NUREG-1795

FAVOR Code Versions 2.4 and 3.1 Verification and Validation Summary Report

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FAVOR Code Versions 2.4 and 3.1 Verification and Validation Summary Report

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ABSTRACT

During plant operation, the walls of reactor pressure vessels (RPVs) are exposed to neutron radiation, resulting in localized embrittlement of the vessel steel and weld materials in the core area. If an embrittled RPV had an existing flaw of critical size and certain severe system transients were to occur, the flaw could very rapidly propagate through the vessel, resulting in a through-wall crack and challenging the integrity of the RPV. The severe transients of concern, known as pressurized thermal shock (PTS), are characterized by a rapid cooling (i.e., thermal shock) of the internal RPV surface in combination with repressurization of the RPV. Advancements in our understanding and knowledge of materials behavior, our ability to realistically model plant systems and operational characteristics, and our ability to better evaluate PTS transients to estimate loads on vessel walls led the U.S. Nuclear Regulatory Commission (NRC) to realize that the earlier analysis, conducted in the course of developing the PTS Rule (10 CFR 50.61) in the 1980s, contained significant conservatisms.

This report, which describes a summary of verification and validation (V&V) of the probabilistic fracture mechanics models in the Fracture Analysis of Vessels-Oak Ridge (FAVOR) code, is one of a series of 21 other documents detailing the results of the NRC study. The V&V involved assuring that the as-built software meets the requirements specified in the theory manual and the user's guide. The V&V activity involved development of test plans, test procedures, acceptance criteria for comparing the FAVOR-generated results with independent calculations, and test reports. The V&V team checked individual computational relationships for programming accuracy, but this V&V effort did not generally include a comprehensive, code line-by-line walkthrough. Based on the validation tests performed and reported results, the Nuclear Regulatory Commission concludes that the as-built software in version 3.1 of the code meets the requirements stated in the associated theory manual and the user's guide with reasonable confidence in the accuracy of the FAVOR-generated results.

FOREWORD

The reactor pressure vessel is exposed to neutron radiation during normal operation. Over time, the vessel steel becomes progressively more brittle in the region adjacent to the core. If a vessel had a preexisting flaw of critical size and certain severe system transients occurred, this flaw could propagate rapidly through the vessel, resulting in a through-wall crack. The severe transients of concern, known as pressurized thermal shock (PTS), are characterized by rapid cooling (i.e., thermal shock) of the internal reactor pressure vessel surface that may be combined with repressurization. The simultaneous occurrence of critical-size flaws, embrittled vessel, and a severe PTS transient is a very low probability event. The current study shows that U.S. pressurized-water reactors do not approach the levels of embrittlement to make them susceptible to PTS failure, even during extended operation well beyond the original 40-year design life.

Advancements in our understanding and knowledge of materials behavior, our ability to realistically model plant systems and operational characteristics, and our ability to better evaluate PTS transients to estimate loads on vessel walls have shown that earlier analyses, performed some 20 years ago as part of the development of the PTS rule, were overly conservative, based on the tools available at the time. Consistent with the NRC's Strategic Plan to use best-estimate analyses combined with uncertainty assessments to resolve safety-related issues, the NRC's Office of Nuclear Regulatory Research undertook a project in 1999 to develop a technical basis to support a risk-informed revision of the existing PTS Rule, set forth in Title 10, Section 50.61, of the Code of Federal Regulations (10 CFR 50.61).

Two central features of the current research approach were a focus on the use of realistic input values and models and an explicit treatment of uncertainties (using currently available uncertainty analysis tools and techniques). This approach improved significantly upon that employed in the past to establish the existing 10 CFR 50.61 embrittlement limits. The previous approach included unquantified conservatisms in many aspects of the analysis, and uncertainties were treated implicitly by incorporating them into the models.

This report is one of a series of 21 reports that provide the technical basis that the staff will consider in a potential revision of 10 CFR 50.61. The risk from PTS was determined from the integrated results of the Fifth Version of the Reactor Excursion Leak Analysis Program (RELAP5) thermal-hydraulic analyses, fracture mechanics analyses, and probabilistic risk assessment. This report summarizes the verification and validation (V&V) of the Fracture Analysis of Vessels, Oak Ridge (FAVOR) code to assure that the as-built software meets the requirements specified in the theory manual and the user's guide.

Brian W. Sheron, Director
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U.S. Nuclear Regulatory Commission

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EXECUTIVE SUMMARY

This report is one of a series of reports that summarize the results of a five year project conducted by the Nuclear Regulatory Commission's Office of Nuclear Regulatory Research. The aim of this study was to develop a technical basis to support revision to the pressurized thermal shock (PTS) rule [10CFR50.61] and the associated PTS screening criteria in a manner consistent with current NRC guidelines on risk informed regulation. The Figure 0.1, included here, shows all of the reports that document this project, and highlights this report.

This document provides a summary of verification and validation (V&V) of the FAVOR (Fracture Analysis of Vessels - Oak Ridge) software. The FAVOR software has been developed at the Oak Ridge National Laboratory (ORNL) under the United States Nuclear Regulatory Commission (NRC) support, and is being used to generate a distribution for frequency of crack initiation and through-wall crack penetration in the reactor pressure vessel for postulated pressurized thermal shock (PTS) events. The software has undergone major modifications to support re-evaluation of the NRC PTS Rule (10CFR50.61) screening criteria. This software also will provide a capability to assess compliance with the PTS risk acceptance criteria for individual plants.

The current FAVOR V&V activity deals with the software validation in accordance with the software V&V plan to demonstrate that the as-built software meets its requirements, as described in the theory manual and user's guide. It includes the development of test plans, test procedures, acceptance criteria for comparing the FAVOR code results with independent calculations, and test reports.

The FAVOR code has been developed under the terms and conditions of the NRC Management Directive 11.7, which requires that all software development, modification, or maintenance are to follow general guidance provided in NUREG/BR-0167. The software V&V has been performed by NRC and Electric Power Research Institute (EPRI) Materials Reliability Program (MRP)-supported engineers from ORNL, Westinghouse Electric Company LLC, Sartrex Corporation, Pacific Northwest National Laboratories (PNNL), and Idaho National Engineering and Environmental Laboratories (INEEL) -- comprising the V&V Team.

During the course of technical basis re-evaluation effort for the PTS rule, FAVOR code development has occurred in several stages. The version 2.4 of the FAVOR code, also termed as the "base version", was used in developing the results for the December 2002 draft PTS NUREG report (ADAMS # ML030090626). A detailed validation testing plan was developed for the base version 2.4 of the FAVOR code. Based on this validation plan, validation testing and reporting of test results was performed.

Individual computational relationships were checked for programming accuracy, but, generally, a comprehensive, code line-by-line walk through is not performed as part of this V&V effort. Instead, a comprehensive review of demonstration test data and observation of the input and output elements from the test is performed to verify all software elements properly actuate.

The FAVOR version 2.4 was subsequently replaced with the revised version 3.1 in which the observed computational errors, as a result of the validation testing, were removed and it also includes additional features, such as the warm pre-stress and upper-shelf ductile tearing models. The version 3.1 of the FAVOR code has been used in generating the results for the present PTS technical basis re-evaluation effort. An incremental validation testing was performed for version 3.1 of the FAVOR code to test those features and corrections that were added relative to the base version 2.4 of the code. The incremental validation of version 3.1 was performed by the INEEL, EPRI/Sartex and EPRI/Westinghouse teams.

Based on the validation tests performed and reported results on FAVOR code versions 2.4 and 3.1, it is concluded that the as-built software in version 3.1 meets the requirements stated in the theory manual and the user's guide with reasonable confidence in the accuracy of the FAVOR-generated results. For the test cases where the acceptance criteria are not satisfied, explanations are provided for the consequences of the differences in the results. The FAVOR code V&V plan specifies a process the users are recommended to follow should they encounter any errors or discrepancies in input/output during the FAVOR code usage.

Engineering and Executive Summary, NUREG-1806

PFM

Models, Validation, & Procedures

- Procedures, Uncertainty, & Experimental Validation: EricksonKirk, M.T., "Probabilistic Fracture Mechanics: Models, Parameters, and Uncertainty Treatment Used in FAVOR Version 04.1," NUREG-1807.
- FAVOR
  - Theory Manual: Williams, P.T. and Dickson, T.L., "Fracture Analysis of Vessels – Oak Ridge, FAVOR v04.1, Computer Code: Theory and Implementation of Algorithms, Methods, and Correlations," NUREG/CR-6854.
  - User Guide: Dickson, T.L. and Williams, P.T., "Fracture Analysis of Vessels – Oak Ridge, FAVOR v04.1, Computer Code: User's Guide," NUREG/CR-6855.
  - V&V Report: Malik, S.N.M., "FAVOR Verification and Validation," NUREG-1795.
- *Flaw Distribution: Simonen, F.A., et al., "A Generalized Procedure for Generating Flaw-Related Inputs for the FAVOR Code," NUREG/CR-6817, Rev. 1, October 2003.*

Results

- Baseline: Dickson, T.L. and Yin, S., "Electronic Archival of the Results of Pressurized Thermal Shock Analyses for Beaver Valley, Oconee, and Palisades Reactor Pressure Vessels Generated with the 04.1 version of FAVOR," ORNL/NRC/LTR-04/18, ADAMS # ML042960465,
- Sensitivity Studies: EricksonKirk, M.T., et al., "Sensitivity Studies of the Probabilistic Fracture Mechanics Model Used in FAVOR Version 04.1," NUREG-1808.

TH

Models, Validation, & Procedures

- TH Model: Bessette, D., "Thermal Hydraulic Analysis of Pressurized Thermal Shock," NUREG-1809.
- RELAP Procedures & Experimental Validation: Fletcher, C.D., et al., "RELAP5/MOD3.2.2 Gamma Assessment for Pressurized Thermal Shock Applications," NUREG/CR-6857.
- Experimental Benchmarks: Reyes, J.N., et. al., Final Report for the OSU APEX-CE Integral Test Facility, NUREG/CR-6856.

Results

- Baseline: Arcieri, W.C., "RELAP5 Thermal Hydraulic Analysis to Support PTS Evaluations for the Oconee-1, Beaver Valley-1, and Palisades Nuclear Power Plants," NUREG/CR-6858.
- Sensitivity Studies: Chang, Y.H., et all., "Thermal Hydraulic Uncertainty Analysis in Pressurized Thermal Shock Risk Assessment," University of Maryland, ADAMS # ML????????.

PRA

Models, Validation, & Procedures

- Procedures & Uncertainty: Whitehead, D.W. and Kolaczkowski, A.M., "PRA Procedures and Uncertainty for PTS Analysis," NUREG/CR-6859.

Results

- Beaver: Kolaczkowski, A.M., et al., "Beaver Valley Unit 1 PTS PRA ," ADAMS # ML042880454.
- Oconee: Kolaczkowski, A.M., et al., "Oconee Unit 1 PTS PRA," ADAMS # ML042880452.
- Palisades: Kolaczkowski, A.M., et al., "Palisades PTS PRA," ADAMS # ML042880473.
- External Events: Kolaczkowski, A.M., et al., "Estimate of External Events Contribution to Pressurized Thermal Shock Risk," ADAMS # ML042880476.
- Generalization: Whitehead, D.W., et al., "Generalization of Plant-Specific PTS Risk Results to Additional Plants," ADAMS # ML042880482.

Figure 0.1. Illustration of the report structure providing the technical basis for PTS rulemaking. This report is marked with a circle.

1. BACKGROUND

This document provides a summary of verification and validation (V&V) of the Fracture Analysis of Vessels, Oak Ridge (FAVOR) software. The Oak Ridge National Laboratory (ORNL) developed the FAVOR software with support from the U.S. Nuclear Regulatory Commission (NRC). The FAVOR software is used to generate a distribution for the frequency of crack initiation and through-wall crack penetration in the reactor pressure vessel (RPV) for postulated pressurized thermal shock (PTS) events. The software has undergone major modifications to support reevaluation of the screening criteria under the NRC PTS rule (Title 10, Section 50.61, of the *Code of Federal Regulations* (10 CFR 50.61) Ref. 1). This software will also provide the capability to assess compliance with the PTS risk acceptance criteria for individual plants.

The current FAVOR V&V activity deals with the software validation in accordance with the software V&V plan to demonstrate that the as-built software meets its requirements, as described in the theory manual and user's guide. It includes the development of test plans, test procedures, acceptance criteria for comparing the FAVOR code results with independent calculations, and test reports.

The FAVOR software uses three distinct computational modules for PTS evaluations. These include a load generator module (FAVLoad), a probabilistic fracture mechanics (PFM) module (FAVPFM), and a postprocessor (FAVPost). The load generator module computes temperature, stress, and flaw stress intensity factors as a function of location in the vessel wall and time during the defined PTS event. The PFM module performs a Monte Carlo analysis by applying deterministic fracture mechanics to many stochastically generated RPVs, containing postulated fabrication-induced flaws, subjected to specified PTS transient conditions imposed on the RPV inner surface. It then performs a deterministic fracture analysis for each flaw by analyzing the temporal relationship between the applied Mode-I stress intensity factor (K_I) and the static cleavage fracture initiation toughness (K_{Ic}) at the crack tip. The result of the PFM analysis is an array containing values of the conditional probability of crack initiation (CPI) ($0 \le$ CPIRPV ≤ 1.0) for each simulated RPV subjected to each PTS transient. The PFM module produces an identically structured array containing values of conditional probability of RPV failure (CPF) ($0 \le$ CPFRPV ≤ 1.0). Probability distributions are determined from the complete arrays of CPIRPV and CPFRPV; associated with each distribution is a mean value and a quantification of uncertainty about that mean. The PFM module calculates stress intensity factors for embedded flaws. The third FAVOR module is the postprocessor that integrates these probability distributions of crack initiation and RPV failure with distributions of transient initiating frequencies derived from plant system and human interaction considerations. Outputs from this process include probability distributions for RPV crack initiation and RPV failure frequencies (events per reactor operating year).

The ORNL performed the software modifications for the NRC. The NRC and Electric Power Research Institute (EPRI) Materials Reliability Program (MRP) supported engineers from ORNL, Westinghouse Electric Company LLC, Sartrex Corporation, Pacific Northwest National Laboratories (PNNL), and Idaho National Engineering and Environmental Laboratories (INEEL) comprised the V&V team and performed the software V&V.

The ORNL developed the FAVOR code under the terms and conditions of NRC Management Directive 11.7 (Ref. 2), which requires that all software development, modification, or maintenance must follow general guidance provided in NUREG/BR-0167 (Ref. 3). The software quality assurance (SQA) guidance in NUREG/BR-0167 applies to technical applications software used in a safety decision by the NRC. Both NRC organization and NRC contractors use this SQA guidance in the development and maintenance of software for the NRC. The SQA program and guidance in NUREG/BR-0167 are based on various industry standards, listed in its Appendix C ("Reference Documents"). The V&V effort has also considered the intent of Appendix B to 10 CFR Part 50 (Ref. 4) to provide reasonable assurance of FAVOR code functionality to support its use in ongoing efforts to reevaluate the PTS screening criteria and for future applications.

