



FAVOR v20.1.12 Software Requirements Document

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Prepared in response to Subtask 1.2 of task order 31310020D0005 / 31310020F0103 entitled FAVOR, REAP, and RPV Analysis by:

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Project Summary

Project Name	Subtask 1.2: Software Requirements Document
Project Number	Subtask 1.2 of task order 31310020D0005 / 31310020F0103
Internal Project Organization	NRC/RES/DE/CIB

Revision History

Revision	Date	Comments
0	09/01/2021	Original

Signatures

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Acronyms and Abbreviations

This section provides abbreviations and acronyms specific to this plan and software project.

ASME	American Society of Mechanical Engineers
BWR	Boiling Water Reactor
CM	Configuration Management
CMMP	Configuration Management & Maintenance Plan
COTS	Commercial Off-The-Shelf
IDE	Integrated Development Environment
NRC	United States Nuclear Regulatory Commission
NQA-1	Nuclear Quality Assurance - 1
PM	Project Manager
PMP	Project Management Plan
PWR	Pressurized Water Reactor
QA	Quality Assurance
SDD	Software Design Document
SOW	Statement of Work
SQA	Software Quality Assurance
SQAP	Software Quality Assurance Plan
SQE	Software Quality Engineer
SRD	Software Requirements Document
STP	Software Test Plan

STRR	Software Test Results Report
SVVP	Software Verification and Validation Plan
SVVR	Software Verification and Validation Report
V&V	Verification and Validation

Definitions

This section provides definitions specific to this plan and software project.

Assessment	A review, evaluation, inspection, test, check, surveillance, or audit to determine and document whether items, processes, systems, or services meet specified requirements and perform effectively. (NQA-1-2015)
Acceptance Testing	The process of exercising or evaluating a system or system component by manual or automated means to ensure that it satisfies the specific requirements and to identify differences between expected and actual results in the operating environment. (NQA-1)
Baseline	A specification or product that has been formally reviewed and agreed upon, that thereafter serves as the basis for use and further development, and that can be changed only by using an approved control process. (NQA-1)
Configuration Item	A collection of hardware or software elements treated as unit for the purpose of configuration control. (NQA-1)
Configuration Management (Software)	The process of identifying and defining the configuration items in a system (i.e., software and hardware), controlling the release and change of those items throughout the system's life cycle, and recording and reporting the status of configuration items and change requests. (NQA-1)
Contractor	The organization or organizations contracted by the NRC to work on the FAVOR project.
Error	A condition deviating from an established baseline, including deviations from the current approved computer program and its baseline requirements. (NQA-1)
Graded Approach	The process of ensuring that the level of analysis, documentation, and actions used to comply with a requirement is commensurate with: <ol style="list-style-type: none"> 1) relative importance to safety, safeguards, and security, 2) magnitude of any hazard involved, 3) the life-cycle stage of a facility or item, 4) programmatic mission of a facility, 5) characteristics of a facility or item, 6) relative importance of radiological and non-radiological hazards, and 7) any other relevant factors (NQA-1)

