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**TECHNICAL SUPPORT DOCUMENT FOR
SECTION 194.23: MODELS AND COMPUTER CODES**

PABC Codes Changes Review

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EXECUTIVE SUMMARY

The U.S. Department of Energy (DOE) conducted a Performance Assessment (PA) to show compliance with the U.S. Environmental Protection Agency's (EPA or the Agency) disposal regulations and compliance criteria under Title 40, Part 194, of the *Code of Federal Regulations* (40 CFR 194) as part of the Waste Isolation Pilot Plant (WIPP) certification process. DOE must demonstrate on an ongoing basis that PA computer software is in compliance with regulations outlined in Section 194.23 – Models and Computer Codes. 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. In September 2004, the Agency published their findings with respect to the qualification of the computer codes on the Compaq ES40 and the Compaq Alpha 8400. At that time the Agency concluded that 38 (of 39) computer codes and 3 libraries migrated to the Compaq ES45 and 8400 using OpenVMS 7.3-1 were approved for use in compliance calculations for the WIPP PA.

In 2005, DOE made revisions to eight of the computer codes; including LHS, POSTLHS, CUTTINGS, DRSPALL, PANEL, SUMMARIZE, PRECCDFGF and CCDFGF. This report presents the Agency's findings with respect to the qualification of these eight computer codes on the Compaq ES40 and ES45. After reviewing that information, the Agency concluded that the most recent versions of these eight codes, as specified in Table 3.1, were approved for use in compliance calculations for the WIPP PA.

1.0 INTRODUCTION

This report describes the results of the U.S. Environmental Protection Agency's (EPA or the Agency) review of Performance Assessment (PA) computer code development and testing activities performed by the U.S. Department of Energy (DOE) in support of their ongoing PA 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 PA computer codes that are documented in DOE's Compliance Certification Application (CCA) (DOE 1996).

DOE conducted a PA to show compliance with EPA disposal regulations as part of the WIPP certification process. DOE must demonstrate on an ongoing basis that PA 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 as follows:

- 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 PA calculation
- Software that is used in managing information or augmenting mission essential decisions
- Software used to collect data (e.g., far-field, near-field, engineered barriers)

DOE executes the PA conceptual models through software applications with parameter value inputs on an infrastructure composed of computers and operating systems that must be periodically updated. For the certification application, performance analyses were run on the DEC Alpha Cluster using the OpenVMS operating system, version 6.1. In 1999 the operating system was updated from OpenVMS 6.1 to 7.1, and a year later from 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 OpenVMS 7.3-1.

In addition to software upgrades, DOE has made hardware changes. The DEC Alpha Cluster was the main platform for performance analyses for the WIPP during the 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 OpenVMS 7.3-1 as the operating system, in conjunction with the Compaq ES40, ES45 and 8400. In June 2003, the Agency presented their findings with respect to their review of 27 codes and 3 libraries that were migrated to the Compaq ES40. The Agency concluded that all of the 27 codes and 3 libraries that were migrated successfully to the Compaq ES40 using OpenVMS 7.3-1, and are approved for use in compliance calculations for the WIPP PA.

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 (Docket A-98-49, II-B3-70), the Agency concluded that 36 (of 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 using OpenVMS 7.3-1 were acceptable and were approved for use in compliance calculations for the WIPP performance assessment. In September 2004 (Docket A-98-49, II-B1-7), the Agency published their findings with respect to the qualification of the computer codes on the Compaq ES45 and the Compaq Alpha 8400. At that time the Agency concluded that 38 (of 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 using OpenVMS 7.3-1 were acceptable and approved for use in compliance calculations for the WIPP performance assessment. SANTOS was the only code not approved for PA calculations.

This report documents the results of the Agency's assessment performed to determine whether the observed DOE PA code activities conform 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 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 the Department of Energy (DOE) implement a Quality Assurance (QA) 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 that require the establishment and implementation of QA programs for all aspects of the WIPP 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, as follows:

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

Life-cycle phases are implemented using an iterative or sequential approach following the process flowchart in Figure 1. Each phase and its 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. Software under configuration control and developed within the scope of these QA requirements do not require a stand-alone SQAP. Following the development of the SQAP, all specified requirements for each phase must be met and not subvert the intent of the requirements. SQAPs may be written for an individual code or a set of codes.

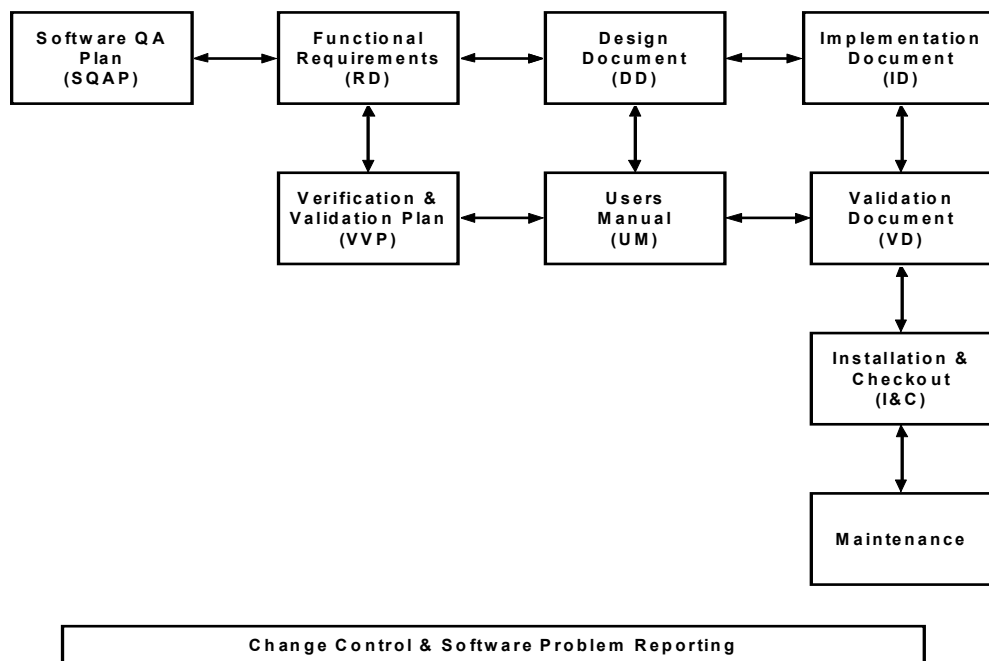


Figure 1. Major Components of DOE's Software Development Process

Requirements Phase

The documents produced during the requirements phase are the Requirements Document and Verification and Validation Plan (RD/VVP), which is a single document that identifies the computational requirements of the code (e.g., MODFLOW 2000 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), 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
- Ranges for data inputs and outputs, in a manner that can be implemented in software

More than one DD may be created during software development. For example, a high-level design may be developed to match the code design to the requirements and define the overall architecture of the code (define modules and subroutines and their purpose, data structures, subroutine-call hierarchy, etc.). Another design document may be developed to define how the

modules will function in detail (define call interfaces between routines, define data types, etc.). A detailed design, as its name implies, is very detailed down to the level of almost writing the code (pseudocode). These separate 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. The UM generally includes the following:

- 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 UM 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 UM 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 UM explains the implementation of these methods in the computer code in sufficient detail so that an independent reviewer can understand them.
- The derivation of the numerical procedure from the mathematical component model. The UM 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 UM 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 PA calculation. Using this information, the computer user can reconstruct the code and/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 previously approved VVP to demonstrate that the developed software meets the requirements defined for it in the RD. The Validation Document (VD), produced during this phase, summarizes the results of the testing activities prescribed in the RD/VVP documents for the individual codes, and provides evaluations based on those results. The VD contains listings of input and output files from computer runs of a model. The VD also contains reports on code verification, bench marking, and validation, and documents the results of the QA 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
- The Approved Users Memorandum

Production Software and/or Baseline Document Change Control

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

- Major changes, including new requirements, new design, new models, and 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 Installation and Checkout Form are used.
- Minor changes do not affect the requirements or design, and can be documented with an addenda (no more than three addenda's per baseline document) or page change to the affected baseline document. In addition to the Change Control Form, the Installation and Checkout Form must be used.
- Patch changes can be used for very small fixes to the code, usually one or two lines of source code or expanding a field's character length, etc. Patch changes can be documented and tested with the Change Control Form and Installation and 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 and at the top of the code prior to the first executable line. The code reviewer should 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 are as follows:

- 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). 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 a *major problem*, the Responsible Manager identifies affected users to be notified of the problem and designates qualified personnel to identify and evaluate the impact of the software problem. The affected analysis 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 a *minor problem*, 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, and provides 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 that necessary components of configuration management are present.

For compliance software, the Software Baseline List contains the following:

- 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
- 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 provides 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 OpenVMS 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 OpenVMS 7.3-1 and Hardware to HP Alpha ES45
- Analysis Report for the ES45 Regression Test
- Analysis Report for the 8400 Regression Test

Regression testing was performed on the upgraded operating systems and hardware that run PA codes to demonstrate the codes continue to 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 UMs, VDs, IDs, and RD/VVPs for each code. The Agency also reviewed all of the Change Control and Software Installation and Checkout forms for code modifications made since the initial certification.

3.0 OVERVIEW OF DOE'S COMPUTER CODE MIGRATION ACTIVITIES

3.1 CURRENT STATUS

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, 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 using OpenVMS 7.3-1 are approved for use in compliance calculations for the WIPP PA. In January 2003, two new hardware systems were added to conduct PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running OpenVMS 7.3-1. This configuration was used for preparing the Compliance Recertification Application (CRA). Because of these changes, regression testing was conducted by DOE for the software codes and three 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 RDs. In September 2004, the Agency published their findings with respect to the qualification of the computer codes on the Compaq ES40 and the Compaq Alpha 8400. At that time the Agency concluded that 38 (of 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 using OpenVMS 7.3-1 were approved for use in compliance calculations for the WIPP PA. In 2005, DOE made revisions to eight of the computer codes; including LHS, POSTLHS, CUTTINGS, DRSPALL, PANEL, SUMMARIZE, PRECCDFGF and CCDFGF. This report presents the Agency's findings with respect to the qualification of these eight computer codes on the Compaq ES40 and ES45. The versions of the computer codes that are approved for use in compliance calculations for the WIPP PA are presented in Table 3.1.

The RD for each software code specifies the validation criteria for the code and the test cases that demonstrate compliance with these criteria. Sandia National Laboratories (SNL) used regression testing to determine whether each code could satisfy the criteria in its RDs when run in the current computing configuration. The regression test was conducted by running every validation test for each code in the current computing configuration (OpenVMS 7.3-1 running on the Compaq ES40 and ES45) and comparing the code's output to the output from the code's previously 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.

Table 3-1. Computer Codes Reviewed by the Agency
(Codes and Version Numbers in **Bold** are not approved by the Agency)

Code Name	Version	Code Name	Version
ALGEBRACDB	2.35	NUTS	2.05A
BLOTADB	1.37	PANEL	4.03
BRAGFLO	5.0	PATTERN	1.0
CCDFGF	5.02	PCCSRC	2.21
CCDFSUM	2.00	PEST	5.5
CUTTINGS_S	6.02	POSTBRAG	4.00
DRSPALL	1.10	POSTLHS	4.07a
DTRKMF	1.0	POSTSECOTP2D	1.04
EPAUNI	1.15A	PREBRAG	7.00
FMT	2.40	PRECCDFGF	1.01
GENMESH	6.08	PRELHS	2.30
GROPECDB	2.12	PRESECOTP2D	1.22
ICSET	2.22	RELATE	1.43
LHS	2.42	SANTOS	2.17
LHS2STEP	1.04	SECOTP2D	1.41
MATSET	9.10	SGSIM	2.0
MODFLOW2000	1.60	SPLAT	1.02
NONLIN	2.00	STEPWISE	2.21
NUCPLOT	1.20	SUMMARIZE	3.00
NUMBERS	1.19		

3.2 DOE'S TEST METHODOLOGY

The test methodology and acceptance criteria described in AP-089 were implemented by the DOE for these regression tests, and the results are presented in Section 5 of this document. The regression tests consisted of running each code on the ES40 and ES45 using OpenVMS 7.3-1. Every test case from each code's RD was run and the results were compared to test results from the previous validation of that code (i.e., Compaq ES40 using OpenVMS 7.3-1). The result was a comprehensive analysis of every test case and every acceptance criterion for each software code.