During the course of technical basis reevaluation effort for the PTS rule, FAVOR code development occurred in several stages. Version 2.4 (Refs. 5 and 6) of the FAVOR code, also termed the base version, was used in developing the results for the December 2002 draft PTS NUREG report (Ref. 7). A validation testing plan (Ref. 8) was developed for the base version 2.4 of the FAVOR code. Based on this validation plan, ORNL (Ref. 9), PNNL (Ref. 10), INEEL (Refs. 11 and 12), and EPRI/Sartrex and EPRI/Westinghouse (Ref. 13) teams performed testing and reporting of test results regarding specific aspects of the code validation.

ORNL subsequently replaced FAVOR Version 2.4 with the revised version 3.1 (Refs. 14 and 15), which removed the observed computational errors as a result of the validation testing. Version 3.1 also includes additional features, such as the warm prestress and upper-shelf ductile tearing models. The V&V team used version 3.1 of the FAVOR code (Refs. 14 and 15) to generate the results for the present PTS technical basis reevaluation effort. The INEEL (Ref. 16) and EPRI/Sartrex and EPRI/Westinghouse (Ref. 17) teams performed incremental validation of version 3.1 of the FAVOR code to test those features and corrections added to the base version 2.4 of the code.

2. OVERVIEW OF SOFTWARE VERIFICATION AND VALIDATION ACTIVITIES

Verification and validation consisted of (1) requirements review, (2) testing activities, and (3) reporting. These steps, as described below, include review of software requirements and process design review, independent testing for validation of the software, and providing software verification and validation reports.

2.1 Software Requirements Verification

Software requirements are the foundation on which the completed calculation system must be designed, built, and accepted. The V&V team examined the software to verify its capability to meet requirements for determining the distribution of failure frequencies for postulated PTS events. The principal goal of this activity is to independently verify that (1) the software design meets the requirements specified for the software (i.e., solution of the right problem) as described in the current version of FAVOR code theory manual and software design description (Refs. 14 and 15), (2) the input requirements are consistent with the application and consistent with information available to the user, and (3) the output is consistent with information needed to evaluate compliance with the NRC PTS risk acceptance criteria. This requirements review also provides the basis for reviewing the software test procedure.

The V&V team performed the design verification by evaluation and analysis of technical reports, documented computer flow diagrams, and logic controls, and use of a top-down analysis to verify subsystem interfaces and to identify potential deficiencies in meeting requirements specified for PTS evaluations. The V&V team checked individual computational relationships for programming accuracy, but this V&V effort did not generally include a comprehensive, code line-by-line walk-through. Instead, the team performed a comprehensive review of demonstration test data and observation of the input and output elements from the test to verify that all software elements properly actuate.

The requirements verification includes the following activities:

- Confirm hardware and software configurations needed to run and test the software (i.e., computer type and processor, operating system, system memory).
- Review source documents used to establish the software requirements.
- Review the major components of the software relative to the software requirements to determine if the software calculation is a complete and correct translation of the requirements (based on review of flow charts and reference documents).
- Review the computational procedures (mathematical models, control flow, data flow, control logic, and data structure) used in the software to satisfy the requirements (based on detailed calculations in each computational algorithm).
- Confirm that the input/output are consistent with the software requirements and are defined for efficient use of the software for inputting field data and assessing compliance with regulatory requirements.

- Confirm the testability of the software for use of sample test data to perform independent calculations and check results with other independently developed software, where applicable.

The V&V Test Plan (Ref. 8) established the test acceptance criteria and mandated the reporting and resolution of any problem identified during requirements verification using a procedure described in the plan's Section 6. Documents on software verification and validation requirements are to be maintained so that future changes are traceable to an approved document.

2.2 Software Validation

The V&V team performed software validation to demonstrate that the performance of the integrated system meets the requirements using two distinct sub activities, (1) test plan and test procedure review and (2) test execution and results analysis. This activity depended on the information derived from the requirements review. The V&V team developed a comprehensive set of validation tests to independently ensure that the software meets all testable requirements identified in the software design specification (Refs. 5, 6, 14, and 15). The team designed the test plan to evaluate all computational algorithms.

Following review of the test procedures, the V&V team performed the actual testing. It performed alternate calculations, exercised the program, and recorded results. The results were compared with the acceptance criteria included in the test procedures to determine acceptability. The team kept records during each validation test to ensure that the test is identified, and the input and outputs are archived with sufficient detail so that the same test could be repeated by others and the results confirmed. All computations were stored and retained electronically and identified with a file name, date, and size.

The V&V team used two software testing methods:

- Perform hand calculations to check the major individual components of the algorithm and verify that the same results are obtained.

- Perform calculations using commercially available software (e.g., ABAQUS, EXCEL, @RISK, SAS) to check the major individual components of the algorithm and verify that results are obtained within defined acceptance criteria.

The team checked the following essential calculations:

- individual variable distributions

- conditional probability of flaw initiation

- conditional probability of vessel failure

- distribution of vessel failure frequencies

- calculations to confirm internally generated distributions

- calculations to confirm the software cannot be used for input outside real physical bounds

- sensitivity calculations to ensure the software properly functions over the range of potential applications
- repetitive calculations for the same conditions to ensure software repeatability

The team included tests of the individual computational modules and end results described in the software specification. These results can be in the form of single value deterministic (SVD) quantities, single value probability (SVP) quantities, or distributions (D).

For FAVOR Version 2.4 (Refs. 5 and 6), the team performed calculations for the variables in each of the three major FAVOR computational modules (i.e., FAVLoad, FAVPFM, FAVPost), described below.

2.2.1 V&V of Deterministic (FAVLoad) Module

The V&V of the deterministic (FAVLoad) module included the following tests:

(a) transient time histories of temperature and stress at specified spatial locations in the RPV wall thickness for variables of (1) temperature, (2) hoop stress, and (3) axial stress

(b) through-wall variation of temperature and stress at specified transient time(s) for variables of (1) temperature, (2) hoop stress, and (3) axial stress

(c) transient time histories of applied K_I (at the deepest point of the flaw) for specified axial and circumferential inner-surface breaking flaw depth(s) for (1) aspect ratio (L/a) of 2, (2) L/a = 6, (3) L/a =10, and (4) L/a = infinity, where L = total flaw length, a = depth of the semi-elliptical inner-surface breaking flaw

(d) through-wall variation of applied K_I (at the deepest point of various flaw depths) for axial and circumferential inner-surface breaking flaws at specified transient time(s) for (1) L/a = 2, (2) L/a = 6, (3) L/a = 10, and (4) L/a = infinity

(e) transient time histories of applied K_I (at the inner crack tip) for various specified axially and circumferentially embedded flaw geometries characterized by the variables of (1) flaw depth, (2) location of inner crack tip, and (3) aspect ratio

Tests (a), (b), (c), and (d) above involve the verification of the FAVLoad module. Test (e) involves verification of the FAVPFM module.

With regard to test (c) above, based on recommendations provided by PNNL staff, all postulated preexisting inner-surface breaking flaws are circumferentially oriented. Therefore, finite length, axially oriented, semi-elliptical surface-breaking flaw geometries would not be encountered during a PFM analysis for currently operating U.S. RPVs. No validation is expected to be performed for finite length, circumferentially oriented, semi-elliptical, surface-breaking flaws with aspect ratios of 2 and 10; only the aspect ratio of 6 is considered for validation. Results obtained during PFM analysis for the Oconee, Unit 1, plant indicate that shallow, circumferentially oriented, semi-elliptical flaws with an aspect ratio of 6 make the most significant contribution to the conditional probability of crack initiation. Therefore, to minimize time and resource requirements, validation of finite length, semi-elliptical flaws is limited to this particular flaw geometry.

2.2.2 V&V of Probabilistic Aspects of the FAVPFM Module

The V&V of the probabilistic aspects of the FAVPFM module included the following tests:

(a) sampling of each embrittlement-related variable for a single RPV subregion (comparing computed and theoretical distributions), including (1) neutron fluence, (2) copper, (3) nickel, (4) phosphorus, and (5) RT_{NDTo}

(b) sampling of each embrittlement-related random variable for multiple subregions, including (1) neutron fluence, (2) copper, (3) nickel, (4) phosphorus, and (5) RT_{NDTo}

(c) sampling of epistemic uncertainty in RT_{NDTo}, ΔRT_{ARREST}, and K_{Ia}

(d) implementation of embrittlement correlation for (1) plate, (2) weld, and (3) forging

(e) sampling of shift in RT_{NDT} (ΔRT_{NDT}), ΔRT_{ARREST}, and K_{Ia}

(f) implementation of methodology for sampling flaw geometry

(g) implementation of methodology for distributing flaws across RPV beltline subregions

(h) implementation of methodology for calculating CPI for each flaw (interaction of applied K_I with fracture initiation toughness)

(i) implementation of methodology for calculating CPF for each flaw

(j) implementation of methodology for treatment of multiple flaws

(k) implementation of methodology for placing flaws in weld regions along fusion line(s) with adjacent plate material

(l-1) PNNL preparation of a report on the generalized flaw distribution algorithm

(l-2) validation of PNNL's generalized flaw distribution algorithm

(m) implementation of the warm prestress methodology

2.2.3 V&V of the FAVPost (Postprocessing) Module

The V&V of the FAVPost (postprocessing) module included the following activities:

(a) sampling of transient initiating frequencies

(b) process of combining sampled transient initiated frequencies with results of PFM analysis

(c) generation of probability distribution for frequency of crack initiation

(d) generation of probability distribution for frequency of RPV failure

(e) generation of descriptive statistics of probability distribution for frequency of crack initiation

(f) generation of descriptive statistics of probability distribution for frequency of RPV failure

Table 2.2-1 lists the organizational teams responsible for developing validation test plans and completing each of the tasks outlined above. The teams presented these plans and discussed their progress in open public meetings.

Table 2.2-1 Summary of Test Program for FAVOR Version 2.4 (Refs. 5 and 6)

Test	Test Responsibility
Deterministic Load Module, Task 2.2.1	ORNL
Probabilistic Analysis Module, Tasks 2.2.2 (a) and (b)	INEEL
Probabilistic Analysis Module, Tasks 2.2.2 (c), (d) and (e)	Westinghouse LLC/EPRI
Probabilistic Analysis Module, Tasks 2.2.2 (f) and (g)	PNNL
Probabilistic Analysis Module, Tasks 2.2.2 (h), (i), (j), (k), and (m)	Sartrex Corp./EPRI
Probabilistic Analysis Module, Task 2.2.2 (l-1)	PNNL
Probabilistic Analysis Module, Task 2.2.2 (l-2)	Westinghouse LLC/EPRI
Probabilistic Postprocessing Module, Task 2.2.3	INEEL

For FAVOR Version 3.1 (Refs. 14 and 15), the team performed an incremental validation of changes made relative to version 2.4 of the code for the FAVOR computational modules. Section 2.2.4 below and Table 2.2-2 summarize the testing tasks performed.

2.2.4 Incremental V&V of FAVOR Version 3.1 Code

The team performed the following testing tasks related to incremental V&V of version 3.1 of the FAVOR code:

(a) unirradiated upper-shelf energy (USE) embrittlement parameter sampling

(b) instantaneous conditional probability of initiation

(c) initiation and arrest toughness scaling factor

(d) vessel failure by plastic collapse or excessive nonductile flaw extension

(e) cleavage reinitiation and arrest

(f) ductile flaw extension and stability

(g) sampled embrittlement-related variables in the PFM module

Table 2.2-2 Summary of Test Program for FAVOR Version 3.1 (Refs. 14 and 15)

Test	Test Responsibility
PFM Module, Task 2.2.4 (a)	INEEL
PFM Module, Tasks 2.2.4 (b), (c), (d), (e), and (f)	Sartrex Corp./EPRI
PFM Module, Task 2.2.4 (g)	Westinghouse LLC/EPRI

3. SUMMARY OF SOFTWARE VERIFICATION AND VALIDATION RESULTS

This section summarizes results from the reports on the V&V tests in Section 2 above. The respective V&V test reports discussed in this section provide further details of the individual tests performed, results obtained, and comparison with the FAVOR-generated results.

3.1 V&V of Deterministic FAVLoad Module

This study (Ref. 9) benchmarked deterministic load-related solutions generated with the FAVOR code for selected PTS transients against solutions obtained from the ABAQUS code (version 6.2-4) (Ref. 18) for the same transients for several representative inner surface breaking and embedded flaws. ABAQUS is a general-purpose, multidimensional, finite element code with fracture-mechanics capabilities. The ABAQUS finite-element models used to generate the analysis results for temperature, stresses, and K_I employed 20-node isoparametric brick elements for the main structure. Collapsed prism elements were used at the crack tip to produce an appropriate singularity for FEM analysis.

3.1.1 Initial Conditions for Analysis

The team performed benchmarking analyses for two transient thermal-hydraulic boundary condition sequences that are representative of important postulated PTS scenarios at the Oconee and Beaver Valley nuclear reactor plants. These boundary conditions consist of time histories defining coolant temperature, internal pressure, and convective heat transfer coefficient applied to the RPV inner wall. The following describes these transients:

- Transient 1, Oconee PTS with repressurization, is the postulated transient 109 from the Oconee PTS analysis. This transient has a complex time history that includes a severe repressurization at 119.5 minutes. The initial cooldown rate is 332 °F/hr for the first 75 minutes, after which the rate slows until the repressurization and then increases at a rate of about 60 °F/hr. In all analyses performed using Transient 1, the stress-free temperature was 468 °F.

- Transient 2, Beaver Valley PTS without repressurization, is the postulated transient sequence 007 from the Beaver Valley PTS analysis. This transient has a complex time history that includes a severe thermal shock having an initial cooldown rate of 1846 °F/hr for the first 15.5 minutes and that quickly reaches a steady state thereafter. No repressurization occurs. In all analyses performed using Transient 2, the stress-free temperature was equal to the initial coolant temperature of 544.8 °F.

3.1.2 Load-Related Output

The load-related transient variables output by the deterministic load module of FAVOR include the following:

- through-wall temperature (T)
- through-wall circumferential (hoop) stress
- through-wall axial stress
- applied Mode I stress intensity factor (K_I) for a range of flaw geometries

These same transient variables are computed and output from the ABAQUS analyses for comparison to the FAVOR solutions.

3.1.3 Acceptance Criteria

This benchmarking exercise sought to illustrate that values of selected parameters computed by FAVOR are within ±10 percent of ABAQUS values. For applications to K_I values, the latter criterion applies only over intervals that are relevant to the application of FAVOR. Specifically, satisfaction of the ±10 percent criterion is required only for K_I value greater than K_{min} = 18.2 ksi-in$^{1/2}$; time histories violating the ±10 criterion only on intervals for which K_I < 18.2 ksi-in$^{1/2}$ will be defined as satisfying the acceptance criteria. Here, K_{min} = 18.2 ksi-in$^{1/2}$ is the location parameter in the three-parameter form of the Weibull statistical model of fracture toughness (Ref. 5). In that Weibull model, the probability of cleavage initiation is zero for crack driving forces below K_{min}.

3.1.4 Summary of Results

3.1.4.1 Temperature and Stress Calculations

All temperature and stress solutions for the Oconee and Beaver Valley thermal-hydraulic transients satisfy the acceptance criteria given in Section 2.6 of the problem statement (Ref. 9). The FAVOR and ABAQUS temperature solutions agree to within 1.2 percent, while the hoop and axial stress solutions agree to within 10 percent.