Independent Reviewer/Tester	Person sufficiently independent with respect to the material/product they are reviewing/testing, who did not perform the work they are reviewing or testing, and who also possess enough subject matter expertise to adequately review/test/evaluate.
Module	A program unit that is discrete and identifiable with respect to compiling; combining with other units, and loading; a logically separable part of a program that can be verified independently and performs a specific limited function, such as modeling physical phenomena, handling user input, output, data storage, etc.; contained, cohesive parts that can be combined to create the final product.
Nonconformance	A deficiency in characteristic, documentation, or procedure that renders the software quality of FAVOR to be unacceptable or indeterminate.
Operating Environment	A collection of software, firmware, and hardware elements that provide for the execution of computer programs. (NQA-1)
Regression Testing	Selective re-testing of a system or component to verify that modifications have not caused unintended effects and that the system or component still complies with its specified requirements.
Software Design Document	A document that describes the design of a system or component. Typical contents include system or component architecture, control logic, data structures, input/output formats, interface descriptions, theoretical bases, embodied mathematical models, control flow, and subroutines used in the software, and the allowed or prescribed ranges for data inputs and outputs in a manner that can be implemented. Currently described in the FAVOR Theory Manual [1].
Software Design Verification	The process of determining if the product of the software design activity fulfills the software design requirements. (NQA-1)
Software Requirements Document	Documentation of the essential requirements (functional performance, design constraints, and attributes (including acceptance criteria)) of the software and its external interfaces.
Software Verification and Validation Plan (SVVP)	A comprehensive, project-level plan which is a roadmap document that describes the elements, processes, and sequence of actions to ensure that the software properly fulfills its intended use as identified in the Software Requirements Document and Software Design Description Document. These actions may include peer reviews, audits, walkthroughs, analyses, architecture evaluations, simulations, testing, and demonstrations.

Test Case	A set of test inputs, execution conditions, and expected results developed for an objective, such as to exercise a program path or to verify compliance with a specific requirement. (NQA-1)
Test Plan	A document that describes the approach to be followed for testing a system or component. Typical contents identify items to be tested, tasks to be performed, and responsibilities for the testing activities. (NQA-1)
Validation	The process of evaluating software to determine whether it satisfies specified requirements, by comparing code predictions to experimental data or independent benchmark standards. Specifically, per the IEEE Std 730™-2014 standard (Reference [2]), the process of providing evidence that the system, software, or hardware and its associated products satisfy requirements allocated to it at the end of each life cycle activity, solve the right problem (e.g., correctly model physical laws and use the proper system assumptions), and satisfy intended use and user needs.
Verification	Mathematical proof of the correctness of algorithms, by confirming that code subroutines and functions produce the expected numerical output as the software goes through each life cycle activity. As Noted in IEEE Std 730™-2014 standard (Reference [2]), “Verified” designates the corresponding status. In design and development, verification includes examining the result of a given activity to determine conformity with the stated requirement for that activity. A system may be verified to meet the stated requirements yet be unsuitable for operation by the actual users.
Unit Test	Process or code developed to test the numeric accuracy and functionality of new or modified subroutines and functions.
Unit Test Suite	Set of unit tests created while developing and maintaining FAVOR.
Verification Test Suite	Set of input files that exercise all the code options, used to verify that code changes do not negatively impact code performance, and that results are as expected.
Validation Test Suite	Set of input files used to validate the codes’ predictions against experimental measurements or independent benchmark standards, to quantify the accuracy, bias, and uncertainty of code predictions.

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1 Purpose, Scope, and Applicability

The purpose is to document the Software Requirements of v20.1.12 of FAVOR. Although this specific work was not done under a qualified SQA program, this document is intended to meet the content and intent of such a program. This document includes the Software Requirements Document (SRD) for FAVLoad, FAVPFM, and FAVPost, including implementing the modernization changes. The software requirements are defined herein for changes to the base version of the FAVOR code v16.1, as distributed by the NRC.

Consistent with the FAVOR Software Quality Assurance Plan (Reference [3]) , the SRD covers the impacted FAVOR function, user input requirements, other data sources, output requirements, interfaces (including any user interactions the software will require), performance requirements, installation considerations, design inputs, and any design constraints for a given module, including operating system, or portability between multiple platforms, as applicable. Applicable references, specifications, codes, standards, regulations, procedures, or instructions are identified that establish software requirements, as well as test, inspection, and acceptance criteria. Acceptance criteria may include a quantification of specified acceptable error range in percent, or a quantitative basis for each required output or feature to be evaluated. Finally, the SRD addresses technical and software engineering requirements, including safety and security features (e.g., vulnerability protection, and cyber-security) for the FAVOR deliverable product. The Software Requirements Description Criteria Form FAVOR-SQA-3 from the FAVOR SQA plan is used as an aide in developing this SRD.

