusions

Since all differences in the regression test results of SUMMARIZE 2.20 are acceptable, the Agency concludes that SUMMARIZE 2.20 meets the acceptance criterion specified in the RD/VVP [1], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS Version 7.3-1.

5.39.5 References

1. WIPP PA (Performance Assessment). 1997. “Requirements Document & Verification and Validation Plan for SUMMARIZE Version 2.20" Sandia National Laboratories. ERMS #246449.
2. WIPP PA (Performance Assessment). 1996. “Requirements Document & Verification and Validation Plan for SUMMARIZE Version 2.10" Sandia National Laboratories. ERMS #237458.
3. WIPP PA (Performance Assessment). 1996. “Validation Document for SUMMARIZE Version 2.10" Sandia National Laboratories. ERMS #237461.
4. WIPP PA (Performance Assessment). 1996. “Requirements Document & Verification and Validation Plan for SUMMARIZE Version 2.15" Sandia National Laboratories. ERMS #240252.
5. WIPP PA (Performance Assessment). 1996. “Validation Document for SUMMARIZE Version 2.15" Sandia National Laboratories. ERMS #240254.
6. WIPP PA (Performance Assessment). 1997 “Software Problem Report 97-016 for SUMMARIZE Version 2.10, 2.15, 2.20" Sandia National Laboratories. ERMS #246511.
7. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
8. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
9. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.

5.40 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.

5.40.1 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.

5.40.1.1 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.

In order to test new operating systems that were added in 2002-03 (Section 1), 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 2.20 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of CAMCON_LIB 2.20 on those operating systems [7]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[8,9]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to CAMCON_LIB 2.20 on the new hardware systems.

5.40.1.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CAMCON_LIB Version 2.2 run on the ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CAMCON_LIB 2.20 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the previous validation of CAMCON_LIB 2.20 with OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.40.1.3 Test Results

The seven test cases for CAMCON_LIB 2.20 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of CAMCON_LIB 2.20 on the Compaq ES45 with OpenVMS 7.3-1 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. The Agency 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.

5.40.1.4 The Agency's Conclusions

Since all differences in the regression test results of CAMCON_LIB 2.20 are acceptable, the Agency 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 ES45 and 8400 with OpenVMS 7.3-1.

5.40.1.5 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.
2. Analysis Plan (AP-065). 2000 "Regression for the Upgrade to Open VMS Version 7.2 on the WIPP DEC Alpha Cluster" Sandia National Laboratories.
3. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for CAMCON_LIB Version 2.16" (Document Version 1.00) Sandia National Laboratories. ERMS #227736.
4. WIPP PA (Performance Assessment). 1999. "Change Control Form for CAMCON_LIB, Version 2.18" Sandia National Laboratories. ERMS #251637.
5. WIPP PA (Performance Assessment). 1999. "Regression testing of CAMCON_LIB Version 2.18" Sandia National Laboratories. ERMS #251629.
6. WIPP PA (Performance Assessment). 1995. "Implementation Document for CAMCON_LIB Version 2.20" (Document Version 1.04) Sandia National Laboratories. ERMS #525736.
7. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
8. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
9. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.40.2 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.

5.40.2.1 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].

In order to test new operating systems that were added in 2002-03 (Section 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 1.25 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of CAMDAT_LIB 1.25 on those operating systems [6]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[7,8]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to CAMDAT_LIB 1.25 on the new hardware systems.

5.40.2.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CAMDAT_LIB 1.25 run on the ES40 with OpenVMS 7.3-1.

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 text file for comparison during the validation process. In the CAMDAT_LIB 1.25 validation, the CDB files are converted using GROPECDB 2.12 which has been validated on a Compaq ES45 and 8400 with OpenVMS 7.3-1 as part of the hardware regression test (see Section 5.10, GROPECDB) [5]. For this regression

test, GROPECDB 2.12 is used to convert the CDB output files from CAMDAT_LIB 1.25 in OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CAMDAT_LIB 1.25 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of CAMDAT_LIB 1.22 on the Compaq ES40 with OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.40.2.3 Test Results

The seven test cases for CAMDAT_LIB 1.25 were executed on the Compaq ES45 and 8400 with OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the previous validation of CAMDAT_LIB 1.22 on the Compaq ES40 with OpenVMS 7.3-1 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. The Agency found that all differences in output acceptable; namely, that the differences are limited to library run date and time, execution statistics, and the directory and file names.

5.40.2.4 The Agency's Conclusions

Since all differences in the regression test results of CAMDAT_LIB 1.25 are acceptable, the Agency 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 ES45 and 8400 with OpenVMS 7.3-1.