3.1.4.2 K_I Calculations

3.1.4.2.1 Surface-Breaking Flaws

For surface-breaking flaws subjected to the Oconee transient, only one out of seven flaw cases does not satisfy the acceptance criteria (i.e., case D1). For the latter case, the study noted the following points:

- FAVOR results are conservative.
- The flaw depth of a = 0.27 in. is near the clad/base metal interface (at 0.25 in.), where three-dimensional finite-element meshing of the crack tip region is a challenge for linear elastic applications of ABAQUS.
- Acceptance criteria are satisfied at peak values of K_I, which would be of interest in PFM calculations.

For surface-breaking flaws subjected to the Beaver Valley transient, five out of seven flaw cases do not satisfy the acceptance criteria (i.e., D1, D2, D3, E2, and E3). For the latter cases, the study observed the following:

- Case D1
    - FAVOR results are conservative.
    - Flaw depth is near clad/base metal interface where three-dimensional finite-element modeling is a challenge.

— K_I at maximum discrepancy exceeds the location parameter value of 18.2 ksi-in$^{1/2}$ by only 4 ksi-in$^{1/2}$.

- Cases D2, D3, E2, and E3

  — K_I at maximum percentage discrepancy is just above 18.2 ksi-in$^{1/2}$.

  — Maximum percentage discrepancies occur at times that are late in the transient.

For all cases, the percent discrepancy (absolute value) at the peak value of K_I is less than 4.5 percent.

3.1.4.2.2 Embedded Flaws

For embedded flaws, all solutions satisfy the acceptance criteria except that of flaw B1 subjected to the Beaver Valley transient. For that B1 Beaver Valley case, the study observed the following:

- FAVOR results are conservative.

- Flaw geometry for case B1 is outside the bounds of applicability for the EPRI K_I methodology for embedded flaws (Ref. 19) employed in FAVOR.

3.1.4.3 Assessment of Deterministic Module

The assessment of V&V results given above included defensible arguments for accepting those limited number of cases that do not satisfy a strict application of the acceptance criteria. Based on that assessment, the V&V team (Ref. 9) concludes that the deterministic module implemented into FAVOR correctly performs the calculations described in the FAVOR software design documentation.

3.2 V&V of PFM Module Tasks 2.2.2 (a) and (b)

The team validated the FAVOR sampling process for both a single RPV subregion (Task 2.2.2 (a)) and multiple RPV subregions (Task 2.2.2 (b)). In addition, because FAVOR treats multiple flaws within a subregion differently from a single flaw, the V&V process examined both the single flaw per subregion and the multiple flaws per subregion cases. This combination of two variations on the number of subregions (single and multiple) with two variations on the number of flaws (single and multiple) results in four sets of case studies. The V&V team examined additional variations within each of the four case groups to validate the treatment of different numbers of flaws and different numbers of subregions.

3.2.1 Basic Approach

To complete this validation, the V&V team extracted the sampled values for each variable from the FAVOR code and compared the resulting distribution to one produced using the commercially available SAS program (Ref. 20). The team compiled a slightly modified version of the FAVOR code that (1) populates flaws in subregions based on an allocation specified in the subregion input and (2) contains write statements to output the sampled embrittlement parameter values. The V&V team then executed this modified version for each test case.

In the second step of the embrittlement sampling validation, the V&V team duplicated the FAVOR sampling algorithms using the SAS programming language (Ref. 20) which is very flexible. In the third step of the FAVOR validation, the team entered the FAVOR output into SAS for comparison to the expected, SAS-generated distribution. Standard goodness-of-fit statistical test statistics (e.g., the chi-squared statistic and the Kolmogorov-Smirnov (K-S) test statistic) were evaluated, as applicable.

Limitations on applicability pertain when, for example, successive generated embrittlement parameters are correlated. Because the SAS and FAVOR sample sizes are large, the statistical tests show even minute differences in the output distributions. Furthermore, the probability of observing high test statistics even when only random variations are present increases with each statistical test that is performed, since each test has that possibility. Therefore, the team used a statistical significance level of greater than 0.1 percent as the acceptance criteria.

The team evaluated 16 cases of the modified FAVOR code, with inputs as indicated in the V&V test plan (Table A-5.3 in Ref. 8). For each embrittlement parameter in each FAVOR run, the team generated density histogram plots that compare the outputs of the two processes. It evaluated percentage differences for the mean, median, 90th percentile, 95th percentile, and 99th percentile of the SAS and FAVOR distributions. In addition, each pair of samples had three statistical tests comparing the distributions:

- a test for whether a statistical difference exists between the mean of the FAVOR sample and the corresponding mean of the SAS sample
- an evaluation of the K-S test of whether the sample cumulative distribution function from FAVOR matches a continuous “theoretical” distribution function determined from the SAS sample
- an evaluation of the chi-squared test statistic (X^2) for each set of histograms

3.2.2 Acceptance Criteria

When the goodness-of-fit tests did not apply, the V&V team compared particular attributes of the FAVOR and SAS distributions for consistency in order to access the acceptability of the FAVOR results. Table 3.2-1 provides details for these assessments.

Table 3.2-1 Comparison of FAVOR and SAS Distribution Attributes

Attribute	Acceptance Criterion
Mean	Relative difference < 1% (See Note a)
Median	Relative difference < 1% (See Note b)
90th percentile	Relative difference < 5% (See Note b)
95th percentile	Relative difference < 5% (See Note b)
99th percentile	Relative difference < 5% (See Note b)

Attribute	Acceptance Criterion

a. The mean of the aggregate distribution for each embrittlement parameter can be calculated directly from the specified inputs. The relative difference is the absolute value of the difference between the associated FAVOR sample average and the calculated mean, divided by the calculated mean. The sample size is large enough to make this comparison achievable. When the specified mean is zero, the absolute difference is evaluated.

b. The relative difference is the absolute value of the difference between the associated FAVOR and SAS attributes, divided by the SAS attribute.

3.2.3 Summary of Results

Table 3.2-2 (Table 1.3.1 in Ref. 11) and Table 3.2-3 (Table 1.3.2 in Ref. 11) provide a summary of the percentage difference results of the validation runs. The first table shows percentage differences for the means and medians, while the second table lists differences for the 90th, 95th, and 99th percentiles. Nearly all the values conform to the criteria specified in the test plan, with percentage differences less than 1 percent for the mean and median and less than 5 percent for the higher percentiles.

The mean and/or median values for three runs with RT_{NDT0} are the only exception for the percentage differences. The percentage differences are above 1 percent because the variation in the distributions is roughly four times the value of the mean. Table 3.2-4 (Table 1.3.3 in Ref. 9) shows the data. The calculated mean and standard deviation values in the second and third columns come directly from the input data and are calculated from simple weighted averages that reflect the mixture distributions being modeled. Even the coefficients of variation for the sample means remain relatively high. A band from one standard deviation to the left of the sample mean to one standard deviation to the right exceeds 1 percent for the FAVOR sample mean. Therefore, these differences are within the range of acceptability.

Table 3.2.5 (Table 1.3.4 in Ref. 11) provides a summary of the more statistical results of the validation runs. The table shows, for each FAVOR run and each relevant embrittlement parameter, the t-test, K-S test, and chi-square test results. The results are indicated in blocks, with “T” preceding the t-test indication, “K” preceding the K-S test indication, and “C” preceding the chi-squared test indication.

Several of the statistical tests (Ref. 11) do show differences in the SAS and FAVOR distributions. None of the differences are notable from a percentage difference standpoint. The differences are all small in magnitude and relate to cases with multiple flaws and dependence in the data. The statistical tests do not consider the intentional dependency in the sampling. The dependency comes from the sampling of fluence based on a vessel-level standard deviation, and from the sampling of chemistry parameters for a flaw based on the parameters of the first flaw in a subregion.

3.3 V&V of PFM Module Tasks 2.2.2 (f) and (g)

This validation (Ref. 10) sought to establish that FAVOR correctly assigns the number, sizes, and locations of flaws to the weld and base metal regions of an RPV in accordance with the PNNL-supplied data files and in a manner consistent with the stated assumptions of the FAVOR code. The verification effort included the following specific elements:

- total number of flaws in a vessel
- total number of flaws in weld regions
- total number of flaws in base metal regions
- numbers of flaws in individual subregions of weld and base metal
- numbers of flaws assigned to Category 1 (surface flaws) and Categories 2 and 3 (buried flaws)
- flaw inner tip locations relative to the inside surface of vessel
- depth dimensions of weld and base metal flaws
- aspect ratios of weld flaws, base metal flaws, and surface flaws

The V&V team performed the validation calculations described in this report using version 2.3 of the FAVOR code. Version 2.3 includes a new treatment of flaws in vessel welds and in vessel cladding in that flaw densities are described on the basis of flaws per unit area of weld fusion surface rather than as flaws per unit volume of metal. The team reviewed later versions of FAVOR (versions 2.4 and 3.1) and determined that the newer versions involve no changes to those parts of the code that simulate flaws.

3.3.1 Basic Approach

The first part of the validation effort was limited to comparisons using the outputs that are part of the standard output files that come from execution of FAVOR. This verification started with the flaw-related input files and independently calculated the numbers and sizes of flaws for an example RPV calculation and then compared these numerical results with outputs from FAVOR.

The second part of the validation effort made comparisons using data from an additional output file generated by a special version of the FAVOR code that ORNL provided. This additional output file allowed verification of the assignment of flaws to subregions of the vessel, verification of the simulated flaw lengths (or aspect ratios), and verification of the simulated locations of flaw inner tips relative to the vessel inside surface.

3.3.2 Summary of Results

3.3.2.1 Verification for Numbers of Flaws Per Vessel

The flaw data from the FAVOR output file (Tables 5, 6, and 7 in Ref. 10) were expressed in terms of flaws per vessel to allow a comparison of validation results for numbers of flaws. The resulting comparisons show excellent agreement (Tables 8 and 9 in Ref. 10). Compared to PNNL's calculation of 8108 flaws per vessel, FAVOR simulated a total of 8106 flaws per vessel. The V&V team concludes that FAVOR correctly simulates the numbers of flaws in welds and base metal and correctly apportions these flaws to the major regions of the vessel consistent with the assigned areas and volumes for the regions.

Table 3.2-2 Percentage Differences for the Mean and Median, Based on 500,000 FAVOR Sample Values for Each Run

Run Name (from Test Plan)	# of plates	# of welds	# of flaws	Difference for mean, followed by difference for median (see Note b)				
				Fluence	RT_{NDT0}	Copper	Nickel	Phosphorus
sssf_w	0	1	1	-0.01 | 0.01	Mean=median=0	0.01 | 0.00	-0.03 | -0.03	-0.02 | 0.00
sssf_w_hm	0	1	1	-0.01 | 0.00	-0.02 | -0.02	0.02 | 0.00	0.00 | -0.02	-0.00 | 0.00
sssf_w_hs	0	1	1	-0.31 | -0.47	Mean=median=0	-0.01 | 0.14	-0.04 | -0.06	-0.07 | 0.08
sssf_w_df	0	1	1	—NA—	—NA—	-0.00 | 0.00	0.01 | 0.00	—NA—
sssf_p	1	0	1	—NA—	—NA—	0.00 | 0.00	-0.01 | -0.01	-0.01 | 0.00
sssf_pa	1	0	1	—NA—	—NA—	-0.00 | -0.00	-0.03 | -0.07	-0.09 | 0.02
mssf_p05	5	0	1	-0.15 | -0.18	**1.20** | **4.10**	-0.12 | -0.03	-0.12 | -0.04	-0.17 | 0.00
mssf_p05a	5	0	1	-0.19 | -0.07	0.57 | 0.02	-0.10 | -0.03	-0.11 | -0.02	-0.15 | -0.05
mssf_w40	0	40	1	0.11 | 0.08	-0.27 | -0.13	0.11 | 0.05	0.06 | 0.11	0.06 | 0.02
mssf_wp45	5	40	1	0.13 | -0.00	-0.31 | **-2.18**	0.02 | -0.00	0.05 | 0.08	0.23 | 0.19
ssmf_w_116	0	1	116	—NA—	—NA—	0.07 | -0.12	-0.08 | -0.13	0.21 | 0.19
ssmf_p_116	1	0	116	—NA—	—NA—	-0.09 | -0.12	0.03 | 0.04	0.45 | 0.57
msmf_p05_116	5	0	116	0.07 | 0.16	0.71 | -0.28	-0.12 | -0.03	-0.09 | -0.06	-0.16 | -0.17
msmf_p05_116_gl	5	0	116	0.22 | 0.13	—NA—	—NA—	—NA—	—NA—
msmf_p05_116_lo	5	0	116	-0.07 | -0.03	—NA—	—NA—	—NA—	—NA—
msmf_wp45_116	5	40	116	-0.20 | -0.10	**1.02** | **1.78**	-0.10 | -0.07	-0.12 | -0.08	-0.25 | -0.19

a. To establish SAS reference distributions for evaluation of the FAVOR sampling, SAS samples of size 5,000,000 were used for each parameter for each run.

b. In each cell, the percentage difference for the mean is shown, followed by the percentage difference for the median. Percentage differences are calculated as the FAVOR value minus the SAS value, multiplied by 100, and divided by the SAS value. The calculation is not applicable for two RT_{NDT0} cases for which the actual mean and median of the sample distribution were zero. It is also not applicable ("—NA—") when the test plan identifies a comparison as not applicable (these are cases where the particular test provides no new comparisons for a particular parameter). Percentage differences with absolute value greater than 1.0 percent are marked in bold.