2 Code Design

Due to the history of FAVLoad, FAVPFM, and FAVPost, existing software design is referenced from the code description documents in the FAVOR Theory and User Manual (Reference [1] and [4]). FAVLoad, FAVPFM, and FAVPost are written in Fortran and should remain that way for new development. For the as-found flaw version of FAVOR, the code design is based on the following:

- The FAVLoad, FAVPFM, and FAVPost codes are written in Fortran and compiled for execution on a Microsoft® Windows PC, a Mac OS system, and an Ubuntu Linux system.
- The Software Requirements Document shall detail the requirements for the new FAVOR software version being released.
- The Software Design Document details how the software shall be structured to satisfy the software requirements.
- An input generator is distributed as a Microsoft® Excel file.
- Separate source codes and executables (FAVLoad, FAVPFM, FAVPost) are produced.
- Executables shall be distributed with each release of the code.

New design features are described in the next revision of the FAVOR Theory and or User's Manual, as applicable.

3 Reference Documents

The following documents were utilized to develop this plan and/or referenced in this document:

- [1] P. T. Williams, T. L. Dickson, B. R. Bass and H. B. Klasky, "ORNL/LTR-2016/309: Fracture Analysis of Vessels – Oak Ridge FAVOR, v16.1, Computer Code: Theory and Implementation of Algorithms, Methods, and Correlations (ML16273A033)," Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, August 2016.
- [2] IEEE Computer Society, "IEEE Standard for Software Quality," The Institute of Electrical and Electronics Engineers, Inc., New York, NY, 2014.
- [3] A. Dyszel and P. A. C. Raynaud, "FAVOR Software Quality Assurance Plan (SQAP)," U.S. Nuclear Regulatory Commission, Washington, DC, 2020.
- [4] P. T. Williams, T. L. Dickson, B. R. Bass and H. B. Klasky, "ORNL/TM-2016/310: Fracture Analysis of Vessels - Oak Ridge, v16.1, Computer Code User's Guide (ML16273A034)," Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, August 2016.
- [5] American Society of Mechanical Engineers (ASME), ASME NQA-1-2015: Quality Assurance Requirements for Nuclear Facility Applications, New York, NY: ASME, 2015.
- [6] American Society of Mechanical Engineers (ASME), "ASME V&V 10-2006: Guide for Verification and Validation in Computational Solid Mechanics," ASME, New York, NY, December 2006, reaffirmed 2016.
- [7] A. Ayszal, T. L. Dickson, M. Smith and P. Raynaud, "TLR-RE/DE/CIB-2020-002: Assessment of V&V Efforts of Fracture Analysis of Vessels – Oak Ridge (FAVOR) Software Product – Version 16.1 (ML20017A170)," U.S. Nuclear Regulatory Commission, Washington, DC, USA, 2020.
- [8] Pacific Northwest National Laboratory, "A Generalized Procedure for Generating Flaw-Related Inputs for the FAVOR Code," Pacific Northwest National Laboratory, Richland, WA, 2004.
- [9] American Society for Testing and Materials, "Standard Test Method for Determination of Reference Temperature, T_0 , for Ferritic Steels in the Transition Range," in *E 1921-97, Annual Book of ASTM Standards Section 3: Metals Test Methods and Analytical Procedures, vol. 03.01, Metals - Mechanical Testing: Elevated and Low-Temperature Tests: Metallography*, West Conshohocken, PA, American Society for Testing and Materials, 1998.
- [10] NUREG/BR-0167: Software Quality Assurance Program and Guidelines (ML012750471), Washington, DC: U.S. Nuclear Regulatory Commission, 1993.
- [11] American Society of Mechanical Engineers (ASME), "ASME NQA-1-2015: Quality Assurance Requirements for Nuclear Facility Applications," ASME, New York, NY, 2015.
- [12] IEEE Computer Society, "IEEE Standard for Software and System Test Documentation," The Institute of Electrical and Electronics Engineers, Inc., New York, NY, 2008.