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 previous validations were often processed through other software codes to produce ASCII files that could then 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. After concluding that a code met the acceptance criteria specified in its RDs, a Software Installation and Checkout Form was completed. The I&C form documents that a code's regression test results met the acceptance criteria specified in its RDs, management's 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, 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 onsite reviews:

- Tabulation of the Agency's code acceptance criteria 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 PA codes to meet the QA 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
- Reviewed the ability of PA codes to accurately reproduce output obtained under the software/hardware configurations in place during the CCA

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

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. “Technical Support Document for Section 194.22 and 23: Review of WIPP Recertification Performance Assessment Computer Codes: CRA Code Review”, September 30, 2004, Environmental Protection Agency, EPA Docket: A-98-49, II-B1-7

5.0 SUMMARY OF INDIVIDUAL COMPUTER CODE MIGRATION

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

5.1 CCDFGF

This section presents the regression test results for the CCDFGF code. The CCDFGF code assembles the results calculated by other codes in the WIPP PA system to produce Cumulative Complementary Distribution Functions (CCDFs) of releases.

5.1.1 Introduction

Since the 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 the OpenVMS 6.1 operating system [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. CCDFGF 3.00 was validated by the DOE's analysis, and the additional acceptance criteria were met. Consequently, the validation of CCDFGF 3.00 relies on 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 relied 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 of CCDFGF 3.01 [8] on the Compaq ES40. In January 2003, two new hardware systems were added to conduct PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running OpenVMS 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]. In September 2004, the Agency concluded that CCDFGF 3.01, 5.0, and 5.0A met the acceptance criteria specified in the VVP [1, 2, 13], and thus was validated on the Compaq ES45 and 8400 using OpenVMS 7.3-1 [14].

In June 2004, the code was changed from Version 5.0A to Version 5.01 to reflect changes involving the confidence intervals assigned to the drilling rate, which were changed from 90% to 99.5 %. The most recent version of the code, however, was issued in December 2004 (Version 5.02). This new version included changes to the Function FindSeries (i.e., a block in the IF-THEN-ELSE construction was removed and a check was made within the remaining block to ensure that 0 was never returned) [17]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to the CCDFGF testing.

5.1.2 Test Methodology

Version 5.01 (ES40 Platforms)

All three of the tests described in the *Validation Plan for CCDFGF Version 5.01* (VP) were performed on the ES40 to test the seven functional requirements [15]. Test Case 1 tested CCDFGF to ensure that it evaluated the different release mechanisms correctly for one future. This test case included five parts; one for each of the following release mechanisms:

- Cuttings and cavings
- Spallings
- Direct brine releases (DBR)
- Culebra releases
- Total releases

The input files for this test case specify only eight vectors, with two futures each. Using only a few vectors and futures allows manual calculation of the correct results. Moreover, each vector tested a different release mechanism, further simplifying the manual calculation. The manual calculation is then compared to the computer generated results.

The objective of Test Case 2 was to ensure that the random number generator was producing a statistically random sequence of numbers, and that the sequence was reproducible. For this test case, CCDFGF 5.01 was run first using the input files for Test Case 2. Next, two utility programs were run; CCGF_CHISQ_TEST.FOR for the Chi-Squared Goodness of Fit test, and CCGF_SERIAL_TEST.FOR for the Serial test. These codes computed the statistics for the output of the random number generator in CCDFGF.

Test Case 2 produced an output file CCGF_QA0501_RND_TEST2.BIN written to the logical RANDOMNUMBERS\$BIN. This binary file contained the sequence of random numbers generated by the random number generator in CCDFGF.

Each utility program used a single input file assigned to the logical CCGF_RANDOM\$INP. For this test case, the logical CCGF_RANDOM\$INP should have the value CCGF_QA0501_RND_TEST2.BIN. This file was unformatted binary data written by CCDFGF, consisting of a sequence of data pairs; each data pair consists of a double precision real number and a three-character string.

Each utility code produced an output file assigned to the logicals CCGF_CHISQ_TEST\$OUT and CCGF_SERIAL_TEST\$OUT. For this test, the logicals were assigned values of CCGF_QA0501_TEST2_CHISQ.OUT and CCGF_QA0501_TEST2_SERIAL.OUT, respectively. These files contain the results of each test by reporting the chi-squared value for each repetition, and whether or not the statistic exceeds the critical value. These files can be found in the library LIBCCGF.

Test Case 3 evaluated the statistical correctness of stochastic futures modeled by CCDFGF. Test Case 3 ran 1,000 futures for each of 8 vectors and examined the following statistics:

- Probability of selecting each CH waste stream
- Probability of brine pocket intrusion
- Probability of an intrusion hitting the excavated region
- Percentage of intrusions hitting the excavated region that hit CH waste
- Probability of each plugging pattern

In addition, Test Case 3 examined the average number of drilling events in each future and the distribution of mining times. When choosing the option to use the volume fraction as a probability for the release of cuttings, Test Case 3 examined the probability of CH waste intrusions that encounter CH waste as well. The input files for this test case specified only eight vectors, with 1000 futures each. The release data for each vector was the same as in Test Case 1. Unlike Test Case 1, the futures for each vector were determined randomly.

Test Case 3 produced four output files. When CCGF_CONTROL_TEST3.INP was used, CCGF_QA0501_TEST3.OUT was assigned to the logical CCGF\$OUT, and CCGF_QA0501_TEST3.PRT was assigned to the logical CCGF_PRT\$OUT. When CCGF_CONTROL_TEST3B.INP was used, CCGF_QA0501_TEST3B.OUT was assigned to the logical CCGF\$OUT, and CCGF_QA0501_TEST3B.PRT was assigned to the logical CCGF_PRT\$OUT. The files assigned to CCGF_QA0501_TEST3.PRT and CCGF_QA0501_TEST3B.PRT contained the data needed to evaluate each release mechanism. The files for CCGF_QA0501_TEST3.OUT and CCGF_QA0501_TEST3B.OUT should be readable by the code CCDFSUM Version 2.00. Both files were too lengthy to include in this document; they can be found in library LIBCCGF class QA0501 in CMS.

Version 5.02 (ES40 and ES45 Platforms)

The CCDFGF code was upgraded from Version 5.01 to Version 5.02 in December 2004. The tests for this code comprised the three test cases described in the VVP for CCDFGF 5.01 [15] and an additional test case for CCDFGF 5.02 described in the *Addendum to the CCDFGF 5.01 Validation Document* (VD) [16]. This additional test case was designed to check that the new interpolation of the drilling rate (90% versus 99.5%) worked properly.

The regression testing of CCDFGF 5.02 on the ES40 platform using OpenVMS 7.3-1 was conducted for Test Cases 1–3. Test results were compared to the results of the validation testing conducted for CCDFGF 5.01 on the ES40 platform using OpenVMS 7.3-1 [16]. Test results for Test Case 4 were compared to the results of the unit testing conducted for CCDFGF 5.02 Test Case 4 [16].

The regression test methodology used the VMS DIFFERENCE command to compare output from CCDFGF 5.02 to the corresponding file from the validation, unit, or regression test results of the previous version. Differences that were limited to code run dates and time, file and directory names, user names, platform names, and execution statistics are acceptable. Differences involving numerical output require 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.

5.1.3 Test Results

Version 5.01 (ES40 Platforms)

Test Case 1 was validated by comparing the output files CCGF_QA0501_TEST1.PRT and CCGF_QA0501_TEST1B.PRT with the known solutions given in the VVP. The only time that CCGF_QA0501_TEST1B.PRT was used to validate Test Case 1 is when the cuttings activity is used to calculate spallings releases. Otherwise, CCGF_QA0501_TEST1.PRT was used to validate Test Case 1. CCGF_QA0501_TEST1.PRT and CCGF_QA0501_TEST1B.PRT can be found in CMS library CCGF. The acceptance criteria were met for each of the five parts; cuttings and cavings, spallings, direct brine releases (DBR), Culebra releases, and total releases.

Test Case 2 was validated by verifying that 90% or more of the Chi-Squared Goodness of Fit test runs and Serial test runs were successes. The Chi-Squared test results, CCGF_QA0501_TEST2_CHISQ.OUT, indicate that one Chi-Squared statistic was greater than the critical value (test 8); thus, acceptance criteria in the VVP requirements were met.

Test Case 3 was validated by comparing the output files CCGF_QA0501_TEST3.PRT and CCGF_QA0501_TEST3B.PRT with the known solutions given in the VVP. CCGF_QA0501_TEST3.PRT and CCGF_QA0501_TEST3B.PRT can be found in the CMS library CCGF.

The 99.5% confidence interval was calculated using two-sided confidence intervals for a population by proportion. The following equation defines the two-sided confidence intervals [8]:

$$\left(p - z_{\alpha/2} \sqrt{\frac{p(1-p)}{n}}, p + z_{\alpha/2} \sqrt{\frac{p(1-p)}{n}} \right)$$

Where p is the probability, n is the number of trials observed, and $z_{\alpha/2}$ is the test statistic. For a confidence interval of 99.5%, $\alpha = 0.005$.

p and n are determined for the following:

- Probability of selecting each CH waste stream
- Probability of brine pocket intrusion
- Probability of an intrusion hitting the excavated region
- Percentage of intrusions hitting the excavated region that hit CH waste
- Probability of each plugging pattern

The observed frequencies for each probability listed above fall within their respective 99.5% confidence intervals. Therefore, CCDFGF met the acceptance criteria in the VVP.

Version 5.02 (ES40 and ES45 Platforms)

Test Cases 1–3 for CCDFGF 5.02 were executed on the COMPAQ ES40 using OpenVMS 7.3-1, and Test Cases 1–4 were executed on the ES45 platform using OpenVMS 7.3-1. Output files from CCDFGF 5.02 test cases were compared to the corresponding files from the validation unit or regression testing of the previous version run on the same platforms. The comparison was performed using the VMS DIFFERENCE command. The comparison found no differences in the output files, with the exception of Test Case 3 on the E840 platform. The difference for Test Case 3 was limited to differences in the callouts for the platform (i.e., ES40 versus ES45).

5.1.4 The Agency's Conclusions

The testing of CCDFGF 5.01 on the ES40 indicated that the acceptance criteria were satisfactorily met as specified for the test cases described in the *Validation Plan for CCDFGF Version 5.01* (VP) [15]. Furthermore, the regression testing of CCDFGF 5.02 (ES40 and ES45) found that all differences were acceptable between the files. The Agency concluded that CCDFGF 5.02 was validated on the Compaq ES40 and ES45 in OpenVMS Version 7.3-1.

5.1.5 References

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5.2 CUTTINGS_S

This section presents the regression test results for the CUTTINGS_S code Versions 5.04A, 5.10, 6.01, and 6.02. 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.

5.2.1 Introduction

Since the 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 using the OpenVMS 6.1 operating system. The validation was accomplished by demonstrating 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 using 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 CUTTINGS_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 that 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 Version 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 were 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 were not used, the INGRES system must be installed on the system for Version 5.04 to run. The linked software was no longer available on the system, so CUTTINGS_S would be relinked to remove these libraries.