Table 3.2-3 Percentage Differences in the 90th, 95th, and 99th Percentiles, Based on 500,000 FAVOR Sample Values for Each Run

Run Name (from Test Plan)	# of plates	# of welds	# of flaws	Percentage difference for 90th percentile, followed by 95th, followed by 99th (see Note b)				
				Fluence	RT_{NDT0}	Copper	Nickel	Phosphorus
sssf_w	0	1	1	-0.01 | -0.04 | -0.11	0.00 | 0.12 | 0.20	0.00 | 0.00 | 0.00	-0.06 | -0.06 | -0.04	-0.02 | -0.04 | -0.01
sssf_w_hm	0	1	1	-0.01 | -0.05 | -0.10	-0.04 | 0.01 | 0.10	0.00 | 0.00 | 0.00	-0.01 | -0.01 | 0.00	-0.00 | -0.00 | -0.00
sssf_w_hs	0	1	1	-0.26 | -0.19 | -0.08	-0.15 | -0.03 | 0.15	0.00 | 0.00 | 0.00	-0.10 | -0.07 | -0.00	-0.10 | -0.18 | -0.03
sssf_w_df	0	1	1	—NA— (see note c)	—NA—	0.04 | -0.05 | 0.00	0.01 | 0.02 | 0.08	—NA—
sssf_p	1	0	1	—NA—	—NA—	-0.01 | -0.01 | -0.01	-0.01 | -0.02 | -0.01	0.02 | -0.02 | -0.11
sssf_pa	1	0	1	—NA—	—NA—	-0.00 | 0.00 | 0.00	-0.05 | -0.15 | -0.14	0.06 | -0.11 | -0.43
mssf_p05	5	0	1	-0.02 | -0.08 | 0.05	-0.17 | -0.05 | -0.06	-0.02 | -0.01 | -0.03	-0.01 | -0.00 | -0.02	-0.01 | -0.01 | -0.02
mssf_p05a	5	0	1	0.03 | 0.06 | -0.02	-0.39 | 0.16 | 0.19	1.29 | -0.00 | -0.01	0.55 | -0.00 | -0.01	0.50 | -0.01 | -0.00
mssf_w40	0	40	1	0.04 | 0.01 | -0.09	0.27 | 0.23 | 0.65	0.00 | 0.00 | 0.00	0.03 | -0.00 | 0.06	-0.01 | -0.06 | -0.02
mssf_wp45	5	40	1	0.22 | 0.16 | 0.17	0.18 | 0.01 | -0.13	0.00 | 0.01 | 0.02	0.03 | 0.02 | 0.01	0.02 | 0.02 | 0.02
ssmf_w_116	0	1	116	—NA—	—NA—	0.00 | 0.00 | 0.00	0.32 | 0.60 | 0.02	-0.06 | -0.04 | -0.18
ssmf_p_116	1	0	116	—NA—	—NA—	0.03 | 0.10 | 0.14	0.14 | 0.14 | 0.15	0.35 | 0.41 | 0.71
msmf_p05_116	5	0	116	0.21 | 0.16 | 0.22	-0.12 | -0.10 | -0.06	0.04 | -0.00 | -0.10	0.00 | -0.03 | -0.10	0.00 | 0.00 | -0.03
msmf_p05_116_gl	5	0	116	0.17 | 0.70 | 0.66	—NA—	—NA—	—NA—	—NA—
msmf_p05_116_lo	5	0	116	0.01 | 0.02 | 0.05	—NA—	—NA—	—NA—	—NA—

Run Name (from Test Plan)	# of plates	# of welds	# of flaws	Percentage difference for 90th percentile, followed by 95th, followed by 99th (see Note b)				
				Fluence	RT_{NDT0}	Copper	Nickel	Phosphorus
msmf_wp45_116	5	40	116	-0.20 | -0.17 | -0.23	-0.34 | -0.31 | -0.06	0.00 | -0.02 | -0.04	0.06 | 0.03 | -0.01	-0.03 | 0.02 | 0.02

To establish SAS reference distributions for evaluation of the FAVOR sampling, SAS samples of size 5,000,000 were used for each parameter for each run.

Each cell shows the percentage difference for the 90th percentile, followed by the percentage difference for the 95th percentile and the percentage difference for the 99th percentile. Percentage differences are calculated as the FAVOR value minus the SAS value, multiplied by 100, and divided by the SAS value. The single percentage difference greater than 1 percent is in bold. All of the percentage differences are small (less than 2 percent).

"—NA—" appears in the table when the test plan identifies a comparison as not applicable (these are cases where the particular test run provided no new comparisons for a particular parameter).

Table 3.2-4 *RT_{NDT0}* Runs with Large Coefficients of Variation

	Mixture Distribution (Calculated from input specifications)			SAS Sample Mean (Sample size 5,000,000)			FAVOR Sample Mean (Sample size 500,000)		
Run Name	Mean	Standard deviation	Coef. of Variation [b]	Std. Dev. [a]	Coef. of Variation [b]	Observed Value	Std. Dev. [a]	Coef. of Variation [b]	Observed Value
mssf_p05	-11.0	53.07	482.5%	0.0237	0.216%	-11.008	0.0751	0.682%	-11.141
mssf_wp45	-13.8	52.12	377.7%	0.0233	0.169%	-13.784	0.0737	0.534%	-13.741
mssf_wp45_116	-13.8	52.12	377.7%	0.0233	0.169%	-13.801	0.0737	0.534%	-13.941

a. The standard deviation divided by the square root of the sample size (5,000,000 for SAS; 500,000 for FAVOR)
b. 100 times the standard deviation of the mean, divided by the mean (calculated from input specifications)

Table 3.2-5 Statistical Test Summary Based on 500,000 FAVOR Sample Values for Each Run

Run Name (from Test Plan)	# of plates	# of welds	# of flaws	Evaluation Results (see Note b)				
				Fluence	RT_{NDT0}	Copper	Nickel	Phosphorus
sssf_w	0	1	1	81%|T-|K-|C-	2.2%|T-|K-|C-df26	58%|T-|K-|C-	96%|T-|K-|C-	63%|T-|K-|C1
sssf_w_hm	0	1	1	90%|T-|K-|C2df37	2.2%|T-|K-|C-df27	51%|T-|K-|C-	82%|T-|K-|C-	38%|T-|K-|C1
sssf_w_hs	0	1	1	82%|T1|K3|C-df38	5.8%|T-|K-|C-df28	37%|T-|K-|C-	82%|T-|K-|C-df38	81%|T-|K-|C1
sssf_w_df	0	1	1	—NA—(see Note c)	—NA—	79%|T-|K-|C-	77%|T-|K-|C-df38	—NA—
sssf_p	1	0	1	—NA—	—NA—	47%|T-|K-|C-df38	77%|T-|K-|C-	63%|T-|K-|C-
sssf_pa	1	0	1	—NA—	—NA—	41%|T-|K-|C-df38	82%|T-|K-|C-	81%|T-|K-|C-df37
mssf_p05	5	0	1	96%|T-|K-|C-	4.6%|T-|K-|C1	86%|T-|K-|C-df37	92%|T-|K-|C-df31	86%|T-|K-|C-df24
mssf_p05a	5	0	1	91%|T-|K2|C-	4.3%|T-|K-|C-	74%|T-|K1|C-df35	89%|T-|K-|C-df31	81%|T-|K-|C-df23
mssf_w40	0	40	1	87%|T-|K3|C3df35	3.9%|T-|K-|C-	69%|T-|K-|C-	88%|T-|K-|C-	75%|T-|K-|C-
mssf_wp45	5	40	1	95%|T-|K-|C-	4.7%|T-|K-|C-	78%|T-|K-|C-	92%|T-|K-|C-	87%|T-|K-|C-df24
ssmf_w_116	0	1	116	—NA—	—NA—	58%|T3|**K4**|**C4**	96%|T-|**K4**|**C4**	66%|**T4**|**K4**|**C4**
ssmf_p_116	1	0	116	—NA—	—NA—	50%|**T4**|**K4**|**C4**	79%|**T4**|**K4**|**C4**	65%|**T4**|**K4**|**C4**
msmf_p05_116	5	0	116	96%|T-|K2|**C4**	4.6%|T-|K-|C-	87%|T-|**K4**|**C4**df37	92%|T-|K-|**C4**df32	87%|T-|**K4**|**C4**df25
msmf_p05_116_gl	5	0	116	4%|T1|K-|**C4**	—NA—	—NA—	—NA—	—NA—
msmf_p05_116_lo	5	0	116	96%|T-|K-|C-	—NA—	—NA—	—NA—	—NA—
msmf_wp45_116	5	40	116	95%|T-|K-|C-	4.7%|T-|K-|C1	78%|T-|K2|**C4**	92%|T-|**K4**|**C4**	87%|T-|K3|**C4**df24

Run Name (from Test Plan)	# of plates	# of welds	# of flaws	Evaluation Results (see Note b)				
				Fluence	RT_{NDT0}	Copper	Nickel	Phosphorus

a. To establish SAS reference distributions for evaluation of the FAVOR sampling, SAS samples of size 5,000,000 were used for each parameter for each run.

b. Entries in the cells are of the form *nn*% | T*y* | K*z* | C*w*, where

- *nn* is the percentage of FAVOR values that were unique (more specifically, differing by less than 1.E-12).
- *y* indicates the significance level for a two-sided t-test for differences in means.
- *z* indicates the significance level of the K-S test.
- *w* indicates the significance level of chi-squared the test. It is followed by "df##," whenever the degrees of freedom of the chi-square test is less than 39. The histograms were constructed with 40 bins, so 39 is the expected degrees of freedom. In some cases, discrete data and truncation result in less than 39 degrees of freedom. In these cases, the number of degrees of freedom is given in the "##" specification.

The significance levels include "-", not significant (p-value greater than 0.05); 1, p-value <=0.05; 2, p-value <=0.01; 3, p-value <=0.001; and 4, p-value <=0.0001. Recall that the p-value is a measure of the likelihood that the calculated statistics are as large as observed when the FAVOR distribution matches the SAS distribution. Thus, small p-values indicate that the distributions differ. The "4" cases are marked in bold.

c. "—NA—" appears in the table when the test plan identifies a comparison as not applicable (these are cases where the particular test run provided no new comparisons for a particular parameter).

3.3.2.2 Verification for Assignment of Flaws to Major Regions

Simonen of PNNL (see Table 15 in Ref. 10) compares the number of weld and base metal flaws, which shows good agreement with the validation calculations for the expected numbers of flaws. It also indicates that FAVOR simulated only four Category 1 surface-breaking flaws in the base metal region of the vessel and zero Category 1 flaws for the weld regions. These numbers are consistent with the validation calculations that give expected flaw counts of 4.512 flaws for the base metal regions and 0.074 flaws for the weld regions. Simonen (see Table 16 in Ref. 10) also made additional comparisons for FAVOR results of flaw counts with the validation calculations for the expected numbers of flaws for Categories 1, 2 (buried flaws within the inner 1/8 of the vessel wall thickness, t), and 3 (buried flaws within the wall from 1/8t to 3/8t) in each of the major vessel regions. Again, the level of agreement is very good, with differences attributed to sampling error from the FAVOR calculations. Category 3 flaws in weld major region #3 show the most notable percentage difference, in that the FAVOR simulation gives 69 flaws versus the expected number of 79.8 flaws.

3.3.2.3 Verification for Flaw Aspect Ratios for Weld and Base Metals Regions

Figures 10 and 11 (Ref. 10) show results from simulations of flaw aspect ratios by the FAVOR code for buried flaws (Categories 2 and 3) of weld and base metal regions, respectively. The plotted lines display the simulated data from the FAVOR output file, whereas the plotted data points are from the validation calculations. The curves from the Monte Carlo calculation by the FAVOR code are in agreement with the data points from the validation calculations. The level of agreement is best for flaws with small through-wall depths (a/t = 1%) because the sample of simulated flaws includes a large number of flaws of the smaller sizes. The apparent level of agreement becomes less satisfactory for flaws of larger through-wall depth dimensions (a/t = 3% and 5%) and for larger flaw aspect ratios. This is the expected trend because the relatively small number of simulated flaws of larger depth dimensions and aspect ratios is insufficient to establish statistically significant trends.

Table 18 (Ref. 10) addresses aspect ratios of surface flaws. The evaluation considered the number of surface flaws in five vessels, for which the independent calculation predicted 22.93 flaws. In contrast, the FAVOR code simulated 17 flaws, which agrees reasonably (considering statistical uncertainties) with the calculated number of flaws. Table 18 (Ref. 10) also lists the expected number of flaws for each of the four flaw aspect ratio categories used by the FAVOR code. The numbers and percentages of flaws from FAVOR and the independent evaluation are in relatively good agreement.

In summary, Simonen (Ref. 10) concludes that the FAVOR code correctly implements flaw-related parameters that enter into the PFM calculations.

3.4 V&V of PFM Module Tasks 2.2.2 (c), (d), (e), and (l)

The validation of Tasks 2.2.2(c), (d), (e), and (l) (Ref. 13) tested the computational algorithms and procedures for the flaw and embrittlement-related parameters in the FAVOR PFM module. The validation included sampling of epistemic uncertainty in initial RT_{NDT} (RT_{NDTo}), various embrittlement correlations for the reactor vessel beltline materials, ΔRT_{ARREST}, crack arrest toughness (K_{Ia}), shift in RT_{NDT} (ΔRT_{NDT}), flaw distribution algorithms, and uncertainties.

3.4.1 Basic Approach

To validate implementation of epistemic uncertainty in RT_{NDTo} that FAVOR used for each subregion, the team copied the FAVOR source code text that uses the epistemic uncertainty into a standalone program that performed the calculation for 1000 samples and wrote the calculated results to a data file. The data were then evaluated independently with the Best-Fit Computer Program (Palisade Corp.) to determine the type of distribution and its controlling parameters (e.g., shape factor for a Weibull distribution) for comparison with the information in the FAVOR theory manual (Ref. 3).

To validate implementation of the embrittlement correlations that FAVOR used for each subregion, the team copied the FAVOR source code text that uses the embrittlement correlations into a standalone program that read the required input data, performed the calculation, and printed the calculated results (e.g., RT_{NDT} shift).

To validate implementation of the RT_{NDT} shift sampling that FAVOR used for each subregion, the team copied the FAVOR source code text that uses the RT_{NDT} shift sampling into a standalone program that performed the calculation for 1000 samples and wrote the calculated results to a data file. The data were then evaluated independently with the Best-Fit Computer Program to determine the type of distribution and its controlling parameters (such as standard deviation of a normal distribution) for comparison with the information in the FAVOR theory report (Ref. 5).

To validate the sampling algorithms for ΔRT_{ARREST} and K_{Ia} in the FAVOR calculation of arrest toughness, the team wrote software to call the appropriate FAVOR subroutines, and the team compared the results to results obtained from independently calculated distributions.

The team performed the following tasks under the V&V plan to validate the flaw distribution algorithm:

- Confirm that the reference size and density distributions used by the PNNL program (Ref. 21) agree with their documented basis. The team considered the distributions for plate, weld, and surface flaws for two types of welds and with and without weld repairs.

- For a representative vessel input (percentage of weld types and repairs), use independent worksheet calculations to validate the representative points (such as largest, smallest, and midpoint sizes) in the best-estimate size/density distributions for plate, weld, and surface flaws.

- For the same representative vessel input, validate the variability of one representative point (such as midpoint size) in the best-estimate size/density distributions for plate, weld, and surface flaws. The team modified the PNNL program to write size or density values from 1000 simulations to their respective files and evaluate the data independently with the Best-Fit Computer Program to determine the type of distribution and its controlling parameters (such as standard deviation of a normal distribution).

3.4.2 Acceptance Criteria

The values computed by FAVOR are acceptable if the difference between the FAVOR and the expected test values was 5 percent or less in the distribution values at the 5th and 95th percentiles are acceptably small.

3.4.3 Summary of Results

The team concludes the following (Ref. 13) as a result of V&V activities performed on FAVOR Version 2.4:

- The combined sampling for the uncertainties in the initial value and epistemic shift in the calculation of initial RT_{NDT} in version 2.4 of the FAVPFM module has been independently verified to produce results of acceptable accuracy per the requirements of Item (II c) of the test plan.

- The sampling for the uncertainties in ΔRT_{ARREST} and K_{Ia} in the calculation of arrest toughness in version 2.4 of the FAVPFM module has been independently verified to produce results of acceptable accuracy per the requirements of Items (II c) and (II i) of the test plan (Ref. 8).

- The deterministic calculations of maximum RT_{PTS} for each region in version 2.4 of the FAVPFM module have been independently verified to produce results of acceptable accuracy per the requirements of Item (II d) of the test plan (Ref. 8). The verification included both types of embrittlement shift options (992 and 993) for plate, weld, and forging materials.

- The combined sampling for the uncertainties in three chemistry values and fluence in the calculation of RT_{NDT} shift in version 2.4 of the FAVPFM module has been independently verified to produce results of acceptable accuracy per the requirements of Item (II e) of the test plan (Ref. 8).