5.40.2.5 References

1. WIPP PA (Performance Assessment). 1995. "Requirements Document & Verification and Validation Plan for CAMDAT_LIB Version 1.22" (Document Version 1.00) Sandia National Laboratories. ERMS #228109.
2. WIPP PA (Performance Assessment). 1995. "Validation Document for CAMDAT_LIB Version 1.22" (Document Version 1.00) Sandia National Laboratories. Sandia WIPP Central Files ERMS #228112.
3. WIPP PA (Performance Assessment). 1995. "Implementation Document for CAMDAT_LIB Version 1.25" (Document Version 1.25) Sandia National Laboratories. ERMS #525734.
4. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12" Sandia National Laboratories. ERMS #237497.
5. WIPP PA (Performance Assessment) 2003. "Analysis Report for the OpenVMS 7.3-1 Regression Test" Sandia National Laboratories. ERMS #525277.

6. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration", June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
7. WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.
8. WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

5.40.2 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.

5.40.2.1 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].

In order to test new operating systems that were added in 2002-03 (Section 1), 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 2.22 run on a DEC Alpha 2100 with OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval with respect to the migration and verification of CAMSUPES_LIB 2.22 on those operating systems [7]. In January 2003, two new hardware systems were added to conduct performance assessments for the WIPP. A Compaq ES45, and a Compaq Alpha 8400 which are both running Open VMS 7.3-1[8,9]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to CAMSUPES_LIB 2.22 on the new hardware systems.

5.40.2.2 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 ES45 and 8400 with OpenVMS 7.3-1 were compared to results from the validation tests of CAMSUPES_LIB Version 2.20 run on the ES40 with OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from CAMSUPES_LIB 2.22 on the Compaq ES45 and 8400 with OpenVMS 7.3-1 to the output from the validation of CAMSUPES_LIB 2.22 on the Compaq ES40 with OpenVMS 7.3-1.

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 2.22 with OpenVMS 7.3-1. The VMS DIFFERENCE command compares two files and identifies records that are different in the two files.

5.40.2.3 Test Results

The two test cases for CAMSUPES_LIB 2.22 were executed on the Compaq ES45 and 8400 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 the Compaq ES40 with OpenVMS 7.3-1 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. The Agency 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.

5.40.2.4 The Agency's Conclusions

Since all differences in the regression test results of CAMSUPES_LIB 2.22 are acceptable, the Agency concludes that CAMSUPES_LIB 2.22 meets the acceptance criteria specified in the VVP [3], and thus is considered as validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1.

5.40.2.5 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.
2. Analysis Plan (AP-065). 2000 "Regression for the Upgrade to Open VMS Version 7.2 on the WIPP DEC Alpha Cluster" Sandia National Laboratories.

3. WIPP PA (Performance Assessment). 1995. “Verification and Validation Plan for CAMSUPES_LIB Version 2.20" (Document Version 1.01) Sandia National Laboratories. ERMS #251633.
4. WIPP PA (Performance Assessment). 1995. “Validation Document for CAMSUPES_LIB Version 2.20" (Document Version 1.02) Sandia National Laboratories. ERMS #251634.
5. WIPP PA (Performance Assessment). 1995. “Implementation Document for CAMSUPES_LIB Version 2.22" (Document Version 1.04) Sandia National Laboratories. ERMS #525738.
6. WIPP PA (Performance Assessment). 1995. “Requirements Document and Verification and Validation Plan for CAMSUPES_LIB Version 2.18" (Document Version 1.00) Sandia National Laboratories. ERMS #227744.
7. EPA, 2003. “Review of WIPP Performance Assessment Computer Code Migration”, June 10, 2003, EPA Docket: A-98-49, II-B3-57. Environmental Protection Agency.
8. WIPP PA – “Analysis Report for the ES45 Regression Test” March 6, 2003 Sandia National Laboratories. ERMS #530290.
9. WIPP PA – “Analysis Report for the 8400 Regression Test” Sandia National Laboratories. ERMS #527280.

6.0 SUMMARY AND CONCLUSIONS

The Agency has reviewed DOE's code migration activities associated with 39 computer codes and three libraries that DOE has migrated to the Compaq ES45 and 8400 with OpenVMS 7.3-1. The Agency 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

- WIPP PA – "Analysis Report for the ES45 Regression Test" March 6, 2003 Sandia National Laboratories. ERMS #530290.

- WIPP PA – "Analysis Report for the 8400 Regression Test" Sandia National Laboratories. ERMS #527280.

In addition to the references cited above, the Agency 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 the Agency.

In March 2004, the Agency concluded that 36 (of the 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 with OpenVMS 7.3-1 were approved for use in compliance calculations for the WIPP performance assessment. As part of this most current technical review of the remaining three codes (i.e., NUMBERS, SANTOS, DRSPALL) the Agency is able to conclude that DRSPALL Version 1.0 is validated on the Compaq ES45 and 8400 with OpenVMS 7.3-1. The Agency also concludes that NUMBERS now meets the QAP 19-1 requirements.