There were no source changes between CUTTINGS_S Version 5.04A and Version 5.04. The only difference was that CUTTINGS_S Version 5.04A would not be linked with SDBREAD_LIB and the INGRES library. The code would 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 would not be used for Version 5.04A. [5]

In order to test the new operating systems that were added in 2002–2003 (Section 1), regression test results from CUTTINGS_S 5.04A run on the ES40 using OpenVMS 7.3-1 were compared to results from the validation tests of CUTTINGS_S 5.04A run on a DEC Alpha 2100 using 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 PAs for the WIPP; a Compaq ES45, and a Compaq Alpha 8400, both running OpenVMS 7.3-1[9,10]. In September 2004, the Agency concluded that CUTTINGS_S 5.04A met the acceptance criteria specified in the RD/VVP [3], and thus was validated on the Compaq ES45 and 8400 using OpenVMS 7.3-1 [11].

The CUTTINGS_S code was upgraded from Version 5.10 to Version 6.00 in January 2005 [12]. CUTTINGS_S was modified to remove unneeded functionality and improve maintainability [13]. The changes reduced the number of input files needed to run CUTTINGS_S and improved the traceability of input parameters to CUTTINGS_S. The new CUTTINGS_S can produce output values for multiple intrusions and cavities, resulting in fewer code executions. Output results on the CAMDAT file may be added, deleted, or renamed.

The validation of CUTTINGS_S Version 6.00 was conducted on a COMPAQ ES40 platform and documented in the *Verification and Validation Plan and Validation Document for CUTTINGS_S Version 6.00* (VVP/VD) [12]. For completeness, regression testing was also conducted by DOE to demonstrate the codes validity on the COMPAQ ES45 platform [14].

In April 2005, the CUTTINGS_S code was upgraded from Version 6.00 to Version 6.01 [16]. In CUTTINGS_S Versions 5.10 and 6.00, the input parameter RNDSPALL was required for use of spall model 4. In version 6.01, use of this parameter is optional. If RNDSPALL is not specified in the input control file, the first spallings vector volume in the spall input file will be used for calculation of spallings releases for the first vector output, the second spallings vector volume will be used for calculation of spallings releases for the second vector output, and so on.

The validation of CUTTINGS_S Version 6.01 was conducted on a COMPAQ ES40 platform and documented in the *Verification and Validation Plan and Validation Document for CUTTINGS_S Version 6.01* (VVP/VD) [16]. For completeness, regression testing was also conducted by DOE to demonstrate the codes validity on the COMPAQ ES45 platform [17].

In June 2005, the CUTTINGS_S code was upgraded from Version 6.01 to Version 6.02 [20]. CUTTINGS_S Version 6.02 was created for the primary purpose of correcting a potential error in calculating the radius at which the drill fluid flow becomes laminar. The code was changed such that the inner radius cannot be greater than the outer radius. In Version 6.02, the subroutine DRILL was modified by adding an IF statement that assigns a value of RORIG to ROUTER if ROUTER becomes less than RINNER. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to the CUTTING_S testing.

5.2.2 Test Methodology

Version 6.0 (ES40 Platform)

The test set for the previous version of the code, CUTTINGS_S Version 5.10, consisted of a total of 10 test cases. Test Cases 1–6 were determined to result in comparable output in the regression testing of Version 5.04 as documented in the VD for CUTTINGS_S Version 5.04 [4]. Test Cases 7–9 were added for CUTTINGS_S Version 5.04, and were determined to result in acceptable output in the validation testing of that version [11]. Test Case 10 was added for CUTTINGS_S Version 5.10, and was determined to result in acceptable output in the validation testing of Version 5.10 [4].

CUTTINGS_S Version 6.00 was the result of extensive code modifications. Because of these changes, several of the existing test cases were no longer relevant, and the input to the remaining test cases must be modified. The major code changes are listed in Table 8-1 [12], along with the effect the changes have on testing.

To test existing functionality, the test set for CUTTINGS_S Version 6.00 included the 5 test cases that were still relevant from the 10 test cases used to validate Version 5.10, with some alterations due to modifications in the CUTTINGS_S code. Test Cases 1, 2, 3, 6, and 9 have been removed, for reasons detailed in Table 8-1 [12]. The remaining test cases (4, 5, 7, 8, and 10) were regression tested against the output from the testing of Version 5.10.

Because of code modifications described in Table 8-1 [12], changes were made to the input files for the existing test cases. For each test case, a new master control file was needed, the "TXT0" file no longer exists, and the input control file was modified. The description of each test case included a listing of the new master control file and the modified input control file, with differences highlighted. There were no changes to any of the input CAMDAT files, the BRAGFLO CAMDAT files, or the spall data file.

The code modifications described in Table 8-1 [12] resulted in changes to the output files. The verification file was no longer generated. Cosmetic changes made to the debug file made it impractical to difference this file. Since this file was used primarily for debugging a CUTTINGS_S run, the file was ignored during testing, except in specific instances where the debug file was examined in the original testing. The primary output file for the original testing was a binary CAMDAT file. Since the binary file cannot be examined directly, the GROPECDB

code [7] was used to produce an ASCII listing of the contents of the CAMDAT file. GROPECDB was run on the output CAMDAT files from the current test execution (Version 6.00) and from the previous validation (Version 5.10), and the resulting files were differenced using the VMS DIFFERENCE utility. Code modifications removed the first time step (time 0.0) and all release variables from the CAMDAT file. To avoid flagging multiple desirable differences, GROPECDB was directed to select only those variables that were of interest from the CAMDAT file output from the previous validation. GROPECDB listed all variables from the CAMDAT file output from the current version. Regression test results were acceptable if all the differences can be attributed to some modification that has been made to the code, or are unrelated to code performance (such as dates, times, file names). Since the changes from Version 5.10 to Version 6.00 do not affect the code exercised by the 5 remaining test cases of the first 10 test cases, regression testing suffices to determine that these test cases continue to produce valid output.

The testing of the Test Cases 4, 5, 7, 8, and 10 must also verify the new functionality described in Table 8-1[12]. A new output data file was generated, and since it contained data written to the output CAMDAT file that has been verified in previous validations, this validation only needs to verify that the correct data has been written to the output data file. A new requirement, R.5, addressed the calculation of BRAGFLO volume-weighted averages. These averages were calculated and written to the output CAMDAT file in previous versions, and the values were verified in the validation testing of Version 5.04 [4]. Thus, this validation only needed to verify that the values of the BRAGFLO volume-weighted average variables were unchanged.

CUTTINGS_S Version 6.00 can process multiple scenarios, vectors, cavities, and intrusions in a single execution. A new Test Case 11 was added to the test set to verify this process. Test Case 11 re-ran a subset of the CUTTINGS_S executions for the CRA1 calculation. The output CAMDAT files generated by the test execution were compared with those generated by the CRA1 PA calculations, and the output data file was hand-checked to verify the format and contents. Thus, this new test case was actually a regression test using CRA1 results.

All test cases were run using the WIPP PA run control system. The scripts, script input files, and all other files related to validation testing of CUTTINGS_S Version 6.00 reside in the SCMS. All test inputs were fetched at run time by the scripts, and test outputs/results and run logs were automatically stored by the scripts in class QA0600 of the CUSP library in the SCMS. A log file that indicated the input/output files was generated by each test case execution.

All the files required to test this code are contained in the QA0600 class of the CUSP library in the SCMS, unless otherwise mentioned. Files may be fetched using the appropriate commands that are defined in the SCMS Plan [14]. Table 8-2 [12] shows the relationship between the functional requirements and the test cases.

Version 6.00 (ES45 Platform)

The test suite for CUTTINGS_S Version 6.00, as described in the VVP/VD [12], consists of Test Cases 4, 5, 7, 8, 10, and 11. (Several test cases were deleted from the test suite because capabilities were removed from CUTTINGS_S Version 6.00 (see Table 8-1) [12].)

The entire test suite for CUTTINGS_S Version 6.00 was executed on the COMPAQ ES45 platform using the OpenVMS 7.3-1 operating system.

CUTTINGS_S needs the following input files: a master control file, an input control file an input CAMDAT file, an optional input BRAGFLO CAMDAT file, and an optional spall data file. All input files used to execute the tests on the COMPAQ ES45 were the same files used in the previous validation of CUTTINGS_S 6.00, except for the master control file. The master control file had to be modified for each test, because it contains the names of the output files.

Each execution of CUTTINGS_S generated the following output files: a text output data file, a binary CAMDAT file (72 CAMDAT files were output for Test Case 11), and a debug file. The regression test methodology used the VMS DIFFERENCE command to compare output from CUTTINGS_S 6.00 on the COMPAQ ES45 platform using OpenVMS 7.3-1 to the output from the validation of CUTTINGS_S 6.00 on the COMPAQ ES40 using OpenVMS 7.3-1. The output CAMDAT file was a binary file and cannot be compared with the VMS DIFFERENCE command. The GROPECDB utility [2] was used to write portions of the CAMDAT file as text so that they could be compared. The debug file was not part of the code's functionality and was not used in verification, so it was not compared. Thus, for each test, the text output data file and the GROPECDB output from each output CAMDAT file were compared using the VMS DIFFERENCE command.

The VMS DIFFERENCE command compares two files and identifies records that were different in the two files. Records with differences were grouped into sections. In the output of the DIFFERENCE command, sections were separated by rows of 12 asterisks; inside a section, the records from the two files were 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. To improve the readability of the difference file, the /NONUMBER and /MERGE=0 options were specified with the DIFFERENCE command. (The DIFFERENCE command issued was listed at the end of each DIFFERENCE file.) The /NONUMBER option eliminated leading line numbers from difference lines; /MERGE=0 suppressed the output of the first matching line as the last line in each section.

Comparing each pair of output files resulted in a list of differences. Differences that were limited to code run dates and time, file and directory names, platform names, and execution statistics were acceptable. Differences involving numerical output required analysis to determine the origin of the differences, and whether the differences affected the code's performance. Numerical differences were determined to be acceptable based on the analysis of each difference.

Version 6.01 (ES40 Platform)

The previous version of the code, CUTTINGS_S Version 6.00, was the result of extensive code modifications. The test set for CUTTINGS_S Version 6.00 consisted of a total of six test cases. Five of these test cases (4, 5, 7, 8, and 10) were regression-tested against the output from the testing of the previous version of CUTTINGS_S. Test Case 11 was introduced for CUTTINGS_S Version 6.00. (Note that Test Cases 1, 2, 3, 6, and 9 were removed from the

CUTTINGS_S 6.00 test set because they tested obsolete features.) The testing for CUTTINGS_S Version 6.00 is documented in the VVP/VD for CUTTINGS_S Version 6.00 [12].

CUTTINGS_S Version 6.01 is the result of a minor change pertaining to spillings model 4. In the older versions, the spillings vector was selected with the RNDSPALL parameter, which usually referenced a random number on the input CAMDAT file. In CUTTINGS_S Version 6.01, the RNDSPALL option is still available, but by default, the spillings vector will have a one-to-one correspondence with the input vector. That is, the first spillings vector volume in the spill input file will be used for calculation of spillings releases for the first vector output, the second spillings vector volume will be used for calculation of spillings releases for the second vector output, etc. CUTTINGS_S will terminate if the number of input vectors exceeds the number of spillings vectors.

To test existing functionality, the test set for CUTTINGS_S Version 6.01 included the six test cases used to validate CUTTINGS_S Version 6.00. The results of the CUTTINGS_S Version 6.01 execution of these tests were compared with the results of the CUTTINGS_S Version 6.00 execution. Test Case 11 was modified to test the one-to-one spillings vector selection. The modification was limited to removing the RNDSPALL command from the input command file and altering the spill data file so that the vectors on the new file correspond to the vectors selected by the RNDSPALL property for the input vectors. Test Case 10 (without modification) tests the older method of selecting the spillings vector with RNDSPALL. A new test case, Test Case 12 verifies that CUTTINGS_S terminates when the number of input vectors exceeds the number of spillings vectors.