- The best-estimate calculations of flaw distribution parameters (density and aspect-ratio percentages) with flaw depth in the PNNL vessel flaw code (Ref. 21) have been independently verified to produce results of acceptable accuracy per the requirements of Item (II I-2) of the test plan (Ref. 8). The verification included two data sources (Shoreham and Pressure Vessel Research Users Facility (PVRUF)), two flaw size categories, three types of flaws (weld, plate, and surface), four types of welds (submerged arc weld (SAW), submerged metal arc weld (SMAW), repair, and composite), and one and two layers of cladding.

- The sampling of uncertainties in flaw density, aspect ratio, percentages, and flaw depth in the PNNL vessel flaw code (Ref. 21) have been independently verified to produce results of acceptable accuracy per the requirements of Item (II I-2) of the test plan (Ref. 8). The verification included two data sources (Shoreham and PVRUF), two flaw size categories, and two types of welds (SAW and SMAW).

Appendix A to this report presents the ORNL and PNNL responses (Ref. 22) to conclusions and recommendations in EPRI Report 1007826 (Ref. 13).

3.5 V&V of PFM Module Tasks 2.2.2 (h), (i), (j), (k), and (m)

This validation (Ref. 13) tested the computational algorithms and procedures in the FAVOR PFM module. The V&V performed computations to calculate the CPI and CPF methodologies for treatment of multiple flaws, placing flaws in weld regions along the fusion line(s) with adjacent plate material, and warm prestress effects.

3.5.1 Basic Approach

The team independently programmed the PFM equations and evaluation procedure contained in Sections 3.3.11 and 4.5 of the FAVOR theory manual (Ref. 5) into a spreadsheet and compared the results to the output from FAVOR. Because the FAVOR software does not print out each variable that should be included in a V&V test, the team added additional write statements to FAVOR to provide appropriate values for testing purposes. The team conducted the testing by randomly selecting a test vessel and flaw size from the Monte Carlo sampling and performing deterministic calculations for that vessel and flaw.

To validate the methodology for calculating the CPI for each flaw, the team performed tests involving only deterministic calculations for the following sample conditions:

- two different vessels
- two different flaw depths
- two different regions of the vessel (two different welds or a plate and a weld)
- two different subregions of each region
- two different transients selected from several that are included in the FAVOR analysis
- different conditions leading to initiation or noninitiation

To validate methodology for calculating the CPF for each flaw, the team performed tests involving both deterministic and sampled values to confirm flaw growth and arrest computational procedures for the following sample conditions:

- two different vessels
- two different flaw depths
- two different regions of the vessel (two different welds or a plate and a weld)
- two different subregions of each region
- two different layers in a weld subregion
- two different transients selected from several that are included in the FAVOR analysis
- different conditions leading to initiation or noninitiation

To validate the methodology for treatment of multiple flaws, the team conducted tests by obtaining individual values of cpi and cpf for a vessel and associated flaws and determining if FAVOR correctly combined the individual cpi and cpf values. (The lower case "cpi" and "cpf" represent the instantaneous value calculated at a specific time step, while upper case "CPI" and "CPF" represent the total value for the RPV.) The values computed by FAVOR were considered acceptable if the difference between the FAVOR and the expected test values was 1 percent or less.

To validate the methodology for placing flaws in weld regions along the fusion line(s) with adjacent plate material in the material having the limiting RT_{NDT}, as described in Section 3.3.3 of the FAVOR theory manual (Ref. 5), the test considered plates and both axial and circumferential welds. The team conducted the tests by changing the copper, nickel, and phosphorous contents and initial RT_{NDT} of the plates and weld materials so that the welds and then the plates were limiting relative to the adjacent welds. FAVOR was then run to determine whether the plate properties would be used for the weld flaws and to confirm that the calculated cpi values were correct.

To validate the methodology for the inclusion of warm prestress effects, the test compared the conditions specified in Section 3.3.4 with values obtained from FAVOR for cpi as a function of K_I and the Weibull parameter of a.

3.5.2 Acceptance Criteria

The values computed by FAVOR were considered acceptable if the difference between the FAVOR and the expected test values was 1 percent or less.

3.5.3 Summary of Results

Appendix A to this report presents the ORNL response (Ref. 22) to conclusions and recommendations on these validation tests (Ref. 13).

3.5.3.1 Instantaneous Conditional Probability of Initiation for Each Flaw

The results indicate very good agreement between the FAVOR calculations related to cpi and the independent calculations obtained from the V&V testing. In general, the difference is 0.01 percent or less for most variables. Even though there are only very small differences in most variables leading up to the computation of cpi, the difference between the computed values for cpi vary from 0.5 to 2 percent. Table 3.4-1 (which reproduces Table 3-11 in Ref. 13) shows a summary of all nonzero cpi values for the vessel, flaw, and transient.

Table 3.5-1 Summary of V&V Testing of cpi for Various Vessels, Flaws, Vessel Materials, and Transients

Vessel No.	Flaw No.	Flaw Location	Trans. No. and Minutes into Trans.	ΔT_{30} V&V Test (Deg. F)	ΔT_{30} FAVOR (Deg. F)	ΔT_{30} % Diff.	cpi V&V Test	cpi FAVOR	cpi % Diff.
26	6	Plate	Transient 1, 9 minutes	192.722	192.692	0.0015	3.2764E-8	3.2211E-8	1.688
26	10	Axial weld	Transient 1, 9 minutes	243.759	243.744	0.006	1.5950E-7	1.5844E-7	0.662
26	35	Axial weld	Transient 1, 6 minutes	263.832	263.814	0.007	1.8013E-6	1.7935E-6	0.432
26	35	Axial weld	Transient 1, 9 minutes	263.832	263.814	0.007	1.2893E-4	1.2882E-4	0.085
26	39	Axial weld	Transient 1, 9 minutes	242.436	242.428	0.003	5.9246E-7	5.9025E-6	0.373
12	26	Circ. weld	Transient 1, 9 minutes	249.863	249.902	-0.015	2.4996E-8	2.5517E-8	2.083
30	16	Axial weld	Transient 2, 30 minutes	259.922	259.875	0.018	1.9784E-9	1.9253E-9	2.686

3.5.3.2 Conditional Probability of RPV Failure for Each Flaw

The results for comparison of ΔT_{30} for the initiation flaw depth and several subsequent depths in the first weld layer indicate that the FAVOR ΔT_{30} value is significantly different from the test value for the first depth following initiation and is in error (see Table 3-12 in Ref. 13). In its response (Ref. 22), ORNL indicated that this issue derives from one of the two bugs that were found in FAVOR; both bugs have been repaired in FAVOR Version3.1.

The ΔRT_{NDT} from the FAVOR and test calculations are in good agreement. However, there can be errors in ΔT_{30}. Because ΔRT_{NDT} is simply the product of a constant and ΔT_{30} (ΔRT_{NDT} = 1.1 x ΔT_{30} for plate), it is not clear why ΔRT_{NDT} is correct when ΔT_{30} is incorrect. Apparently there is some mismatch in the manner in which FAVOR computes or obtains ΔT_{30} relative to ΔRT_{NDT} (see Table 3-12 in Ref. 13). In its response (Ref. 22), ORNL indicated that this issue derives from one of the two bugs that were found in FAVOR; both bugs have been repaired in FAVOR Version 3.1.

The team performed additional testing to assess the FAVOR computational accuracy for flaw depths beyond the first weld layer (see Table 3-13 in Ref. 13). The results show that FAVOR indicates the correct weld layer, selects the appropriate random number, and generally generates accurate results, except for possibly ΔT_{30}. In its response (Ref. 22), ORNL indicated that this issue derives from one of the two bugs that were found in FAVOR; both bugs have been repaired in FAVOR Version 3.1.

The team tested FAVOR to assess its ability to accurately predict vessel failure for a weld (see Table 3-17 in Ref. 13). The results of this test indicate that FAVOR correctly moved through the four weld layers, resampled the residual element contents, selected the appropriate random numbers, and predicted vessel failure.

There is some indication that the appropriate arrest toughness is not selected in Step P7 of the propagation model. For example (see results in Table 3-14 of Ref. 13), it appears that Equation 99 in Section 4.5 of the theory manual was used to compute K_{Ia} for a flaw propagating in a plate. Interpretation of the theory manual suggests that Equation 102 of Section 4.5 should have been used to determine K_{Ia} for plate material. In its response (Ref. 22), ORNL stated that, based on test results (see Ref. 17), the arrest calculations performed in FAVOR Version 3.1 resolve this comment.

3.5.3.3 Treatment of Multiple Flaws

Testing showed that FAVOR accurately calculates CPI and CPF for multiple flaws in accordance with the specifications in Section 3.3.10 of the theory manual.

3.5.3.4 Placing Flaws in Weld Regions Along the Fusion Line(s) With Adjacent Flaws

Testing indicates that changing the copper, nickel, and phosphorous contents and initial RT_{NDT} of the plates and weld materials so that the plates are limiting relative to the adjacent welds also changes the location of a specified flaw in a vessel (see Table 3-18 in Ref. 13). It is not clear from the theory manual that the flaw position is intended to change based on changes in residual element content or initial RT_{NDT} alone. In its response (Ref. 22), ORNL indicated that this problem has been fixed in version 3.1 of the FAVOR code.

Based on observed abnormal changes in calculated ΔT_{30} values in limiting plates (see Tables 3-18 and 3-19 in Ref. 13), FAVOR may not correctly implement the weld fusion line calculation described in Section 3.3.3 of the theory manual. In its response (Ref. 22), ORNL stated that this problem has been fixed in version 3.1 of the FAVOR code.

3.5.3.5 Warm Prestress Methodology

Test results indicate that FAVOR correctly implements the warm prestress methodology in Section 3.3.4 of the theory manual.

3.6 V&V of Postprocessing (FAVPost) Module Task 2.2.3

The V&V team tested the postprocessor module in FAVOR Version 2.4 to validate its outputs for the conditional frequency of crack initiation (CFI) and conditional frequency of vessel failure (CFF). The team created a mimic process in SAS (Ref. 20) that receives the FAVPost input and combines the PFM results.

3.6.1 Basic Approach

This test combined the CPI and the CPF with the probability distributions on the frequencies of the thermal/hydraulic transients. More specifically, for each vessel, the mimic process sampled from each transient initiating frequency distribution (Task 2.2.3 (a)) and then summed the products of the resulting frequencies and the conditional probabilities of failure for the vessel (Task 2.2.3 (b)). This calculation was performed for each failure mode (CPI and CPF). With

10,000 FAVOR simulated vessels, the team evaluated 10,000 CPI frequencies and 10,000 CPF frequencies and sorted them from small to large (Tasks 2.2.3 (c) and (d)). Alternately, a straightforward algebraic combining of multiple probability distributions into a composite distribution for the frequency of crack initiation and the frequency of RPV failure led to estimates of the mean and other output quantities for comparison with FAVPost. For each set of data, quantities such as the mean, standard deviation, standard error, and 99th percentile were evaluated and compared with the corresponding FAVPost outputs (Tasks 2.2.3 (e) and (f)).

3.6.2 Acceptance Criteria

A simple comparison in which the FAVOR and the computed test values agree within 5 percent was used as an acceptance criteria.

3.6.3 Summary of Results

3.6.3.1 Conditional Probabilities and Initiating Event Frequencies

The first set of rows in Table 3.6-1 reproduces the first table in the FAVPost output. The second set of rows shows the corresponding SAS output. The means and ratios of means are identical for the conditional probabilities for the FAVOR and SAS values. The 99th percentiles for the FAVOR and SAS values differ by approximately 5 percent. The 95th percentiles between the FAVOR and SAS values show the largest differences, by a factor of 2.

Table 3.6-1 Conditional Probabilities of Crack Initiation and Vessel Failure for 10K Test Case

	Conditional probability of initiation CPI=P(I|E)			**Conditional probability of failure CPF=P(F|E)**			
Transient Number	Mean CPI	95th % CPI	99th % CPI	Mean CPF	95th % CPF	99th % CPF	Ratio = (CPFmean/ CPImean)
FAVOR output							
102	1.5849E-05	6.6485E-07	1.8549E-04	2.9033E-06	2.4324E-10	8.1642E-06	0.1832
103	1.2620E-04	1.3623E-04	1.9851E-03	3.2337E-05	2.3888E-05	4.5388E-04	0.2562
104	1.5849E-05	6.6485E-07	1.8549E-04	2.9035E-06	2.4324E-10	8.1642E-06	0.1832
105	1.2620E-04	1.3623E-04	1.9851E-03	3.2337E-05	2.3888E-05	4.5388E-04	0.2562
SAS output							
1 (#102)	1.5849E-05	1.3291E-06	1.8962E-04	2.9033E-06	4.8107E-10	8.1287E-06	0.1832
2 (#103)	1.2620E-04	2.7244E-04	2.0984E-03	3.2337E-05	4.7658E-05	4.8278E-04	0.2562
3 (#104)	1.5849E-05	1.3291E-06	1.8962E-04	2.9035E-06	4.8107E-10	8.1287E-06	0.1832
4 (#105)	1.2620E-04	2.7244E-04	2.0984E-03	3.2337E-05	4.7658E-05	4.8278E-04	0.2562
These results do not use the transient frequency distributions. They are calculated from the data from the 10,000 vessels simulated in FAVOR. The mean values are identical for SAS and FAVOR. In this example, the vessel responses under transients 102 and 104 are identical, and the vessel responses under transients 103 and 105 are identical.							

3.6.3.2 Histograms of Conditional Frequency of Crack Initiation and Vessel Failure

The team plotted the histograms from the FAVOR postprocessor in a spreadsheet and included similar data from the SAS sampling process. Figures 3.6-1 and 3.6-2 show the FAVOR and SAS values for the CFI and CFF for the distribution tails. The FAVOR and SAS curves converge closely as the cumulative distribution approaches 100 percent, but differ noticeably at 95 percent.

3.6.3.3 Descriptive Statistics for Frequency of Crack Initiation and Vessel Failure

Tables 3.6-2 and 3.6-3 show statistics, such as the mean, variance, and the upper tail, from the FAVOR and SAS computations for frequencies of initiation and failure, respectively. The tables include key FAVOR outputs along with the results from four SAS sampling runs. There is complete agreement between FAVOR and SAS for the probability that each frequency would be zero. The 5th percentile and medians do not appear in these two tables because they are all zero. As with the CFI and CFF histograms, the largest difference is for the 95th percentile.

Overall, the SAS and FAVOR outputs for the FAVPost module agree closely in nearly all cases. Since the primary results are outputs from sampling the transient frequency distributions, exact agreement is not expected. For both failure modes of crack initiation and vessel failure, the mean of the FAVOR conditional frequency is within the range of results from the four SAS sampling runs. The same statement applies to the other basic sampling statistics such as the variance estimates, skewness, and kurtosis. The probability of zero failures is identical for the SAS and FAVOR outputs. (See Ref. 12 for further discussion of the differences in SAS and FAVOR outputs.)