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- [13] IEEE Computer Society, "IEEE Standard for System, Software, and Hardware Verification and Validation," The Institute of Electrical and Electronics Engineers, Inc., New York, NY, 2017.
- [14] American Society of Mechanical Engineers (ASME), ASME Boiler and Pressure Vessel Code – Section XI Rules for Inservice Inspection of Nuclear Power Plant Components, Two Park Avenue, New York, New York, USA.: ASME, 2017.
- [15] American Society of Mechanical Engineers (ASME), Alternative Characterization Rules for Quasi-Laminar Flaws," ASME Boiler and Pressure Vessel Code, Case N-848, Section XI, Division 1, April 30, 2015, New York, New York: ASME, 2015.
- [16] V. Lacroix, P. Dulieu and D. Couplet, "Alternative Characterization Rules for Quasi-Laminar Flaws," in *Proceedings of ASME 2014 Pressure Vessels and Piping Division Conference, July 20-24, 2014*, Anaheim, CA, 2014.
- [17] V. Lacroix, P. Dulieu and A. S. Bogaert, "Alternative Characterization Rules for Quasi-Laminar Flaws Based on 3-D X-FEM Calculations," in *Proceedings of ASME 2015 Pressure Vessels and Piping Division Conference, July 19-23, 2015*, Boston, MA., 2015.
- [18] B. R. Bass, T. L. Dickson, S. B. Gorti, H. B. Klasky, R. K. Nanstad, M. A. Sokolov and P. T. Williams, "ORNL Evaluation of Electrabel Safety Cases for Doel 3 / Tihange 2: Final Report (R1)," Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, 2015.

4 Roles & Responsibilities

The organizational structure and responsibility assignments shall be such that:

- Software development and maintenance is well planned, verified, and documented under quality assurance procedures.
- Quality is achieved and maintained by those who have been assigned responsibility for performing work, and
- Quality achievement is verified by those not directly responsible for performing the work.

The responsibilities are laid out in the FAVOR Software Quality Assurance Plan (Reference [3]) and not repeated herein. Overall, code development is performed by the NRC and/or the Contractor. The NRC is responsible for high level oversight and direction and assigns work based on staffing resources and knowledge.

A summary of the project team responsibilities is shown in Table 4-1, and a list of key documents that the project team creates during the life cycle of FAVOR development are shown in Table 4-2. This report focuses on the two green highlighted documents shown in these tables.

Table 4-1: Functional Responsibility Matrix¹

P=Prepare/Perform A=Approve I=Input R=Review S=Surveillance OD=Own & Distribute	NRC PM	Contractor PM	Code Custodian	Records Custodian	Software Developer	Software Tester	SQE ²	QA Manager ²
Documents/Actions								
FAVOR Software QA Plan (SQAP)	I, R, A	I, A	I	I, OD	I, R	I, R	P, R ⁴	I, R, A
Configuration Mgmt. Plan and Procedures (CMMP)	I, R, A	I, A	I	I, OD	I, R		P, R ⁴	I, R, A
Software Requirements Document (SRD)	I, R, A	I, R	P, I, R ⁴	OD	P, I, R ⁴		I, R ⁴	S
Software Design Document (SDD)	I, R	I, R, A	I, OD		P			
Source Codes	I, R	I, R, A	I, OD		P			
Acceptance test input files	I, R	I, R, A	I, OD		I, R	P		
Software Test Plans ³ (STPs)		A	I, R ⁴		I, R	P		
V&V Plan (SVVP)	I, R, A	I, R, A	R ⁴	OD	I, R	P	I, R ⁴	R, A
Software Test Results Reports ³ (STRRs)		R, A	I, R ⁴	OD	I, R	P		
V&V Tests and Results Reports (SVVR)	R, A	I, R, A	R ⁴	OD	I, R	P	S	S
Technical Reviews (e.g., assessments/surveillances)	P, I	P					S	S

¹ Note that this document does not meet the full requirements of this matrix as the document was not developed under a fully qualified Software QA program.