All input files for the test cases were the same files used in the previous validation of CUTTINGS_S 6.00, except for the master control file (and the files mentioned above for Test Case 11). The master control file was modified for each test case, because it contained the names of the output files. The new master control file for each test case was listed in this document.

A successful CUTTINGS_S execution produced the output files; the output data file, a set of output CAMDAT files, and a debug file. The output data file was compared to the Version 6.00 output using the VMS DIFFERENCE utility. The output CAMDAT file was a binary file that could not be examined directly. The GROPECDB code [7] was used to produce an ASCII listing of the contents of the CAMDAT file. GROPECDB was run on the output CAMDAT files from the current test execution (Version 6.01) and from the previous validation (Version 6.00), and the resulting files are compared by differencing them using the DCL DIFFERENCE utility. Acceptable differences in the GROPECDB files were limited to the GROPECDB run time, CUTTINGS_S run date and time, CUTTINGS_S version, and CAMDAT file names. Since the debug file was not part of the code's functionality and was not used in verification, DOE did not examine or difference this file, with the exception of Test Case 12.

All test cases were run using the WIPP PA run control system. The scripts, script input files, and all other files related to validation testing of CUTTINGS_S Version 6.01 reside in the SCMS. All test inputs were fetched at run time by the scripts, and test outputs/results and log files were

automatically stored by the scripts in class QA0601 of the CUSP library in the SCMS. A log file that indicated the input/output files was generated by each test case execution.

Version 6.01 (ES45 Platform)

The test suite for CUTTINGS_S Version 6.01 was described in the VVP/VD [16], and consists of Test Cases 4, 5, 7, 8, 10, 11, and 12. (Several test cases were deleted from the test suite when CUTTINGS_S Version 6.00 was validated, because capabilities were removed from the code.) The entire test suite for CUTTINGS_S Version 6.01 was executed on the Compaq ES45 platform using the OpenVMS 7.3-1 operating system.

CUTTINGS_S needed the following input files: a master control file, an input control file, an input CAMDAT file for each vector, an optional input BRAGFLO CAMDAT file for each scenario-vector pair, and a spall data file for spall model 4 only. All input files used to execute the tests on the Compaq ES45 were the same files used in the previous validation of CUTTINGS_S 6.01 except for the master control file. The master control file had to be modified for each test because it contains the names of the output files.

Each successful execution of CUTTINGS_S generated the following output files: an output data file, a binary output CAMDAT file (72 CAMDAT files were output for Test Case 11), and a debug file. The regression test methodology for all tests except Test Case 12 used the VMS DIFFERENCE command to compare output from CUTTINGS_S 6.01 on the Compaq ES45 platform using OpenVMS 7.3-1 to the output from the validation of CUTTINGS_S 6.01 on the Compaq ES40 using OpenVMS 7.3-1. The output CAMDAT file was a binary file and could not be compared with the VMS DIFFERENCE command. The GROPECDB utility [2] was used to write portions of the CAMDAT file as text so that they can be compared. The debug file was not part of the code's functionality and was not used in verification. Thus, the output data file and the GROPECDB output from each output CAMDAT file were differenced.

The regression test methodology used the VMS DIFFERENCE command to compare output from various versions of the codes. Comparing each pair of output files results in a list of differences. Differences that were limited to code run dates and time, file and directory names, platform names, and execution statistics were acceptable. Differences involving numerical output required analysis to determine the origin of the differences and whether the differences affected the code's performance. Numerical differences may be determined to be acceptable based on the analysis of each difference. If all differences were found to be acceptable, it follows that the output of CUTTINGS_S 6.01 met the acceptance criteria specified in the VVP/VD [16].

A different test methodology must be used for Test Case 12. This test case validated that CUTTINGS_S terminates on a specific error condition without generating an output data file or an output CAMDAT file. For this test case, the debug file and the log file were examined to verify that the test case met the acceptance criteria specified in the VVP/VD [16] for this test case.

Version 6.02 (ES40 and ES45 Platforms)

The tests for CUTTING_S Version 6.02 comprise the test cases described in the *Verification and Validation Plan/Validation Document CUTTINGS_S Version 6.01* (VVP/VD) [16] and an additional test case for CUTTINGS_S 6.02 described in the *Addendum to the CUTTINGS_S Version 6.01 Verification and Validation Plan/Validation Document* (VVP/VD Addendum) [21]. Per the VVP/VD [16], Test Cases 1, 2, 3, 6, and 9 are obsolete, leaving eight test cases as described in the VVP/VD [16] and its addendum [21].

The regression testing of CUTTINGS_S 6.02 on the ES40 platform using OpenVMS 7.3-1 was conducted for seven test cases. Test results were compared to the results of the validation testing conducted for CUTTINGS_S 6.01 on the ES40 platform using OpenVMS 7.3-1 [16]. Test case 13, added when CUTTINGS_S was upgraded to Version 6.02, was subject to unit testing rather than regression testing. Results of the unit testing for CUTTINGS_S 6.02 test case 13 on the ES40 platform using OpenVMS 7.3-1 can be found in VVP/VD Addendum [21].

The regression testing of CUTTINGS_S 6.02 on the ES45 platform using OpenVMS 7.3-1 was conducted for all eight test cases. Test results for the seven test cases (above) were compared to the results of the regression testing conducted for CUTTINGS_S 6.02 on the ES40 platform using OpenVMS 7.3-1. Test results for Test Case 13 were compared to the results of the unit testing conducted for CUTTINGS_S 6.02 [16].

CAMDAT database files (CDB) were produced in most the CUTTINGS_S test cases. The output CDB files were converted from a binary CDB file to an ASCII GROPE file for comparison during the validation process. The CDB files were converted using GROPECDB 2.12. GROPECDB 2.12 was validated [3] on a COMPAQ ES40 and ES45 following the same process described in this document using OpenVMS 7.3-1. For this regression test of CUTTINGS_S 6.02, GROPECDB 2.12 was used to convert the CDB output files from CUTTINGS_S 6.01 in OpenVMS 7.3-1, as well as CUTTINGS_S 6.02 in OpenVMS 7.3-1.

The regression test methodology uses the VMS DIFFERENCE command to compare output from various versions of the codes. Comparing each pair of output files results in a list of differences. Differences that were limited to code run dates and time, file and directory names, platform names, and execution statistics were acceptable. Differences involving numerical output required analysis to determine the origin of the differences and whether the differences affected the code's performance. Numerical differences may be determined to be acceptable, based on the analysis of each difference.

5.2.3 Test Results

Version 6.0 (ES40 Platform)

The CUTTINGS_S execution generated three output files; the output data file (new to this version), the output CAMDAT file, and the debug file. The binary CAMDAT file was compared with the corresponding CAMDAT file from the previous validation (Version 5.10). The contents of the new data file were hand-compared to verified results from the output CAMDAT file.

The binary output CAMDAT file was GROPEd, using GROPECDB, to produce a text listing of its contents. The corresponding binary file from Version 5.10 was also GROPEd. Time 0.0 and the release variables, which were not output by Version 6.00, were not listed for Version 5.10. The two GROPECDB output files were then compared with the DCL DIFFERENCE utility.

The difference file of the GROPECDB output of the output CAMDAT files was examined to verify that no unacceptable differences were found. The following acceptable differences were expected in GROPECDB comparisons: the GROPECDB run date and time, the CAMDAT file name, and the CUTTINGS_S version and run date and time. In addition, because of changes to CUTTINGS_S Version 6.00 as detailed in Table 8-1 [12], time step 1 corresponds to time step 2 from Version 5.10 (GROPECDB did not list time step 1 for the Version 5.10 file). All values must match to at least five significant digits (with rounding).

Testing for CUTTINGS_S Version 6.00 was completed, and DOE concluded that the acceptance criteria for all test cases were successfully met. DOE also concluded that testing verified that CUTTINGS_S satisfies all the requirements listed in the CUTTINGS_S RD [18].

Version 6.0 (ES45 Platform)

All six test cases for CUTTINGS_S 6.00 were executed on the COMPAQ ES45 platform using OpenVMS 7.3-1. Output files from the test cases were compared to the corresponding output files from the validation of CUTTINGS_S 6.00 on a COMPAQ ES40 using OpenVMS 7.3-1 by using the VMS DIFFERENCE command. 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.

DOE concluded that all differences in output were acceptable; namely, that the differences were 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 were acceptable; namely, that the differences were limited to code run date and time, file and directory names, platform names, system version numbers, and execution statistics.

Version 6.01 (ES40 Platform)

The CUTTINGS_S execution for this test case generated three output files: the output data file, the output CAMDAT file, and the debug file. The output data file and the binary output CAMDAT file were compared with the corresponding files from the previous validation

(Version 6.00). The output data file from the current test execution was compared to the output data file from the Version 6.00 test execution with the DCL DIFFERENCE utility.

The binary output CAMDAT file was GROPEd, using GROPECDB, to produce a text listing of its properties and global variable values. The corresponding binary file from Version 6.00 was also GROPEd. The two GROPECDB output files were then compared with the DCL DIFFERENCE utility. The difference file of the GROPECDB output and the output CAMDAT files were examined to verify that no unacceptable differences are found. The following acceptable differences were expected in GROPECDB comparisons: the GROPECDB run time, the CAMDAT file name, and the CUTTINGS_S run date and time. If all the differences were acceptable, the acceptance criteria were met for this portion of the test case.

Testing for CUTTINGS_S Version 6.01 was completed, and DOE concluded that the acceptance criteria for all test cases were successfully met. DOE also concluded that the testing verified that CUTTINGS_S satisfied all the requirements listed in the CUTTINGS_S RD [18].

Version 6.01 (ES45 Platform)

All seven test cases for CUTTINGS_S 6.01 were executed on the Compaq ES45 platform using the OpenVMS 7.3-1 operating system. For all test cases except Test Case 12, output files from the test cases were compared to the corresponding output files from the validation of CUTTINGS_S 6.01 on a Compaq ES40 using OpenVMS 7.3-1 by using the VMS DIFFERENCE command. 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. Since only acceptable differences were detected between the results of CUTTINGS_S 6.01 executed on the Compaq ES45 platform using OpenVMS 7.3-1 and CUTTINGS_S 6.01 executed on the Compaq ES40 platform using OpenVMS 7.3-1, DOE concluded that CUTTINGS_S 6.01 met the acceptance criteria specified in the VVP/VD [16] for these test cases.

For Test Case 12, the debug file and the log file from the test cases were examined according to the acceptance criteria specified in the VVP/VD [16]. From this examination, DOE concluded that CUTTINGS_S 6.01 met the acceptance criteria for this test case.

Version 6.02 (ES40 and ES45 Platforms)

Seven test cases for CUTTINGS_S 6.02 were executed on the COMPAQ ES40 using OpenVMS 7.3-1 and eight test cases were executed on the ES45 platform using OpenVMS 7.3-1. All test case output files (.CDB and .TBL files for all except Test Case 12 were compared, and Test Case 12 .DBG file was compared) from CUTTINGS_S 6.02 test cases were compared to the corresponding files from the validation, unit, or regression testing of the previous version run on the same platform. The comparison was performed using the VMS DIFFERENCE command. The comparison found no unacceptable differences in the output files.

Since all differences are acceptable between the files, DOE concluded that CUTTINGS_S 6.02 met the acceptance criteria specified in the VVP/VD [16], and thus was validated on the COMPAQ ES40 and ES45 platforms using OpenVMS 7.3-1.