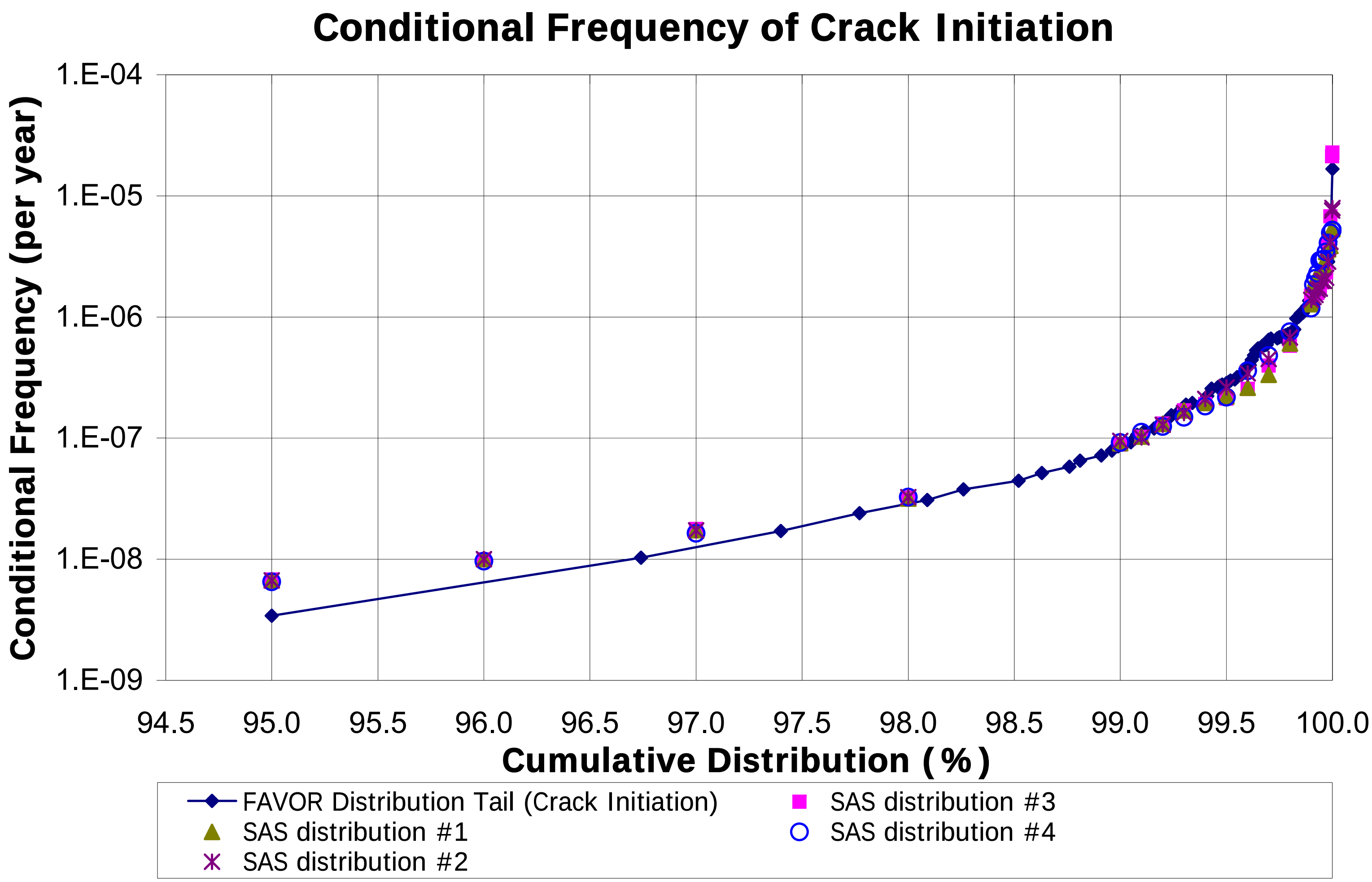

Figure 3.6-1 Comparison of SAS and FAVOR simulated outputs for upper tail of distribution of conditional frequency of crack initiation

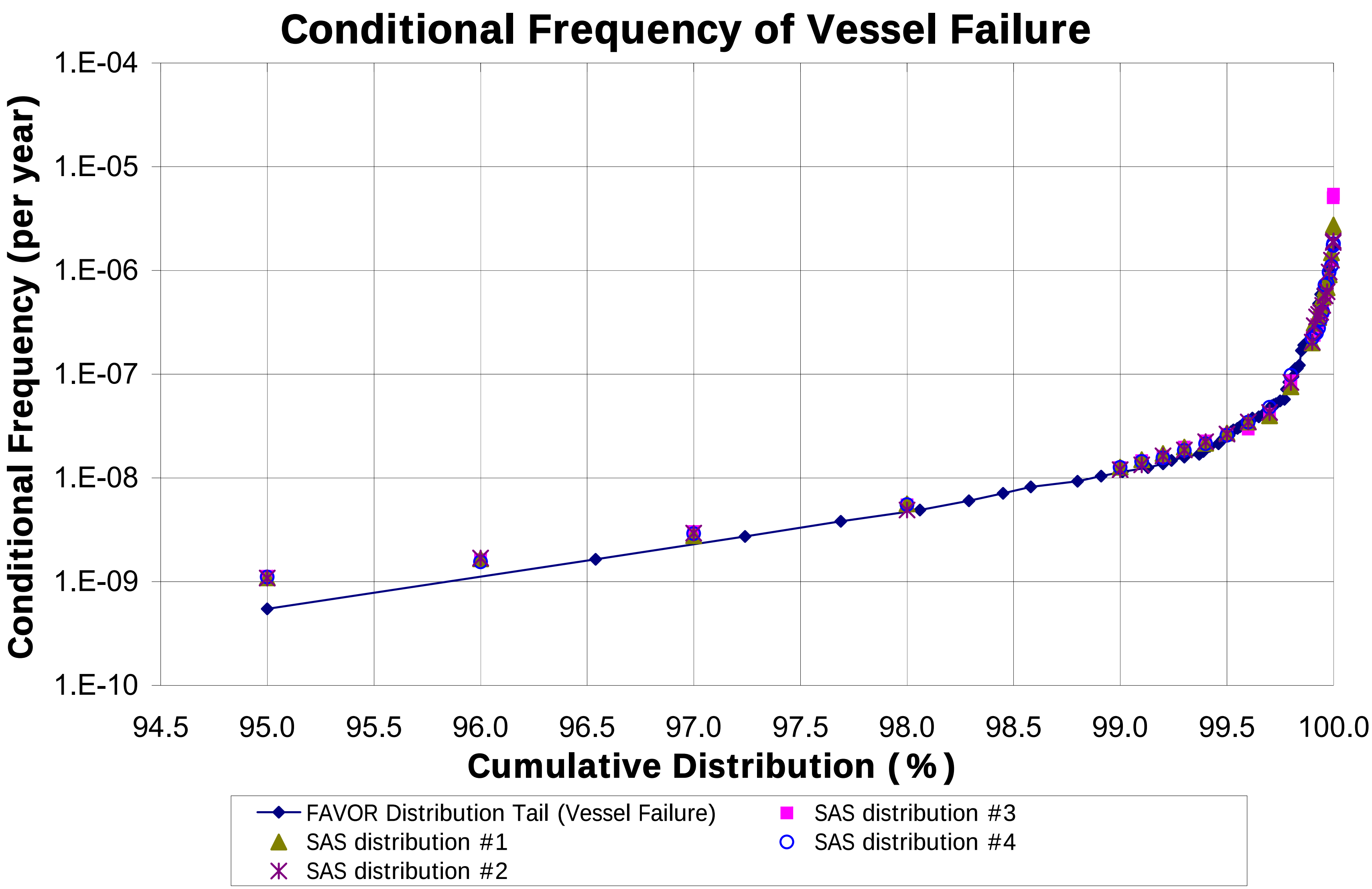

Figure 3.6-2 Comparison of SAS and FAVOR simulated outputs for upper tail of distribution of conditional frequency of vessel failure

Table 3.6-2 Statistics for Frequency of Crack Initiation

Statistics	FAVOR	SAS Runs				SAS Average
		SAS 1	SAS 2	SAS 3	SAS 4	
Minimum	0	0	0	0	0	0
Maximum	1.6724E-05	2.2807E-05	5.4573E-06	5.2172E-06	7.9371E-06	—
95.0th Percentile	3.4238E-09	6.8239E-09	6.6838E-09	6.5209E-09	6.6990E-09	—
99.0th Percentile	8.6737E-08	8.8313E-08	9.1243E-08	9.1892E-08	9.5078E-08	—
99.9th Percentile	1.3935E-06	1.5202E-06	1.5606E-06	1.5131E-06	1.4231E-06	—
Mean	**8.2935E-09**	8.6736E-09	6.8668E-09	7.5121E-09	7.1539E-09	**7.5516E-09**
Standard Deviation	1.8712E-07	2.4921E-07	1.0731E-07	1.1648E-07	1.1478E-07	7.9201E-08 (See Note a)
Standard Error	1.8712E-09	2.4921E-09	1.0731E-09	1.1648E-09	1.1478E-09	3.9601E-10
Variance (unbiased)	3.5012E-14	6.2102E-14	1.1514E-14	1.3566E-14	1.3173E-14	6.2722E-15
Variance (biased)	3.5009E-14	6.2108E-14	1.1516E-14	1.3567E-14	1.3174E-14	6.2728E-15
Moment Coeff. of Skewness	7.3711E+01	7.9349E+01	3.1783E+01	3.0713E+01	4.3263E+01	—
Pearson's 2nd Coeff. of Skewness	1.3297E-01	1.0441E-01	1.9197E-01	1.9348E-01	1.8698E-01	—
Kurtosis	6.4089E+03	7.0683E+03	1.2080E+03	1.1031E+03	2.5439E+03	—

a. For the SAS average, the standard deviation is the square root of the (biased) variance, the variances are the sums of the variances across the k = 4 runs, each divided by 16 (k^2), and a divisor of 200 (the square root of k, times the square root of 10,000) was used for the standard error.

Table 3.6-3 Statistics for Frequency of Vessel Failure

Statistics	FAVOR	SAS Runs				SAS Average
		SAS 1	SAS 2	SAS 3	SAS 4	
Minimum	0	0	0	0	0	0
Maximum	1.6332E-06	5.4380E-06	2.7414E-06	1.8117E-06	1.9310E-06	—
95.0th Percentile	5.4629E-10	1.1314E-09	1.0926E-09	1.1105E-09	1.0865E-09	—
99.0th Percentile	1.1363E-08	1.2612E-08	1.2900E-08	1.2632E-08	1.2033E-08	—
99.9th Percentile	2.6167E-07	2.3468E-07	2.5532E-07	2.3388E-07	2.4903E-07	—
Mean	**1.3284E-09**	1.6078E-09	1.4029E-09	1.2755E-09	1.2748E-09	**1.3903E-09**
Standard Deviation	2.7747E-08	5.7813E-08	3.5474E-08	2.7135E-08	2.8243E-08	1.9581E-08 (See Note a)
Standard Error	2.7747E-10	5.7813E-10	3.5474E-10	2.7135E-10	2.8243E-10	9.7905E-11
Variance (unbiased)	7.6990E-16	3.3420E-15	1.2583E-15	7.3624E-16	7.9760E-16	3.8338E-16
Variance (biased)	7.6982E-16	3.3423E-15	1.2584E-15	7.3632E-16	7.9768E-16	3.8342E-16
Moment Coeff.	3.9998E+01	8.4820E+01	5.7387E+01	4.5853E+01	4.7991E+01	—

Statistics	FAVOR	SAS Runs				SAS Average
		SAS 1	SAS 2	SAS 3	SAS 4	
of Skewness						
Pearson's 2nd Coeff. of Skewness	1.4363E-01	8.3432E-02	1.1864E-01	1.4102E-01	1.3541E-01	—
Kurtosis	1.8816E+03	7.8506E+03	3.9455E+03	2.5270E+03	2.7637E+03	—

a. For the SAS average, the standard deviation is the square root of the (biased) variance, the variances are the sums of the variances across the k = 4 runs, each divided by 16 (k^2), and a divisor of 200 (the square root of k, times the square root of 10,000) was used for the standard error.

3.7 Incremental V&V of Version 3.1 Code Task 2.2.4 (a)

The team developed, implemented, and obtained results using a test plan for validation of the unirradiated USE embrittlement parameter sampling in FAVOR Version 3.1 (Refs. 13, 14 and 15). The team based the test plan on the embrittlement sampling validation for version 2.4 of FAVOR (Tables A-5.1 through A-5.5 in Ref. 8).

3.7.1 Basic Approach

The team reviewed the sample input decks on the FAVOR Version 3.1 distribution compact disc to identify typical values for the USE parameter that could be added to the input decks of the 16 FAVOR input scenarios developed and executed (Ref. 11) for FAVOR Version 2.4. The review identified five runs as able to provide unique displays of the sampling of the USE parameter. The USE parameter sampling protocol from the FAVOR theory manual (Ref. 14) was implemented as an addition to the SAS Institute, Inc. (Ref. 20) program that mimics the FAVOR sampling processes for other embrittlement parameters. The SAS application also compares the resulting samples.

Using SAS, the team generated a USE sample size of 5 million for each run. The FAVOR sample size was taken to be an order of magnitude less (500,000), so that the SAS sample could be regarded as the theoretical distribution. The evaluation considered various combinations of sample sizes less than or equal to these limits. The results were similar even for sample sizes as small as 10,000 SAS values with 1,000 FAVOR values. The large sample sizes ensured that the mixtures of distributions generated would have some stability and smoothness.

Table 3.7-1 provides an overview of the five runs specified for testing the sampling of the USE parameter. The five runs consider the USE parameter at a nominal value (112 ft-lbf), a case with a higher mean (150 ft-lbf), a case with a higher standard deviation (achieved by making the USE mean small—4 ft-lbf), a five-subregion plate case (with specified mean USE values of 4, 84, 90, 112, and 150 ft-lbf), and the same five-subregion case with an unequal allocation among the subregions. Unirradiated USE is an embrittlement attribute of a subregion that is sampled in exactly the same manner for plates and welds.

For each of the five runs showing unique aspects of the USE sampling, the team generated density histogram plots that compare the outputs of the two processes. Percentage differences were evaluated for the mean, median, 90th percentile, 95th percentile, and 99th percentile of the SAS and FAVOR distributions. In addition, the following statistical tests comparing the distributions were considered for each pair of samples:

- a test for whether a statistical difference exists between the mean of the FAVOR sample and the corresponding mean of the SAS sample
- an evaluation of the K-S test to determine if the sample cumulative distribution function from FAVOR matches a continuous theoretical distribution function determined from the SAS sample
- an evaluation of the chi-squared test statistic (X^2) for each set of histograms

Table 3.7-1 Summary of FAVOR 3.1 USE Validation Runs

USE Run #	FAVOR Version 2.4 Run #	Run	Run Name	Subregion number and type	Weight of each subregion	Purpose of Run
1	5	Base case	*sssf_p*	1 plate	1	Observe sampling for baseline region unirradiated USE.
2	2	Higher mean	*sssf_hm*	1 weld	1	Observe embrittlement sampling for USE with a higher specified mean.
3	3	Lower mean (or higher standard deviation)	*sssf_hs*	1 weld	1	Observe embrittlement sampling for USE with a lower specified mean. Observe truncation at zero.
4	11	Single flaw among five plates	*mssf_5p*	5 plates	Equal	Observe mixing of USE distributions for five different regions.
5	12	Single flaw among five plates, with unequal weights	*mssf_5pa*	5 plates	Unequal	Observe effect of different weighting of regions.