5.2.4 The Agency's Conclusions

The testing of CUTTING_S 6.0, 6.01 on the ES40 indicated that the acceptance criteria were satisfactorily met as specified for the test cases described in the *Verification and Validation Plan/Validation Document CUTTINGS_S Version 6.01* (VVP/VD) [16]. Furthermore, the regression testing of CUTTING_S 6.0 (ES45), 6.01(ES45) and 6.02 (ES40 and ES45) found that all differences were acceptable between the files. The Agency concluded that CUTTING_S 6.0, 6.01, and 6.02 were validated on the Compaq ES40 and ES45 in OpenVMS Version 7.3-1.

5.2.5 References

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5.3 DRSPALL

This section documents the validation and verification results for the DRSPALL computer code. 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 can 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.

5.3.1 Introduction

DRSPALL calculates the spillings 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 drillbit and cavings removed by shear forces of the drilling mud against the drilled cavity wall are calculated 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 DRSPALLMODFLOW software; the Software QA plan, an RD, VVP, UM, DD, ID, and the 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 Windows. However, for implementation in WIPP and other similar PAs, the code was ported to the WIPP Alpha-Cluster running OpenVMS. 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 PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running the OpenVMS 7.3-1 operating system. In September 2004, the Agency concluded that DRSPALL Version 1.0 met the acceptance criteria specified in the RD/VVP, and thus was validated on the Compaq ES45 and 8400 using OpenVMS 7.3-1 [7].

In January 2004, modifications to DRSPALL Version 1.00 were made, which included cosmetic changes and bypassing the bounds checking, and the upper bound on the farfield stress was changed from 15E6 to 18E6 to accommodate future initial conditions [8]. The most recent version of DRSPALL is 1.1. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to DRSPALL.

5.3.2 Test Methodology

The test set for DRSPALL consisted of four test cases that were designed to address the requirements established in Section 2 of the VVP\VD [4]. The test cases were 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 was used to perform the CRA calculations.) The production executable is generated as described in the DRSPALL ID [3]. All files used in functional testing are stored in class QE0100 of the DRS library of the 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 required that DRSPALL be executed one or more times. Each execution was referred to by DOE as a "case" or "subcase" or "run." For example, Test Case 5 had six subcases, labeled Case 5.1 through 5.7 (5.4 is not defined), and the files for the test case were distinguished by "TC51 " through "TC57" in their names.

The initial tests for DRSPALL Version 1.1 consisted of the two subcases of Test Case 4 described in the VVP and VD for DRSPALL 1.00 (VVP/VD) [4]. Test Case 4 was identified in the VVP/VD as suitable for future regression testing. Regression test results from DRSPALL 1.10 run on the ES45 using OpenVMS 7.3-1 were then compared to results from the validation tests of DRSPALL 1.10 run on the ES40.

Once the testing of Test Case 4 was complete, the entire test suite for DRSPALL was executed with DRSPALL 1.10 on the COMPAQ ES40 platform using OpenVMS 7.3-1 [9]. The test suite consists of Test Case 1 (1.1, 1.2), Test Case 2 (2.1, 2.2, 2.3, 2.4, 2.5, 2.6), Test Case 4 (4.1, 4.2) and Test Case 5 (5.1, 5.2, 5.3, 5.5, 5.6, 5.7), where each number in parentheses represents a subcase. (As noted above there is no Test Case 3 defined for DRSPALL.) Each subcase was a

separate execution of DRSPALL and resulted in output files that must be included in the regression test. The DRSPALL output files were a binary CAMDAT file, a diagnostics file, and, for some test cases, a set of validation files.

The regression test methodology used the VMS DIFFERENCE command to compare output from DRSPALL 1.10 on the COMPAQ ES40 platform using OpenVMS 7.3-1 to the output from the validation of DRSPALL 1.00 on the COMPAQ ES40 using OpenVMS 7.3-1. The output CAMDAT file was a binary file and cannot be compared with the VMS DIFFERENCE command. The GROPECDB utility code [4] was used to write portions of the CAMDAT file as text so that they can be compared. The diagnostics file was not part of the code's functionality and was not used in verification. However, since several of the version 1.10 code changes alter the diagnostics file, the file from the validation of DRSPALL 1.10 for Test Case 4.1 only was compared to the corresponding output file from the validation of DRSPALL 1.00.

After completing the testing of DRSPALL 1.1 on the ES40, regression tests were performed of DRSPALL 1.1 on the ES45 using OpenVMS 7.3-1 and were compared to results from the validation tests of DRSPALL 1.10 run on the ES40 using OpenVMS 7.3-1 [11].

5.3.3 Test Results

DRSPALL reads its run parameters from an input control file (file extension “.DRS”). The DRSPALL UM [5] provided instructions on constructing and interpreting the input control file. Each subcase of the four test cases had its own input control file. The input control file contained the test subcase number (as “Validation Test Case”). DRSPALL responded to the test case number by creating special output files that contained 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 DD for DRSPALL [2] described any non-standard processing that was dependent on the test case. Each execution of DRSPALL generated an output CAMDAT file (“.CDB”) and an output diagnostics file (“.DBG”). The DRSPALL UM [5] described the variables output in the CAMDAT file. Variables on a CAMDAT file may be extracted in tabular form using the GROPECDB utility or plotted using the BLOTADB utility. In addition to the standard output files, a particular test case may generate additional files to be used for validation only. These validation files were described under the relevant test case section.

Most test cases compared the results of the DRSPALL execution with those generated by analytical and other numerical solutions. These solutions were described in detail in the relevant test case section in the VVP\VD [4].

The DRSPALL test cases were run with a set of procedure files. Each test case had its own procedure file, and each subcase had a procedure file. The procedure file for the test case (e.g., DRS_TC5.COM) executed all subcases. It created a subdirectory for the subcase, fetched the subcase procedure file from the SCMS, and executed the subcase procedure file, usually by submitting a job to a batch queue. The procedure file for the subcase (e.g., DRS TC5I.COM) fetched the DRSPALL input file(s), and executed DRSPALL with the appropriate input and output file designations. The subcase procedure file may also do some simple post-processing

on the CAMDAT file, but most post-processing was done manually by the tester. The test cases were designed to meet the requirements coverage presented in Section 6 of the VVP\VD.

All subcases of the four test cases for DRSPALL Version 1.10 were executed on the COMPAQ ES40 and ES45 using OpenVMS 7.3-1. Output from the test cases were compared to the corresponding output files from the validation of DRSPALL Version 1.0 on a COMPAQ ES40 and ES45 using OpenVMS 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.

5.3.4 The Agency's Conclusions

The comparison of the regression tests found that all differences in output were acceptable; namely, that the differences were limited to the test details (output file name, test date and time, test node). Therefore, the Agency concluded that DRSPALL Version 1.10 meets the acceptance criteria specified in the RD/VVP, and was validated on the Compaq ES40 and 45 using OpenVMS 7.3-1.

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5.4 LHS

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

5.4.1 Introduction

LHS Version 2.32ZO was validated in August 1996 on a DEC Alpha 2100 using the OpenVMS 6.1 operating system using 10 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 using 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 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 using OpenVMS 7.3-1 were compared to results from the validation tests of LHS 2.41 run on a DEC Alpha 2100 using OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval of LHS 2.41 on those operating systems [6]. In January 2003, two new hardware systems were added to conduct PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running OpenVMS 7.3-1 [7,8]. In September 2004, the Agency concluded that LHS 2.41 met the acceptance criteria specified in the RD/VVP [1], and thus was considered as validated on the Compaq ES45 and 8400 using OpenVMS 7.3-1 [9].

In January 2005, the LHS code was revised in order to accurately describe the normal, lognormal, student, and logstudent distributions [10]. Version 2.42 of the code was subsequently validated to run on the COMPAQ ES40 using OpenVMS 7.3-1 [11]. Following the validation of the code on the ES40, it was regression tested to run on the ES45 [12]. The discussion below documents the test methodology and results, and the Agency's conclusions with respect to LHS 2.42.

5.4.2 Test Methodology

The tests for this code comprised the 11 test cases described in the RD/VVP for LHS Version 2.41 (RD/VVP) [1]. All of the test cases were run on the ES40 and the results compared to the evaluation criteria. Previous versions of LHS were validated using a now-retired code called PLOTLHS. This code constructed a cumulative distribution function (CDF) plot for a sampled distribution, and overlaid that plot onto the plot of the theoretical CDF. However, it was determined that PLOTLHS incorrectly handled truncated distributions, specifically truncated normal and lognormal distributions. Thus, it was not a feasible method to validate the current version of LHS.

To verify that LHS meets the acceptance criteria for Test Cases 1 through 4, the software EXCEL was employed to construct CDF plots from the sampled distributions. These plots were overlaid on the plots of the expected CDFs of the distributions. (These CDFs were also calculated using EXCEL).

Once LHS Version 2.41 was verified on the ES40 using OpenVMS 7.3-1, regression test results from LHS 2.42 run on the ES45 using OpenVMS 7.3-1 were compared to results from the validation tests of LHS 2.42 run on the ES40 using OpenVMS 7.3-1.

5.4.3 Test Results

The 11 test cases for LHS 2.42 were executed on the Compaq ES45 using 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 using OpenVMS 7.3-1 by using the VMS DIFFERENCE command. No differences were found.

5.4.4 The Agency's Conclusions

Since no differences were found, the Agency concluded that LHS 2.42 met the acceptance criteria specified in the RD/VVP [1], and thus was considered as validated on the Compaq ES40 and ES45 using OpenVMS 7.3-1.

5.4.5 References

1. WIPP PA (Performance Assessment) 1996. "Requirements Document & Verification and Validation Plan for LHS Version 2.41." Sandia National Laboratories. Sandia WIPP Central Files WPO # 30731.

2. WIPP PA (Performance Assessment) 1995. "Requirements Document & Verification and Validation Plan for LHS Version 2.32ZO." Sandia National Laboratories. Sandia WIPP Central Files WPO # 23533.
3. WIPP PA (Performance Assessment) 1995. "Validation Document for LHS Version 2.32ZO." Sandia National Laboratories. Sandia WIPP Central Files WPO # 23536.
4. WIPP PA (Performance Assessment) 1996. "Validation Document for LHS Version 2.41." * Sandia National Laboratories. Sandia WIPP Central Files WPO # 30734.
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." Environmental Protection Agency.
7. WIPP PA – "Analysis Report for the ES45 Regression Test, March 6, 2003." Sandia National Laboratories. Sandia WIPP Central Files. ERMS 530290.
8. WIPP PA – "Analysis Report for the 8400 Regression Test." Sandia National Laboratories. Sandia WIPP Central Files. ERMS 527280.
9. USEPA – "Review of WIPP Performance Assessment Computer Code Migration Activities –Version 2." September 2004.
10. WIPP PA (Performance Assessment) 2004. "Change Control Form for LHS, Version 2.41." WIPP Central Files WPO # 538375.
11. WIPP PA (Performance Assessment) 2005. "Verification and Validation Plan & Validation Document for LHS (Version 2.42)." Sandia National Laboratories. Sandia WIPP Central Files ERMS 538370.
12. WIPP PA (Performance Assessment) 2005. Analysis Report for the ES45 Regression Test of LHS Version 2.42. Sandia National Laboratories.

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

5.5 PANEL

This section presents the regression and validation test results for the PANEL code. PANEL takes the source term data and computes the solubility 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.

5.5.1 Introduction

PANEL 3.50ZO was initially validated in September 1995 on a DEC Alpha 2100 using the OpenVMS 6.1 operating system 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 using 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 CCA. In June 1998, PANEL was revised to Version 4.00 and was validated on a DEC Alpha 2100 using 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 that 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 2002–2003 (Section 1), regression test results from PANEL 4.00 run on the ES40 using OpenVMS 7.3-1 were compared to results from the validation tests of PANEL 4.00 run on a DEC Alpha 2100 using 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 consisted 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 of PANEL 4.00 on those operating systems [10].

In January 2003, two new hardware systems were added to conduct PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running OpenVMS 7.3-1[11, 12]. In September 2004, the Agency concluded that PANEL 4.02 met the acceptance criteria specified in the RD/VVP [3], and thus were considered as validated on the Compaq ES45 and 8400 using OpenVMS 7.3-1[16].

In April 2005, the PANEL code was revised to Version 4.03 in order to be able to set the default panel brine volume via MATSET [17]. To ensure that this version was working properly, the DOE regression-tested Version 4.03 against Version 4.02 on the COMPAQ ES40 and ES45 using OpenVMS 7.3-1[2]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to PANEL 4.03.

5.5.2 Test Methodology

The test suite for PANEL, as described in the VVP [14], consisted of Test Cases 1 through 9, with Test Case 4 requiring two executions. The entire test suite for PANEL Version 4.03 was

executed on the Compaq ES40 platform using OpenVMS 7.3-1, and then executed again on the Compaq ES45 platform using OpenVMS 7.3-1.

PANEL needed the following input files: a CAMDAT file containing source term and inventory data, and an optional CAMDAT file containing brine flow and volume data. PANEL also needed a run type option input on the command line. All input files and options used to execute the PANEL 4.03 tests were the same files and options used in the previous validation of PANEL 4.02.

Each successful execution of PANEL generated the following output files: a binary output CAMDAT file and a debug file. The regression test methodology used the VMS DIFFERENCE command to compare output from the current execution to the output from a validation of PANEL. The output CAMDAT files were binary files and could not be compared using the VMS DIFFERENCE command. The GROPECDB utility code [4] was used to write portions of the CAMDAT files as text, so that they could be compared. Thus, the debug file and the GROPECDB output from the output CAMDAT file were differenced. The output from PANEL 4.03 on the Compaq ES40 platform is compared with the VMS DIFFERENCE command to the output from the validation of PANEL 4.02, and the output from PANEL 4.03 on the Compaq ES45 platform was compared to the output from the validation of PANEL 4.03 on the Compaq ES40.

5.5.3 Test Results

All test cases for PANEL 4.03 were executed twice: first on the Compaq ES40 platform using OpenVMS 7.3-1, and then on the Compaq ES45 platform using OpenVMS 7.3-1. The output from PANEL 4.03 on the Compaq ES40 platform was compared to the output from the validation of PANEL 4.02, and the output from PANEL 4.03 on the Compaq ES45 platform was compared to the output from the validation of PANEL 4.03 on the Compaq ES40.

Output files from the test cases run on the ES40 platform were compared to the corresponding output files from the validation of PANEL 4.02 by using the VMS DIFFERENCE command. The comparison found that the differences in the output files were limited to code run dates and times, PANEL versions and build dates, file and directory names, and a new message. The new error message “ELBNAM REFCON AND PROP NAM PANDFVOL NOT FOUND!! SET TO 4.000E+03” in the debug file is a result of an intentional source change to PANEL 4.03, so this difference is expected.

Output files from the test cases run on the ES45 platform were compared to the corresponding output files from PANEL 4.03 on the ES40 platform by using the VMS DIFFERENCE command. The comparison found that the differences in the output files were limited to code run dates and times, platforms, and file names.

Since PANEL 4.03 executed on the Compaq ES40 and ES45 platforms using OpenVMS 7.3-1 met the acceptance criteria specified in the VVP [14] for all test cases, PANEL 4.03 was considered as validated on the Compaq ES40 and ES45 platforms using OpenVMS 7.3-1.

5.5.4 The Agency's Conclusions

Since PANEL 4.03 executed on the Compaq ES40 and ES45 platforms using OpenVMS 7.3-1 met the acceptance criteria specified in the VVP [14] for all test cases, PANEL 4.03 was considered as validated by the Agency on the Compaq ES40 and ES45 platforms using OpenVMS 7.3-1.

5.5.5 References

1. Analysis Plan (AP-042) 1998. "Regression for the Upgrade to OpenVMS Version 7.1 on the WIPP COMPAC Alpha Cluster." Sandia National Laboratories.
2. Analysis Plan (AP-065) 2000. "Regression for the Upgrade to OpenVMS Version 7.2 on the WIPP DEC Alpha Cluster." Sandia National Laboratories.
3. WIPP PA (Performance Assessment) 1998. "Requirements Document and Verification and Validation Plan for PANEL Version 4.00." Sandia National Laboratories. Sandia WIPP Central Files WPO # 48787.
4. WIPP PA (Performance Assessment) 1995. "Requirements Document and Verification and Validation Plan for PANEL Version 3.50ZO." Sandia National Laboratories. Sandia WIPP Central Files WPO # 24326.
5. WIPP PA (Performance Assessment) 1995. "Validation Document for PANEL Version 3.50ZO" Sandia National Laboratories. Sandia WIPP Central Files WPO # 24328.
6. WIPP PA (Performance Assessment) 1996. "Requirements Document and Verification and Validation Plan for PANEL Version 3.60." Sandia National Laboratories. Sandia WIPP Central Files WPO # 37358.
7. WIPP PA (Performance Assessment) 1998. "Validation Document for PANEL Version 3.60." Sandia National Laboratories. Sandia WIPP Central Files WPO # 37362.
8. WIPP PA (Performance Assessment) 1998. "Validation Document for PANEL Version 4.00." Sandia National Laboratories. Sandia WIPP Central Files WPO # 48791.
9. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12." Sandia National Laboratories. Sandia WIPP Central Files WPO # 37497.
10. EPA, 2003. "Review of WIPP Performance Assessment Computer Code Migration, June 10, 2003." Environmental Protection Agency.
11. WIPP PA - "Analysis Report for the ES45 Regression Test, March 6, 2003." Sandia National Laboratories. Sandia WIPP Central Files. ERMS 530290.

12. WIPP PA – “Analysis Report for the 8400 Regression Test.” Sandia National Laboratories. Sandia WIPP Central Files. ERMS 527280.
13. WIPP PA (Performance Assessment) 2003. “Change Control Form for PANEL.” Sandia National Laboratories. Sandia WIPP Central Files WPO # 526499.
14. WIPP PA (Performance Assessment) 2003. “Requirements Document and Verification and Validation Plan for PANEL Version 4.02.” Sandia National Laboratories. Sandia WIPP Central Files WPO # 526649.
15. WIPP PA (Performance Assessment) 2003. “Analysis Report for PANEL Version 4.02 Regression Testing for the ES45 and 8400 Platforms.” Sandia National Laboratories.
16. USEPA – “Review of WIPP Performance Assessment Computer Code Migration Activities –Version 2.” September 2004.
17. WIPP PA (Performance Assessment) 2005. “Change Control Form for PANEL, Version 4.03 Sandia National Laboratories. Sandia WIPP Central Files WPO # 539452.
18. WIPP PA (Performance Assessment) 2005. “Installation and Checkout for PANEL Version 4.03 Regression Testing for the Compaq ES40 and ES45 Platforms.” Sandia National Laboratories.

5.6 POSTLHS

This section presents the regression test results for the POSTLHS 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.

5.6.1 Introduction

POSTLHS Version 4.06ZO was validated in October 1995 on a DEC Alpha 2100 using the OpenVMS 6.1 operating system by demonstrating that the results of two test cases met the acceptance criteria defined in the RD/VVP for POSTLHS 4.06ZO [1]. In February 1996, POSTLHS was revised to Version 4.07 and was validated on a DEC Alpha 2100 using 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 CCA PA.

In order to test new operating systems that were added in 2002–2003 (Section 1), regression test results from POSTLHS 4.07 run on the ES40 using OpenVMS 7.3-1 were compared to results from the validation tests of POSTLHS 4.07 run on a DEC Alpha 2100 using OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency’s approval of

POSTLHS 4.07 on those operating systems [4]. In January 2003, two new hardware systems were added to conduct PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running OpenVMS 7.3-1[5,6].

In September 2004, the Agency concluded that POSTLHS 4.07 met the acceptance criteria specified in the RD/VVP [3], and thus were considered as validated on the Compaq ES45 and 8400 using OpenVMS 7.3-1[7]. In April 2005, the POSTLHS code was revised to Version 4.07A in order to re-index the CAMDAT output files [8]. To ensure that this version was working properly, the DOE regression-tested Version 4.07 against Version 4.07A on the COMPAQ ES40 and ES45 using OpenVMS 7.3-1[9]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to POSTLHS 4.07A.

5.6.2 Test Methodology

The test suite for POSTLHS, as described in the VVP [1], consists of Test Cases 1 and 2. The entire test suite for POSTLHS Version 4.07A was executed on the Compaq ES40 platform using OpenVMS 7.3-1, and then executed again on the Compaq ES45 platform using OpenVMS 7.3-1.

POSTLHS needs the following input files: an LHS output file, an input control file, and an input CAMDAT file. All input files used to execute the POSTLHS 4.07A tests were the same files used in the previous validation of POSTLHS 4.07.

Each successful execution of POSTLHS generated the following output files: a set of binary output CAMDAT files and a debug file. The regression test methodology used the VMS DIFFERENCE command to compare output from the current execution to the output from a validation of POSTLHS. The output CAMDAT files were binary files and could not be compared with the VMS DIFFERENCE command. The GROPECDB utility was used to write portions of the CAMDAT files as text, so that they could be compared. Thus, the debug file and the GROPECDB output from each output CAMDAT file were differenced. The output from POSTLHS 4.07A on the Compaq ES40 platform was compared to the output from the validation of POSTLHS 4.07, and the output from POSTLHS 4.07A on the Compaq ES45 platform was compared to the output from the validation of POSTLHS 4.07A on the Compaq ES40.

5.6.3 Test Results

Both test cases for POSTLHS 4.07A were executed twice, first on the Compaq ES40 platform using OpenVMS 7.3-1 and then on the Compaq ES45 platforms using OpenVMS 7.3-1. The output from POSTLHS 4.07A on the Compaq ES40 platform was compared to the output from the validation of POSTLHS 4.07, and the output from POSTLHS 4.07A on the Compaq ES45 platform was compared to the output from the validation of POSTLHS 4.07A on the Compaq ES40.

Output files from the test cases run on the ES40 platform were compared to the corresponding output files from the validation of POSTLHS 4.07 by using the VMS DIFFERENCE command. The comparison found that the differences in the output files were limited to code run dates and

time, POSTLHS version and build date, file and directory names, platform and system names, and execution statistics.

Output files from the test cases run on the ES45 platform were compared to the corresponding output files from POSTLHS 4.07A on the ES40 platform by using the VMS DIFFERENCE command. 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.

Since POSTLHS 4.07A executed on the Compaq ES40 and ES45 platforms using OpenVMS 7.3-1 met the acceptance criteria specified in the VVP [1] for all test cases, POSTLHS 4.07A was considered validated on the Compaq ES40 and ES45 platforms using OpenVMS 7.3-1.

5.6.4 The Agency's Conclusions

Since only acceptable differences were detected between the results of POSTLHS 4.07A on the ES40 and ES45 and POSTLHS 4.07, the Agency concluded that POSTLHS 4.07A on the ES40 and ES45 met the acceptance criteria specified in the VVP [1] for these test cases.