3.7.2 Acceptance Criteria

Table 3.2-1 shows the acceptance criteria that include percentage differences less than 1 percent for the mean and median values and less than 5 percent for the higher percentiles.

3.7.3 Summary of Results

Table 3.7-2 provides a summary of the percentage difference results of the validation runs. The center column in the table shows USE percentage differences for the means and medians, while the column at the far right lists differences for the 90th, 95th, and 99th percentiles. Nearly all the values conform to the criteria specified in the test plan, with percentage differences less than 1 percent for the mean and median and less than 5 percent for the higher percentiles. The mean values for the run present the only exception, with the USE mean set at 4 ft-lbf. With both positive and negative values, the FAVOR sample mean is 4 ft-lbf. In the presence of truncation on the left, the aggregate mean from SAS is, of course, higher.

Table 3.7-2 Unirradiated USE Percentage Differences Based on 500,000 FAVOR Sample Values for Each Run

Run Name (from Test Plan)	# of plates	# of welds	# of flaws	Percentage difference for mean, followed by difference for median (see Note b)	Percentage difference for 90th percentile, followed by 95th, followed by 99th (see Note c)
sssf_p	1	0	1	-0.03|-0.03	-0.03| 0.04| 0.01
sssf_w_hm	0	1	1	0.00|-0.01	0.02|-0.00| 0.08
sssf_w_hs	0	1	1	-11.2|-0.05	-1.25|-0.96|-0.31
mssf_p05	5	0	1	-0.14| 0.00	-0.20|-0.19|-0.07
mssf_p05a	5	0	1	-0.11|-0.04	-0.23|-0.21|-0.23

a. To establish SAS reference distributions for evaluation of the FAVOR sampling, SAS samples of size 5,000,000 were used for each parameter for each run.

b. Each cell shows the percentage difference for the mean, followed by the percentage difference for the median. Percentage differences are calculated as the FAVOR value minus the SAS value, multiplied by 100, and divided by the SAS value. The single large difference is marked in bold.

c. Each cell shows the percentage difference for the 90th percentile, followed by the percentage difference for the 95th percentile and the percentage difference for the 99th percentile. All of the percentage differences are less than 0.4 percent in absolute value except for the high standard deviation (low mean) test case, where they are less than 1.5 percent.

For the case with a specified USE mean of 4 ft-lbf, percentage difference for mean is the largest (11.2 percent). Apparently, FAVOR does not ensure that the generated USE values are nonnegative. Of course, the specified mean for this run is much lower than the 80 to 130 ft-lbf values found in the FAVOR input decks. With the higher means, the probability of generating a negative value is extremely small. Adding the check to ensure nonnegative values would still improve the reliability of the sampling protocol. In the SAS mimic process, negative values were set equal to zero. The FAVOR algorithm should also ensure that the sampled standard deviation used in the calculation is greater than zero. The SAS process uses a rejection method, resampling if necessary until a positive standard deviation is obtained.

One other observation about FAVOR Version 3.1 that arose in the evaluation of the USE parameter sampling is whether the unirradiated USE is defined as an attribute of a major beltline region, as indicated in the theory manual (e.g., in Item 1 on page 43, Ref. 14), or is an attribute of a subregion. The mean values for this parameter are entered at the subregion level, indicating that the parameter could vary within a major region. The manual must clarify this issue. In the FAVOR runs performed for the validation, different major beltline region numbers were given for each subregion in the two multiple-subregion cases.

In summary, the FAVOR results agree with the SAS mimic process, except for the possibility of generating negative USE values and standard deviations. In addition, since the mean value for unirradiated USE is specified as an input and sampled in the FAVOR code at the subregion level, the FAVOR documentation that defines this parameter must explain how it could differ between subregions within a major beltline region.

In its response (Ref. 22), ORNL indicated the following:

- Future releases of FAVOR will eliminate the possibility of sampling negative values unirradiated USE. However, this issue is academic because the mean values and standard deviations for USE are such that negative values would probably never be sampled. It can easily be shown that this had no impact on any PTS analysis results generated as part of the PTS reevaluation program.

- In future releases of FAVOR, the theory and user manuals will provide further clarification regarding how USE can have different values for various subregions within the same major beltline region.

3.8 Incremental V&V of Version 3.1 Code Tasks 2.2.4 (b), (c), (d), (e), (f)

Validation testing (Ref. 17) under this task included the computational algorithms and procedures in the FAVOR Version 3.1 PFM module. The V&V effort covered five distinct computational sections, including (1) instantaneous conditional probability of initiation, (2) initiation and arrest toughness scaling factor, (3) vessel failure by plastic collapse or excessive nonductile flaw extension, (4) cleavage reinitiation and arrest, and (5) ductile flaw extension and stability. The V&V used procedures similar to those employed during V&V of FAVOR Version 2.4 (Ref. 13).

3.8.1 Basic Approach

The V&V team used the LOAD and PFM data files employed to test FAVOR Version 2.4 (see Section 2.2 of Ref. 5) to test version 3.1, but it modified the PFM data file to include the material unirradiated USE input for the ductile fracture analysis.

The team performed the validation testing by independently programming the PFM equations and evaluation procedure contained in Sections 3.3.3 through 3.3.14 and 4.5 of the FAVOR theory manual into a spreadsheet and comparing the results to the output from FAVOR. Because the FAVOR software does not write each variable that should be included in a V&V test, the team added write statements to the software to provide appropriate values for testing purposes. The team selected a transient, test vessel, and flaw size from the Monte Carlo sampling and performed deterministic calculations for that transient, vessel, and flaw. The calculations included the conditional probability of flaw extension, the flaw growth, arrest and failure predictions, and various intermediate variables needed to compute flaw extension and growth.

The FAVOR PFM output files TRACE and Flaw-Track aided the decisions for selecting vessels and flaws for V&V testing. These files list the vessels and flaws that have positive, nonzero conditional probabilities of initiation and failure, and summarize the propagation history (arrest, reinitiation, and failure by either nonductile cleavage or ductile tearing instability) for the vessels and flaws.

3.8.2 Acceptance Criteria

The values computed by FAVOR were considered acceptable if the difference between the FAVOR and the expected test values was 1 percent or less.

3.8.3 Summary of Results

The conclusions and recommendations from this validation testing (Ref. 17) follow, with ORNL responses noted:

- FAVOR accurately predicts the instantaneous conditional probability of initiation, cpi(t)(i,j,k), for a specified transient, i, vessel, j, flaw, k, and time step, t.

- FAVOR accurately predicts the conditional probability of initiation, CPI(i,j,k), for a specified transient, i, vessel, j, and flaw, k.

- FAVOR accurately calculates the conditional probabilities of initiation and failure, CPI(i,j) and CPF (i,j), for a specified transient, i, and vessel, j, with multiple flaws, as defined in Sections 3.3.9 and 3.3.10 of the theory manual (Ref. 14).

- The theory manual should specify that values for $\sigma_{\ln(KIa)}$ and $\mu_{\ln(KIa)}$ in the equation for $\Phi_{KI\text{-}initiation}$ on page 54 of the theory manual (Ref. 14) are calculated for the initiation location, while the values for $\sigma_{\ln(KIa)}$ and $\mu_{\ln(KIa)}$ used in the equation for K_{Ia} shown on page 55 of the theory manual are calculated for the flaw location being evaluated.

In response, ORNL stated that future releases of FAVOR theory manual will provide the requested clarification.

- ORNL should explain why the ΔRT_{NDT} for a flaw at one mesh location appears to be determined from ΔT_{30} for a flaw at the next larger mesh location. Clarify the reason for this occurrence or confirm that the software is intended to operate in this manner.

In response, ORNL stated that FAVOR has an option (TRACE) to print out detailed data as the flaw propagates through the wall. The data in Tables 5-A and 5-B, generated using the trace option and reproduced below, illustrate that the ΔRT_{NDT} at each mesh point is correctly calculated from the ΔT_{30} at the same mesh point. ORNL provided an example for weld and plate material. It added write statements to FAVOR Version 3.1 to generate these data. ORNL suspects that there was an inconsistency in the placement of the write statement(s) or in the interpretation of the data generated by those write statements for ΔT_{30}.

ORNL Table 5-A Example of Through-Wall Data Taken from FAVOR-Generated File for Plate Material

Flaw position (i)	Flaw depth (inch)	ΔT_{30} (F)	ΔRT_{NDT} (F)	$(\Delta RT_{NDT})_i/(\Delta T_{30})_i$
6	0.482	280.25	308.28	1.10
8	0.643	277.70	305.47	1.10
10	0.804	275.19	302.71	1.10
12	0.964	272.72	300.00	1.10
14	1.125	270.30	297.33	1.10
16	1.286	267.92	294.71	1.10
18	1.446	265.58	292.13	1.10
20	1.607	263.27	289.60	1.10
22	1.768	261.01	287.11	1.10
24	1.929	258.79	284.67	1.10
26	2.259	254.33	279.77	1.10
28	2.759	247.88	272.67	1.10
30	3.259	241.76	265.94	1.10

ORNL Table 5-B Example of Through-Wall Data Taken from FAVOR-Generated File for Weld Material

Flaw position (i)	Flaw depth (inch)	ΔT_{30} (F)	ΔRT_{NDT} (F)	$(\Delta RT_{NDT})_i/(\Delta T_{30})_i$
5	0.431	190.54	188.63	0.99
7	0.604	189.54	187.64	0.99
9	0.776	188.53	186.64	0.99
11	0.949	187.52	185.64	0.99
13	1.121	186.50	184.63	0.99
15	1.294	185.48	183.62	0.99

- The theory manual and software provide different equations for membrane stress. ORNL must change either the software or theory manual to incorporate the desired computational algorithm for membrane stress.

In response, ORNL noted that the equations for membrane stress in the theory manual and the software are indeed different. The application of the membrane stress (to determine if a cracked vessel has failed because of ligament instability) in the software is used in an expression that is equivalent to the expression in the theory manual. In the manual, the equation for membrane stress is

$$\sigma_m(t) = \frac{p_i(\tau)\left(R_i + a\right)}{\beta\left(R_o - R_i - a\right)}; \quad \beta = \begin{cases} 1 & \text{hoop stress} \\ 2 & \text{axial stress} \end{cases},$$

where $p_i(\tau)$ is the time-dependent internal pressure, R_i and R_o are the inner and outer vessel radii, respectively, and a is the current flaw depth. However, the membrane stress is identical in the software, except that the denominator does not include the flaw depth a.

The manual specifies a check to determine if the above membrane stress is greater than the flow stress. On the other hand, the software provides a check to determine if the membrane stress (without the flaw depth term a in the denominator) is greater than the flow stress multiplied by (1 – (a/(Ro – Ri))). A simple algebraic manipulation (i.e., to move the common denominator to the side of equation containing the product of flow stress and the above multiplier) illustrates that the checks (for failure because of ligament instability) in the theory manual and software produce the identical result.

For clarity, future releases of the FAVOR code will have equations identical to those in the theory manual used to check for ligament instability.)

- The multiplier, 0.019, in the equation for m on page 45 of the theory manual is incorrect and should be changed to 0.0019.

In response, ORNL agreed to correct future releases of the FAVOR theory manual.

- The meaning, application, and computational procedure for J_R^* in steps D1 and D3 are not clear, and ORNL should revise the theory manual to better explain the meaning and application of J_R^*. The relationship for Δa in the second equation in step D4 of the theory manual (Ref. 14) is not the value used to compute T_R from the fourth equation in step D4. ORNL should modify the theory manual to better explain the crack extension value used to calculate T_R.

In response, ORNL agreed to provide further clarification on the meaning, application, and computational procedure for J_R^* in steps D1 and D3 in future releases of the FAVOR theory manual. J_R^* is the value of $J_{applied}$ corresponding to a previous time step at which a stable ductile tear occurred. For a ductile tear to occur at the current time, it is necessary for $J_{applied}$ to be equal to or greater than J_R^*.

Regarding the relationship for Δa in the second equation in step D4 of the FAVOR theory manual, ORNL noted that FAVOR has a through-wall mesh of discrete points at which values of $K_I(t)$ and $T(t)$ have been calculated. The flaw is propagated through the wall along these mesh points (i.e., flaw growth is always from one mesh point to another mesh point). In this case, the equations in the theory manual predict a ductile flaw extension of 0.0638 in.; however, FAVOR propagated the flaw to the next mesh point, which was a distance of 0.25 in. This accounts for the observed differences in Δa and T_R.

ORNL maintained that step D4 of the ductile tearing submodel (page 59 of FAVOR theory manual) currently (and sufficiently) states the following:

The IGA Propagation submodel is searched to find the closest node n to the current flaw position. The flaw is then repositioned to this node point. Based on this new position of the flaw, the applied tearing modulus is estimated from a second-order finite-difference ratio.

- Results from one of the tested flaw growth trials for vessel 43, flaw 9, and transient 1 at 9 minutes indicate that the flaw initiated, grew to 6.9065 in. (175.4 mm), arrested, and subsequently had neither ductile tearing nor cleavage reinitiation. In this instance, the node points associated with the J values for the ductile fracture calculation were nominally 4.5 in, (114.3 mm) rather than 6.9 in. (175.4 mm) for the indicated flaw depth. ORNL should investigate and correct the discrepancy between the arrested flaw position and position of the node points for the ductile fracture analysis.

In response, ORNL reconstructed and investigated this case using a through-wall analysis trial to determine if an initiated flaw propagates through the wall to failure. It uncovered a programming logic error that was not properly accounting for the unique case of a stable ductile tear such that the crack tip location exceeded the user-specified wall depth corresponding to the failure criteria but was less than the total wall thickness. In some cases, this flaw could eventually have a stable arrest when it should have been counted as a failure.

ORNL corrected the FAVPFM code such that a stable tear that exceeds the wall-depth failure criteria is considered an unstable ductile tear and results in failure. It performed some PFM analyses with the corrected code to determine the impact of this error on the analysis results. The results of these analyses verified that the impact of this error on the integrated analysis results was very small (i.e., 1 percent or less). ORNL will correct this error in future releases of FAVOR.

- When evaluating flaws along the weld fusion line, FAVOR uses the limiting embrittlement properties of adjacent plates and welds to determine the weld fracture toughness as described in Section 3.3.3 of the theory manual. ORNL should revise Section 3.3.3 of the theory manual to state that the weld chemistry resampling procedure is maintained when the plate embrittlement properties are used to define weld fracture toughness.

In response, ORNL noted that future releases of the FAVOR theory manual will provide this clarification.

- FAVOR accurately implements the warm prestressing strategy described in Section 3.3.4 of the theory manual.

3.9 <u>Incremental V&V of Version 3.1 Code Task 2.2.4 (g)</u>

The V&V team tested several sampled embrittlement related variables used in the PFM analysis, including (1) irradiation induced shift in T30 (i.e., ΔT30), (2) irradiated flow stress, (3) unirradiated and irradiated USE, (4) RT_{PTS} (i.e., the value of RT_{NDT} at the vessel inner surface as defined in 10 CFR 50.61), and (5) the current delta probability of flaw initiation (CDCPI) and current delta conditional probability of vessel failure (CDCPF) from the transient time distribution report.