5.6.5 References

1. WIPP PA (Performance Assessment) 1995. "Requirements Document & Verification and Validation Plan for POSTLHS Version 4.06ZO." Sandia National Laboratories. Sandia WIPP Central Files WPO # 23552.
2. WIPP PA (Performance Assessment) 1996. "Software Installation and Checkout Form, POSTLHS Version 4.07." Sandia National Laboratories. Sandia WIPP Central Files WPO # 230717.
3. WIPP PA (Performance Assessment) 1996. "Validation Document for GROPECDB Version 2.12." Sandia National Laboratories. Sandia WIPP Central Files WPO # 37497.
4. EPA 2003. "Review of WIPP Performance Assessment Computer Code Migration, June 10, 2003." Environmental Protection Agency.
5. WIPP PA – "Analysis Report for the ES45 Regression Test, March 6, 2003." Sandia National Laboratories. Sandia WIPP Central Files. ERMS 530290.
6. WIPP PA – "Analysis Report for the 8400 Regression Test." Sandia National Laboratories. Sandia WIPP Central Files. ERMS 527280.
7. USEPA – "Review of WIPP Performance Assessment Computer Code Migration Activities –Version 2." September 2004.
8. WIPP PA (Performance Assessment) 2005. "Change Control Form for POSTLHS, Version 4.07. Sandia National Laboratories.

9. WIPP PA (Performance Assessment) 2005. "Installation and Checkout for POSTLHS Version 4.07A Regression Testing for the Compaq ES40 and ES45 Platforms." Sandia National Laboratories.

5.7 PRECCDFGF

This section presents the regression test results for the PRECCDFGF. PRECCDFGF collates output from all other WIPP PA codes, and formats this output into the RELTAB input file for CCDFGF.

5.7.1 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 VP on the COMPAQ ES40 and 8400 using the Open the VMS 7.3-1 [1] operating system. 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 using OpenVMS 7.3-1[2]. In September 2004, the Agency concluded that PRECCDFGF Version 1.00B met the acceptance criteria specified in the VVP [1], and thus, was considered as validated on the COMPAQ ES45 and 8400 platforms using OpenVMS 7.3-1[4].

In July 2005, PRECCDFGF was updated to Version 1.01 with three significant modifications [5]. The first was that PRECCDFGF 1.01 would read the text output file of release tables written directly by CUTTINGS_S Version 6.00 or higher. This file replaced a set of files that were created by SUMMARIZE from the output of the previous versions of CUTTINGS_S. Secondly, when reading the release tables from the other codes written by SUMMARIZE and the CUTTINGS_S text output file, PRECCDFGF 1.01 would read the header records at the start of the files to ensure that the fields in the files correspond to the values expected by the READ statements in the code itself. Failure of the header to match the expected text would cause PRECCDFGF to abort its execution with appropriate error messages being logged. Finally, whereas PRECCDFGF version 1.00B read a text output file from LHS to get data about the sampled parameter GLOBAL:PBRINE, version 1.01 would read a set of CAMDAT files generated by POSTLHS to obtain this data. Thus, PRECCDFGF was no longer required to read output files from LHS.

Version 1.01 of the code was subsequently validated to run on the COMPAQ ES40 using OpenVMS 7.3-1 [5]. Following the validation of the code on the ES40, it was regression-tested to run on the ES45 [6]. The discussion below documents the test methodology and results, and the Agency's conclusions with respect to PRECCDFGF Version 1.01.

5.7.2 Test Methodology

Both test cases described in the VVP [1] were validated on the COMPAQ ES40 using the WIPP PA run control system [5]. The first test case demonstrated that PRECCDFGF correctly consolidates input data, retrieved parameters, and created an output file for use by CCDFGF. It validated that PRECCDFGF terminated and logged the appropriate error message when one of the SUMMARIZE input files had an invalid header. Specifically, this test case verified that an error was detected and reported when the order of data indicated in the header of an input file did not match the order required by PRECCDFGF. The VMS DIFFERENCE utility compared the output file assigned to the logical CCGF_RELTAB\$OUT with the file CCGF_QA0100D_RELTAB_T1.DAT.

This second test case was used to test that PRECCDFGF terminated if one of the SUMMARIZE input files had an incorrectly formatted header [5]. The code passed this test if PRECCDFGF recognized the problem and terminates. Appropriate error messages were written to the log file name assigned to the logical ERROR\$LOG. The test evaluator manually inspected the error log file to determine if the correct error message was recorded.

The regression tests for PRECCDFGF Version 1.01 comprised the two test cases described in the VVP [1]. Test results from PRECCDFGF 1.01 run on the Compaq ES45 platform using OpenVMS 7.3-1 were compared to results from the validation tests of PRECCDFGF 1.01 on the ES40 platform.

5.7.3 Test Results

Both test cases for PRECCDFGF 1.01 were executed by DOE on the COMPAQ ES40 platform using OpenVMS 7.3-1[5]. In the first test case, the only differences observed between CCGF_QA0101_RELTAB_T1.DAT and CCGF_QA0100D_RELTAB_T1.DAT were the file names. Furthermore, the results of the second test case indicated that the error in the log file message was written correctly.

All test cases for PRECCDFGF 1.01 were executed on the Compaq ES45 platform using OpenVMS 7.3-1 [6]. The output from PRECCDFGF 1.01 on the Compaq ES45 platform was compared to the output from the validation of PRECCDFGF 1.01 on the Compaq ES40.

Output files from the test cases run on the ES45 platform were compared to the corresponding output files from PRECCDFGF 1.01 on the ES40 platform by using the VMS DIFFERENCE command. The comparison found that there were no differences in the output files. Since no differences were detected between the results of PRECCDFGF 1.01 on the ES45 and the ES40, we concluded that PRECCDFGF 1.01 on the ES45 met the acceptance criteria specified in the VVP [1] for these test cases.

Since PRECCDFGF 1.01 executed on the Compaq ES45 platform using OpenVMS 7.3-1 met the acceptance criteria specified in the VVP [1] for all test cases, PRECCDFGF 1.01 is considered validated on the Compaq ES45 platform using OpenVMS 7.3-1.

5.7.4 The Agency's Conclusions

Since PRECCDFGF 1.01 executed on the Compaq ES40 platform using OpenVMS 7.3-1 met the acceptance criteria specified in the VVP [1] for all test cases, PRECCDFGF 1.01 was considered by the Agency as validated on the Compaq ES40 platform using OpenVMS 7.3-1. Furthermore, since no differences were detected between the results of PRECCDFGF 1.01 on the ES45 and the ES40, the Agency concluded that PRECCDFGF 1.01 on the ES45 met the acceptance criteria specified in the VVP [1] for these test cases.

5.7.5 References

1. WIPP PA (Performance Assessment) 2003. "Verification and Validation Plan for PRECCDFGF Version 1.00A Document Version 1.02." Sandia National Laboratories. Sandia WIPP Central Files 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. Sandia WIPP Central Files 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.
4. USEPA – "Review of WIPP Performance Assessment Computer Code Migration Activities Version 2." September 2004.
5. WIPP PA (Performance Assessment) 2003. "Validation Document for PRECCDFGF Version 1.01 Document Version 1.05." Sandia National Laboratories. Sandia WIPP Central Files ERMS 539296.
6. WIPP PA (Performance Assessment) 2005. "Installation and Checkout for PRECCDFGF Version 1.01 Regression Testing for the Compaq ES45 Platforms. Sandia National Laboratories.

5.8 SUMMARIZE

This section presents the regression test results for the SUMMARIZE code. SUMMARIZE reads ordered sets of sampled CAMDAT (CDB) data files. For the current regulatory calculations, there are 100 different input CAMDAT files in each ordered set. These files would normally constitute the principal output from one of the WIPP-PA analytical codes. SUMMARIZE can extract a single item (or set of items) from each of its 100 input files and write the 100 item values to a single output file. If the input data constitute time histories, SUMMARIZE will select the one value from each input file that corresponds most closely to a user-selected time or set of times from the time history. If requested, SUMMARIZE can interpolate input data to the exact time specified by the user. As a result of this process, selected

data that originally resided on 100 different binary CAMDAT files are rearranged and reported on a single ASCII output file.

SUMMARIZE reports its results in any of several convenient ASCII formats that can be read by commercial and WIPP PA analysis and plotting codes. SUMMARIZE's output format is normally selected by the user to be compatible with the analysis and/or plotting code that will be applied next in the run sequence.

5.8.1 Introduction

Since the 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 using 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 using the OpenVMS 6.1 operating system [5, 6]. Test Cases 2, 3, 5, 6 and 7 for the validation of SUMMARIZE 2.15 were identical to the 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 using 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 2002–2003 (Section 1), regression test results from SUMMARIZE 2.20 run on the ES40 using OpenVMS 7.3-1 were compared to results from the validation tests of SUMMARIZE 2.20 run on a DEC Alpha 2100 using OpenVMS 6.1. In June 2003, the Agency completed a report documenting the Agency's approval of SUMMARIZE 2.20 on those operating systems [7]. In January 2003, two new hardware systems were added to conduct PAs for the WIPP; a Compaq ES45 and a Compaq Alpha 8400, both running OpenVMS 7.3-1 [8, 9]. In September 2004, the Agency concluded

that SUMMARIZE 2.2 met the acceptance criteria specified in the VVP [1], and was considered as validated on the COMPAQ ES45 and 8400 platforms using OpenVMS 7.3-1[10].

During an August 9, 2004, technical exchange meeting, the Agency requested additional information regarding how data transfer between process model codes and CCDFGF was verified (CRA Response Activity Tracking Number 08/09/04A was assigned to this verbal request). DOE responded to this request by describing a procedure for inspecting WIPP PA Run Control log files to verify that the correct files were fetched from CMS libraries and used by SUMMARIZE [16, 17]. Subsequent to the response, DOE discovered several problems with data transfer across the SUMMARIZE interface, which were discovered, reported, and corrected [11]. The problems encountered fell into two categories:

- Certain releases were miscalculated because information in certain SUMMARIZE output tables were not in the column that PRECCDFGF expected (Kirchner and Vugrin 2004).
- Releases to the Culebra were estimated in several cases, because SUMMARIZE wrote zeros to the output table when it could not locate an input CAMDAT database file.

The impact of the first class of errors on the results and conclusions of the CRA-2004 were determined to be minimal (Yugrin 2004). An informal review of the second type of error indicated that the impact was minimal. A formal review is in progress. Regardless, DOE recognized that the SUMMARIZE interface needed to be improved in future PAs [14].

Both classes of problems outlined can be traced back to errors in the SUMMARIZE input files, not with the SUMMARIZE code itself. Nearly 600 SUMMARIZE input files were used in the CRA-2004 PA. Since each one was prepared manually, the probability of errors was considerable. However, it was determined that improving the SUMMARIZE code was an important part of improving the interface between process model codes and CCDF construction codes. The following steps were followed to improve the SUMMARIZE interface:

The SUMMARIZE code was updated to Version 3.00 [12].

- A PRECCDFGF driver was added to the set of output drivers in SUMMARIZE. This driver writes header information at the top of the output table. The header information identifies the data that appears in the rest of the table.
 - SUMMARIZE was modified to incorporate strict checking of the vector list, removing the possibility that vectors are inadvertently skipped due to errors in COB file specification.
 - The PRECCDFGF code was updated to Version 1.01 (Section 5.7). PRECCDFGF was modified to read the header information produced by SUMMARIZE 3.00 to verify that the data in the input file is in the order required by PRECCDFGF.

- The WIPP PA Run Control scripts were re-written to automate the generation of the SUMMARIZE input files and eliminate errors introduced during manual editing of the files.

The steps outlined above were implemented and used in the CRA-2004 PABC. In order to demonstrate that the improvements made to the SUMMARIZE interface eliminated the errors discussed above, a verification study was performed. The procedures and results of this verification of the SUMMARIZE interface in the CRA are discussed below.