3.9.1 Basic Approach

Testing of the sampled embrittlement related variables involved independently generating variable distributions and comparing the results with values from FAVOR at various locations within the distributions (e.g., 5th percentile, 50th percentile, 95th percentile).

3.9.2 Acceptance Criteria

The values computed by FAVOR were considered acceptable if the difference between the FAVOR and test values are as specified in Appendix A to EPRI 1010953 (Ref. 17).

3.9.3 Summary of Results

The conclusions and recommendations from this validation testing follow (see also the detailed results in Ref. 17):

- The combined sampling for the uncertainties in the calculation of DT30 and irradiated flow stress in version 3.1 of the FAVPFM module has been independently verified to produce results of acceptable accuracy per the requirements of Sections A-9 and A-10 of the incremental V&V test plan (i.e., an acceptable accuracy is agreement in the independently calculated values (e.g., the 5th, 50th, and 95th percentile values) within 5 percent).

- The sampling for the uncertainties in the calculation of initial and irradiated USE in version 3.1 of the FAVPFM Module has been independently verified to produce results of acceptable accuracy per the requirements of Section A-7 of the incremental V&V test plan (i.e., an acceptable accuracy is agreement in the independently calculated values (e.g., the 5th, 50th, and 95th percentile values) within 5 percent).

- The deterministic calculations of maximum RT_{PTS} for each type of region in version 3.1 of the FAVPFM module have been independently verified to produce results of acceptable accuracy per the requirements of Section A-8 of the incremental V&V test plan for embrittlement shift option 992 (Regulatory Guide 1.99, Revision 2 [Ref. 23]) (i.e., an acceptable accuracy is agreement of the calculated values within 5 percent).

- For representative RPV load and PFM input for several dominant PTS transient sequences, the V&V team confirmed that the percentages of total CDCPI and CDCPF with time step that are given in the transient time distribution report for FAVOR Version 3.1 are accurately calculated per the requirements of Section A-11 of the incremental V&V test plan (i.e., an acceptable accuracy is agreement of the calculated probabilities within 1 percent).

- ORNL should correct Section 4.2.1 of the FAVOR Version 3.1 theory manual (Ref. 14) to state that ΔRT_{PTS} for the 993 shift option is calculated by ΔRT_{NDT} of Equation 75 instead of ΔT_{30} of Equation 74. As a result, the FAVOR Version 3.1 calculated results would be of acceptable accuracy per the requirements of Section A-8 of the incremental V&V test plan (i.e., an acceptable accuracy is agreement of the calculated values within 5 percent).

- ORNL should revise Section 3.3.3 of the theory manual to state that the weld chemistry resampling procedure is maintained when the plate embrittlement properties are used to define weld fracture toughness.

- ORNL should modify the theory manual to better explain the crack extension value used to calculate T_R in step D4.

- ORNL should revise the theory manual to better explain the meaning and application of J_R^* in steps D1 and D3.

4. CONCLUDING REMARKS

Based on the validation tests and reported results for FAVOR Versions 2.4 and 3.1, the NRC concludes that the as-built software in version 3.1 meets the requirements stated in the theory manual and the user's guide with a reasonable confidence in the accuracy of the FAVOR-generated results. FAVOR Versions 2.4 and 3.1 satisfy the acceptance criteria for most of the validation tests. For the test cases where the code does not satisfy the acceptance criteria, ORNL provided explanations for the consequences of the differences in the results.

5. REFERENCES

1. 10 CFR 50.61, “Fracture tough new requirements for protection against pressurized thermal stock events”, Title 10 of the Code of Federal Regulations Part 50, Section 61, U.S. Government Printing Office, Washington, 2004.

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APPENDIX A: COMMENTS AND REPLIES FOR REFERENCE 13

This appendix provides the V&V team comments, followed by the ORNL and PNNL response to each comment.

A.1 Conclusions

(1) The combined sampling for the uncertainties in the initial value and epistemic shift in the calculation of initial RT_{NDT} in Version 02.4 of the FAVPFM Module has been independently verified to produce results of acceptable accuracy per the requirements of Item (II c) of the Test Plan.

ORNL response: No action required.

(2) The sampling for the uncertainties in the ΔRT_{ARREST} and K_{Ia} in the calculation of arrest toughness in Version 02.4 of the FAVPFM Module has been independently verified to produce results of acceptable accuracy per the requirements of Items (II-c) and (II-i) of the Test Plan.

ORNL response: No action required.

(3) The deterministic calculations of maximum RT_{PTS} for each region in Version 02.4 of the FAVPFM Module have been independently verified to produce results of acceptable accuracy per the requirements of Item (II-d) of the Test Plan. The verification included both types of embrittlement shift options (992 and 993) for plate weld and forging materials.

ORNL response: No action required.

(4) The combined sampling for the uncertainties in three chemistry values and fluence in the calculation of RT_{NDT} shift in Version 02.4 of the FAVPFM Module has been independently verified to produce results of acceptable accuracy per the requirements of Item (II-e) of the Test Plan.

ORNL response: No action required.

(5) The best-estimate calculations of flaw distribution parameters (density and aspect-ratio percentages) with flaw depth in the March 2002 version of the PNNL Vessel-Flaw Code have been independently verified to produce results of acceptable accuracy per the requirements of Item (II-1-2) of the Test Plan. The verification included two data sources (Shoreham and PVRUF), two flaw size categories, three types of flaws (weld, plate, surface), four types of welds (SAW, SMAW, Repair, and Composite) and both one and two layers of cladding.

ORNL response: No action required.

(6) The sampling of uncertainties in flaw density, aspect-ratio percentages and flaw depth in the March 2002 version of the PNNL Vessel-Flaw Code have been independently verified to produce results of acceptable accuracy per the requirements of Item (II-1-2) of the Test Plan. The verification included two data sources (Shoreham and PVRUF), two flaw size categories and two types of welds (SAW and SMAW).

ORNL response: No action required.

(7) Independent calculations by Sartrex and ORNL using the same PFM source code, PFM and load input files, and compiler version, but different versions of Windows 2000, gave different results for individual vessels and flaws. There is an apparent operating system dependency.

ORNL response: ORNL has not been provided sufficient information to evaluate this assertion. For example, we would want to know whether the different versions of Windows referred to above produce significantly different converged solutions. Our approach would be to test the program for convergence on different versions of Windows. Although the Windows 2000 operating system has been tested at ORNL, the following text appears in Section 1.4 of the FAVOR User's Guide:

> **The recommended computer for execution of FAVOR, v03.1, is a Pentium III or IV (or equivalent) with the Windows XP Professional operating system and 1024 Mbytes of RAM. The installation requires approximately 165 Mbytes of free disk space for executables, documentation, source code, and example input files.**

All three FAVOR modules make use of dynamic memory management where the required internal memory is calculated based on the size of the problem and then allocated from the global heap memory at run time; therefore, the only limitation on the number of thermal hydraulic transients, RPV trials, or subregions employed in the model is the memory capacity of the computer being used. For all of the models tested by the developers to date, 1024 MB of RAM was sufficient to run FAVOR; however, be advised that larger models in the future may require more memory. In addition, some problems have been encountered when running large cases (e.g., 20,000 subregions with 30 transients) on a PC with Windows 2000 Professional and 512 Mbytes of RAM. Windows XP (with the latest Service Pack installed) is the recommended operating system."

All calculations carried out to date at ORNL for the PTS Re-Evaluation Study have been performed on a PC with the Windows XP Professional operating system.

(8) The results indicated very good agreement between the FAVOR calculations related to cpi and the independent calculations obtained from the V&V testing. In general, the difference was 0.01% or less for most variables. Even though there were only very small differences in most variables leading up to the computation of cpi, the difference between the computed values for cpi varied from 0.5% to 2%.

ORNL response: No action required.

(9) The value of *cpi* was found to be quite sensitive to differences in ΔT_{30}, and the values used in computing ΔT_{30}, and difference is calculated *cpi* could result from round-off error.

ORNL response: It is not made clear in this statement just how different are calculated values of cpi. Again, it would be helpful to have more information concerning the basis of this observation. It can be noted here that FAVOR utilizes

double-precision arithmetic for calculations. Based on the draft results (Ref. 2), it appears that FAVOR ver 3.1 resolves this comment.

(10) According to the theory manual the probability that a flaw will initiate is determined by Equation 94. However, the FAVOR software limits use of Equation 94 to conditions where K_I > the Weibull parameter a_k. If this condition is not satisfied then the probability of initiation is set equal to zero. This restriction on the use of Equation 94 is not stated in the theory manual.

ORNL response: This issue has been addressed in the latest version of the Theory Manual, v03.1. It is understood that a Weibull distribution, as a lower-bounded continuous statistical distribution, has a lower limit (referred to in the Theory Manual as the location parameter, a_{KIc}) such that any value below the location parameter has a zero probability of occurrence associated with it. For clarity, the updated Theory Manual has been modified to reflect that the applied K_I must be greater than the Weibull K_{Ic} location parameter, a_{KIc}, to have a non-zero probability of crack initiation. Figure 11 in Sect. 3.3.7 has been revised along with the discussion of Fig. 11. Equations (7) and (9) in Sect. 3.3.7, Eq. (87) in Sect. 4.2.7 (Eq. (68) in ver. 2.4), **and Eq. (114) of Step 7 of Sect. 4.5** (Eq. (94) in Step 7 of Sect. 4.5 in ver. 2.4) **have also been revised to reflect the above comment.**

(11) The results for comparison of ΔT_{30} for the initiation flaw depth and several subsequent depths in the first weld layer indicate that the FAVOR ΔT_{30} value is significantly different from the test value for the first depth following initiation, and is in error.

ORNL response: This issue derives from one of the two bugs that were found recently in FAVOR; both bugs have been repaired.

(12) The ΔRT_{NDT} from the FAVOR and test calculations are in good agreement. However, because there can be errors in ΔT_{30}, and ΔRT_{NDT} is the product of a constant and ΔT_{30}, there appears to be a mismatch in the manner in which FAVOR obtains ΔRT_{NDT} relative to ΔT_{30}.

ORNL response: See the response to item 11 above—both bugs have been repaired.

(13) Additional testing was performed to assess the FAVOR computational accuracy for flaw depths beyond the first weld layer. The results show that FAVOR indicates the correct weld layer, selects the appropriate random number, and generally generates accurate results, except for possibly ΔT_{30}.

ORNL response: No action required (also, see response to item 11).

(14) Favor was tested to assess its ability to accurately predict vessel failure for a weld. The results of this test indicate FAVOR correctly moved through the four weld layers, re-sampled the residual element contents, selected the appropriate random numbers, and predicted vessel failure.

ORNL response: No action required.

(15) Testing showed that FAVOR accurately calculates *CPI* and *CPF* for multiple flaws in accordance with the specifications in Section 3.3.10 of the theory manual.

ORNL response: No action required.

(16) Testing indicated that changing the *Cu*, *Ni*, *P* contents and initial RT_{NDT} of the plates and weld materials so the plates were limiting relative to the adjacent welds also changed the location of a specified flaw in a vessel. It is not clear from the theory manual that it is the intent for the flaw position to change based on changes in residual element content or initial RT_{NDT} alone.

ORNL response: This problem was fixed when repairs were made to FAVOR ver. 02.4.

(17) Based on observed abnormal changes in calculated the ΔT_{30} values in limiting plates FAVOR may not implementing correctly the weld fusion line calculation described in Section 3.3.3 of the theory manual (Ref. 2).

ORNL response: This problem was fixed when repairs were made to FAVOR ver. 02.4.

(18) There is some indication that the appropriate arrest toughness is not selected in Step P7 of the propagation model.

ORNL response: More detail is required to address this comment. Step P7 of the Initiation-Growth-Arrest (IGA) Submodel states the following:

Step P7. Check the current applied K_I for the advancing flaw against the current value of the arrest fracture toughness K_{Ia}.

if $K_1 < K_{1a}$ then

the flaw has arrested

proceed to Step P8

else

the flaw has not arrested

proceed to Step P2

Where, the value of K_{Ia} is calculated in Step P6.

(19) V&V test results indicate that FAVOR correctly implements the warm pre-stress methodology in Section 3.3.4 of the theory manual.

ORNL response: No action required.

A.2 Recommendations

(1) The April 2003 version of the documentation (PNNL-14268 Report) for the Vessel-Flaw code should be reviewed to ensure that the discrepancies in reported values for the distribution parameters in the March 2002 documentation were corrected.

PNNL response: The issue is with the documentation as issued in March 2002. The 2003 report (Ref. 5) has corrected the problem.

(2) The theory manual should be revised to indicate that Equation 94 is applicable when K_I > the Weibull parameter ak, and if this condition is not satisfied then the probability of initiation is set equal to zero.

ORNL response: This has been done.

(3) The software should be reviewed to ensure the ΔT30 computation is performed correctly subsequent to flaw initiation.

ORNL response: This has been done.

(4) The software should be reviewed to ensure that the algorithms for placing and evaluating flaws along the weld fusion line are operating correctly.

ORNL response: ORNL has performed such a review and is satisfied things are working correctly.

(5) The software should be reviewed to ensure that the appropriate arrest toughness is being selected in Step P7.

ORNL response: ORNL has performed such a review and is satisfied things are working correctly.

(6) The software should be reviewed to determine what effect, if any, there is on the accuracy of the CPI and CPF relative to operating system dependence.

ORNL response: Our approach would be to test the program for convergence on different versions of Windows.

(7) A software design assessment should be made to determine if it is the intent that flaw location in a specified vessel can change based on changes in residual element content or initial RT_{NDT} alone.

ORNL response: This problem was fixed when repairs were made to FAVOR ver. 02.4.

A.3 <u>List of References</u>

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11. ABSTRACT *(200 words or less)*

During plant operation, the walls of reactor pressure vessels (RPVs) are exposed to neutron radiation, resulting in localized embrittlement of the vessel steel and weld materials in the core area. If an embrittled RPV had an existing flaw of critical size and certain severe system transients were to occur, the flaw could very rapidly propagate through the vessel, resulting in a through-wall crack and challenging the integrity of the RPV. The severe transients of concern, known as pressurized thermal shock (PTS), are characterized by a rapid cooling (i.e., thermal shock) of the internal RPV surface in combination with repressurization of the RPV. Advancements in our understanding and knowledge of materials behavior, our ability to realistically model plant systems and operational characteristics, and our ability to better evaluate PTS transients to estimate loads on vessel walls led the U.S. Nuclear Regulatory Commission (NRC) to realize that the earlier analysis, conducted in the course of developing the PTS Rule (10CFR50.61) in the 1980s, contained significant conservatisms.

This report, which describes a summary of verification and validation (V&V) of the probabilistic fracture mechanics models in the Fracture Analysis of Vessels-Oak Ridge (FAVOR) code, is one of a series of 21 other documents detailing the results of the NRC study. The V&V involved assuring that the as-built software meets the requirements specified in the theory manual and the user's guide. The V&V activity involved development of test plans, test procedures, acceptance criteria for comparing the FAVOR-generated results with independent calculations, and test reports. The V&V team checked individual computational relationships for programming accuracy, but this V&V effort did not generally include a comprehensive, code line-by-line walkthrough. Based on the validation tests performed and reported results, the Nuclear Regulatory Commission concludes that the as-built software in version 3.1 of the code meets the requirements stated in the theory manual and the user's guide with reasonable confidence in the accuracy of the FAVOR-generated results.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

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