Version 3.00 of the code was subsequently validated to run on the COMPAQ ES40 using OpenVMS 7.3-1 [12]. Following the validation of the code on the ES40, it was regression-tested to run on the ES45 [13]. The discussion below documents the test methodology, regression test results, and the Agency's conclusions with respect to SUMMARIZE 3.00 on the new hardware systems.

5.8.2 Test Methodology

The tests for this code comprised the 13 test cases described in the *Requirements & Design Document for SUMMARIZE Version 3.0* (RD/DD) [17].

There are a number of differences in functionality between SUMMARIZE Version 2.20 [1] and SUMMARIZE Version 3.00. The following functionality is new to SUMMARIZE Version 3.00:

- A new driver has been added to interface to the PRECCDFGF code.
- A new SKIP command in the *VECTORS will allow the user to designate the vectors that do not have a corresponding input data file. If SKIP is issued, the code will abort if a vector that is not on the skip list does not have an input data file. If SKIP is not issued, the code prints a warning message to the log file and continues.
- A new HEADER command in the *OUTPUT environment allows the user to control whether a header will be written to the output file. If HEADER is not issued, the header is always written.
- If any item is not found on any CAMDAT file, SUMMARIZE will abort by default. A new IGNORE_MISSING command in the *ITEMS environment allows the user to instruct the code to print a warning message to the log file and continue.

The following functionality has been changed:

- A separate error log file is no longer generated. All error messages are written to the log file. The log file output is reduced and modified to make it more useful for debugging.
- Several small changes are noted in the format of the output data table files, particularly in the table headers. The data itself (that is, the values represented) will remain unchanged.

- The MULTIPLES_FILES and SINGLE_FILES commands in the *OUTPUT environment are combined into a SETS command. The same options will be selected (although the option keywords may be different). A new option requests that a blank line be inserted between tables. This is the new default now. The old commands and options still function.
- The FIRST and LAST options of the *TIMES environment commands select the first and last time on each CAMDAT file, not just on the first CAMDAT file.
- The bug in the SURFER GRID output driver is fixed. However, this driver is still not tested and documented.

The following functionality was removed:

- NAME command option GET_FROM_INPUT_FILE in the *OUTPUT environment. A filename must be specified.
- The NAME command in the *INPUT environment is exactly equivalent to the TEMPLATE command. The NAME command is no longer allowed to list multiple input data files.
- Code for the SURFER STREAM output driver.
- Code for the SURFER LOGICAL output driver.

ES40 Test Methodology

The test set for SUMMARIZE Version 2.20 consisted of eight test cases. The test set and evaluation of test results for SUMMARIZE Version 2.20 were documented in "Validation Document for SUMMARIZE Version 2.10," [3]. Test Case 3 was removed from the test set because it verified untested functionality, and the previous test results contained a known error. The other seven test cases were regression-tested by running SUMMARIZE Version 3.00 on the ES40 and comparing its output with the output from the validation of SUMMARIZE Version 2.20 also run on the ES40.

Five new test cases were added to test functionality new to SUMMARIZE Version 3.00. For the first three of these test cases, the tester must examine the output data file for content and format. The last two of the new test cases check error conditions that should cause SUMMARIZE to abort. If SUMMARIZE aborts, no output data file is generated. The tester must examine the log file to verify that SUMMARIZE detected the error condition and aborted.

SUMMARIZE needs the following input files: an input control file and a set of CAMDAT data files. The SUMMARIZE input control files must always be modified slightly for each test case because they contain the name of the output data file, which should include the program class or version. Two other changes to the input control files were made to make future testing easier;

the hard-coded directory location for the input data files were removed in most test cases and the output data file names have been changed to indicate the test number. The input control files were changed (in some tests) to replace the obsolete commands with the new form of the command. The new control file for each test case was listed in this document. The differences between the SUMMARIZE Version 3.00 and Version 2.20 input control files were also included, with annotations of any command changes. (The differences were listed with the VMS DIFFERENCE utility outside of the normal test procedure.) The CAMDAT data files were the same files used in the previous validation of SUMMARIZE Version 2.20.

A successful SUMMARIZE execution generated the following output files: one or more ASCII output data files and a log file. The log file was not part of the code's functionality and was usually not examined or compared. Each output data file was compared to the corresponding file from the previous validation of SUMMARIZE Version 2.20 using the VMS DIFFERENCE utility. Changes to SUMMARIZE Version 3.00, as described in the Change Control Form [11], cause differences in the test output data files. The following cosmetic differences were considered by the Agency to be acceptable:

- Headers should appear for all drivers and styles, unless the HEADER OFF command is issued.
- Blanks may be added or removed from header lines. In some drivers, blanks were added so that the header information appeared over the column of data it described.
- Commas may be removed from header lines if they do not separate column headings.
- Times in the header may be written in "F" format.
- The comment lines (which start with "!") for the CCDF and STEPWISE driver output should now be replaced by a single comment line (the CAMDAT title). The release name and description for the CCDF driver output may also be changed.
- Blanks may be added or removed from data lines.
- Blanks lines may be added or removed.
- "*BREAK" lines may be replaced by blank lines or "!*BREAK" lines.
- Trailing commas on data lines should be removed.
- The vector number previously output at the start of some data lines as a real number may be output as an integer.
- The "*" that sometimes followed the vector number in the data lines (if there was no input CAMDAT file for the vector) should no longer appear. (The "*" may still appear after the vector number in the header.)

- Real numbers may be written with greater precision, and “F” format numbers may be written in “E” format. The numeric values may not change.

All test cases were run using the WIPP PA run control system. The scripts, script input files, and all other files related to validation testing of SUMMARIZE Version 3.00 reside in QC0300 class of the SUM library in the SCMS. All test inputs were fetched at run time by the scripts, and test outputs/results and run logs were automatically stored by the scripts in class QC0300 of the SUM library in the SCMS. A log file that indicates the input/output files was generated by each test case execution.

ES45 Test Methodology

The test suite for SUMMARIZE, as described in the VVP/VD [12], consisted of 12 test cases: Test Cases 1, 2, and 4–13 (i.e., there is no Test Case 3). The entire test suite for SUMMARIZE Version 3.00 was executed on the Compaq ES45 platform using OpenVMS 7.3-1.

SUMMARIZE needed the following input files: an input control file and a set of CAMDAT data files. All input CAMDAT files used to execute the SUMMARIZE 3.00 ES45 tests were the same files used in the previous validation of SUMMARIZE 3.00 on the ES40. The SUMMARIZE input control files for all test cases were modified slightly to add “ES45” to the name of the output data file. The new input control files were shown in this document, along with the differences from the control files used in the previous validation of SUMMARIZE 3.00 on the ES40.

Each successful execution of SUMMARIZE generated the following output files: one or more ASCII output data files and a log file. The regression test methodology used the VMS DIFFERENCE command to compare output from the current execution to the output from the validation of SUMMARIZE on the ES40. Each output data file was differenced. The log file was not part of the code’s functionality and was usually not differenced. However, Test Cases 12 and 13 abort without generating an output data file. In these two cases, the log file was differenced. The VMS DIFFERENCE command was used to compare the output from SUMMARIZE 3.00 on the Compaq ES45 platform to the output from the validation of SUMMARIZE 3.00 on the Compaq ES40.

Verification of the SUMMARIZE Interface in the CRA-2004 PABC

In 2005, DOE performed a verification exercise to determine whether the data used to compute estimated releases in the CRA-2004 PABC was correctly transferred across the SUMMARIZE interface between the process model COB files and the CCDFGF input REL TAB file [14]. Because DOE’s objective was to verify data transfer across the SUMMARIZE interface, DOE focused their attention on data from process models that produce binary output files in the CAMDAT database (COB) format that are read using SUMMARIZE (i.e., PANEL, NUTS, BRAGFLO, and SECOTP2D). The transfer of information from process models that interface directly with PRECCDFGF (i.e., EPAUNI, and CUTTINGS_S) was not investigated. The correct transfer of this information was addressed in the validation and verification testing for PRECCDFGF (Section 5.7).

The basic approach DOE used to verify data transfer across the SUMMARIZE interface was to extract data from the CDB files using a code other than SUMMARIZE, and compare that data with corresponding entries in the CCDFGF RELTAB file. The data was extracted from the CDB files using the code GROPECDB, Version 2. To make the extraction process tractable, traceable, and reproducible, Digital Command Language (DCL) scripts were written to automate the process. For similar reasons, a FORTRAN utility was written to automate the process of extracting data from the RELTAB file. The two independent data sets were then loaded into a Microsoft Access database (CheckReltab) to facilitate the comparison.

A slight complication in the data comparison was introduced by the fact that GROPECDB does not perform interpolation in time, while SUMMARIZE does. If GROPECDB receives a request for the value of a variable at a time that does not exist in the CDB file, it returns the value at the nearest time. When this situation occurred, the SUMMARIZE behavior was emulated by interpolating the data within the CheckReltab database before comparison to the REL TAB data value.

5.8.3 Test Results

Testing for SUMMARIZE Version 3.00 was completed and the acceptance criteria for all test cases were successfully met. Testing verified that SUMMARIZE satisfied all the requirements listed in the SUMMARIZE Requirements and Design Document [17] and the additional functionality listed in this document.

Output files from the test cases were run on the ES45 and compared to the corresponding output files from the validation of SUMMARIZE 3.0 on the Compaq ES40 using OpenVMS 7.3-1 by using the VMS DIFFERENCE command. All differences in output were limited to code run date and time, file and directory names, platform names, and system version numbers.

Data transfer across the SUMMARIZE interface in the CRA-2004 PABC was verified by extracting the data from the process model CDB files using a code other than SUMMARIZE and comparing that data with corresponding entries in the CCDFGF RELTAB file. To make the extraction process tractable, traceable, and reproducible, Digital Command Language (DCL) scripts were written to automate the CDB data extraction process. For similar reasons, a FORTRAN utility was written to automate the process of extracting data from the RELTAB file. The two independent data sets were then loaded into a Microsoft Access database to facilitate comparing them. The data sets could be efficiently compared by constructing database queries. The data extraction and comparison exercise was performed on replicate R1 of the CRA-2004 PABC.

Performing the data extraction and comparison exercise revealed that, except for a minor flaw in the interpolation algorithm used in SUMMARIZE, the data values in process model CDB files matched that found in the RELTAB file very well. The flaw in the SUMMARIZE interpolation algorithm affected only a very small number of data values, and was only observed when the dependent variable interval was smaller than can be represented in the single precision data format of CDB files. Thus, the flaw should have no impact on computed releases.

5.8.4 The Agency's Conclusions

Testing for SUMMARIZE Version 3.00 on the ES40 was completed and the acceptance criteria for all test cases were successfully met. The testing verified that SUMMARIZE satisfied all the requirements listed in the SUMMARIZE Requirements and Design Document [17] and the additional functionality listed. Since all differences in the regression test results of SUMMARIZE 3.00 on the ES45 were acceptable, the Agency concluded that SUMMARIZE 3.0 was validated on the Compaq ES40 and ES45 using OpenVMS Version 7.3-1. Furthermore, DOE's verification exercise demonstrated that data from the process model CDB files were transferred across the SUMMARIZE interface with sufficient accuracy.

5.8.5 References

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6.0 SUMMARY AND CONCLUSIONS

In 2005, DOE made revisions to eight of the computer codes, including LHS, POSTLHS, CUTTINGS, DRSPALL, PANEL, SUMMARIZE, PRECCDFGF, and CCDFGF. The revised computer codes have been qualified on the Compaq ES40 and ES45 using OpenVMS 7.3-1. After completing the Agency's review, the Agency has concluded that the most recent versions of these computer codes (Table 3.1) are approved for use in compliance calculations for the WIPP PA on the Compaq ES40 and ES45 using OpenVMS 7.3-1.