² Positions in the Quality Assurance Organization of the Contractor. These positions can be filled by one person, depending on the organization and simplicity of the code change.

³ Per NUREG/BR-0167, these are classified as informal.

⁴ Independent Technical Review

P=Prepare/Perform A=Approve I=Input R=Review S=Surveillance OD=Own & Distribute	NRC PM	Contractor PM	Code Custodian	Records Custodian	Software Developer	Software Tester	SQE ²	QA Manager ²
Documents/Actions								
Software Changes	R, A	I, R	I, R ⁴		P			
Change Documents (Appendices D – L)	R, A	I, R	P, I, R ⁴	OD	P		I	S
User Input Guide, Theory Manual	I, R, A	I, R	P, I, R ⁴	OD	P, I, R ⁴		S	S
Maintaining Problem Reporting, Corrective Action, & Change Control	R, A	R	P	OD	I		S	S
QA Records	A	I, R	R ⁴	OD			S	S

Table 4-2: Key Process Documents/Outputs

Process Document/Output
Software Quality Assurance Plan (SQAP)
Configuration Management and Maintenance Plan (CMMP)
Software Requirements Document (SRD)
Software Verification & Validation Plan (SVVP)
Software Verification & Validation Report (SVVR)
Software Design Document (SDD) – may be a part of the FAVOR Theory Manual
Software Test Plan(s) (STPs)
Software Test Results Report(s) (STRRs)
GitHub Testing Issues
<i>Implementation Documentation</i>
1. FAVLoad, FAVPFM, FAVPost source code and executables
2. User's Manual
3. FAVOR Theory Manual
4. Acceptance Test Problems

5 Software Release

A typical software release shall consist of delivering the following items to approved FAVOR users:

1. FAVLoad, FAVPFM, FAVPost executables (*.exe files);
2. FAVOR Theory Manual;
3. FAVOR User's Manual; and
4. Acceptance Test Problems along with their solutions.

On case-by-case basis only, if deemed in the interest of the NRC: FAVLoad, FAVPFM, FAVPost source code may be distributed in ASCII format so normal text editors can view and edit the source.

6 Software Description

The **Fracture Analysis of Vessels – Oak Ridge (FAVOR)** computer program has been developed to perform deterministic and probabilistic risk-informed analyses of the structural integrity of a nuclear reactor pressure vessel (RPV) when subjected to a range of thermal-hydraulic events. The focus of these analyses is on the beltline region of the RPV. Development of FAVOR originated under the NRC-sponsored Heavy Section Steel Technology (HSST) program and, more recently, continued under the Probabilistic Structural and Material Modeling (ProSaMM) Program, both at Oak Ridge National Laboratory (ORNL).

Thermal-hydraulic events addressed by the FAVOR code include both overcooling accidents and normal operating transients. Overcooling events, where the temperature of the coolant in contact with the inner surface of the RPV wall rapidly decreases with time, produce time-dependent temperature gradients that induce biaxial stress states varying in magnitude through the vessel wall. Near the inner surface and through most of the wall thickness, the stresses are tensile, thus generating Mode I - opening driving forces that can act on possible existing internal surface-breaking or embedded flaws near the wetted inner surface. If the internal pressure of the coolant is sufficiently high, then the combined thermal plus mechanical loading results in a transient condition known as a pressurized-thermal shock (PTS) event. Normal planned reactor operational transients, such as start-up, cool-down, and leak-test can also present challenges to the structural integrity of the RPV.

As shown in Figure 6-1, FAVOR, written in Fortran, is composed of three computational modules: (1) a deterministic load generator (**FAVLoad**), (2) a Monte Carlo PFM module (**FAVPFM**), and (3) a post-processor (**FAVPost**). Also shown are the data streams that flow through the three modules.

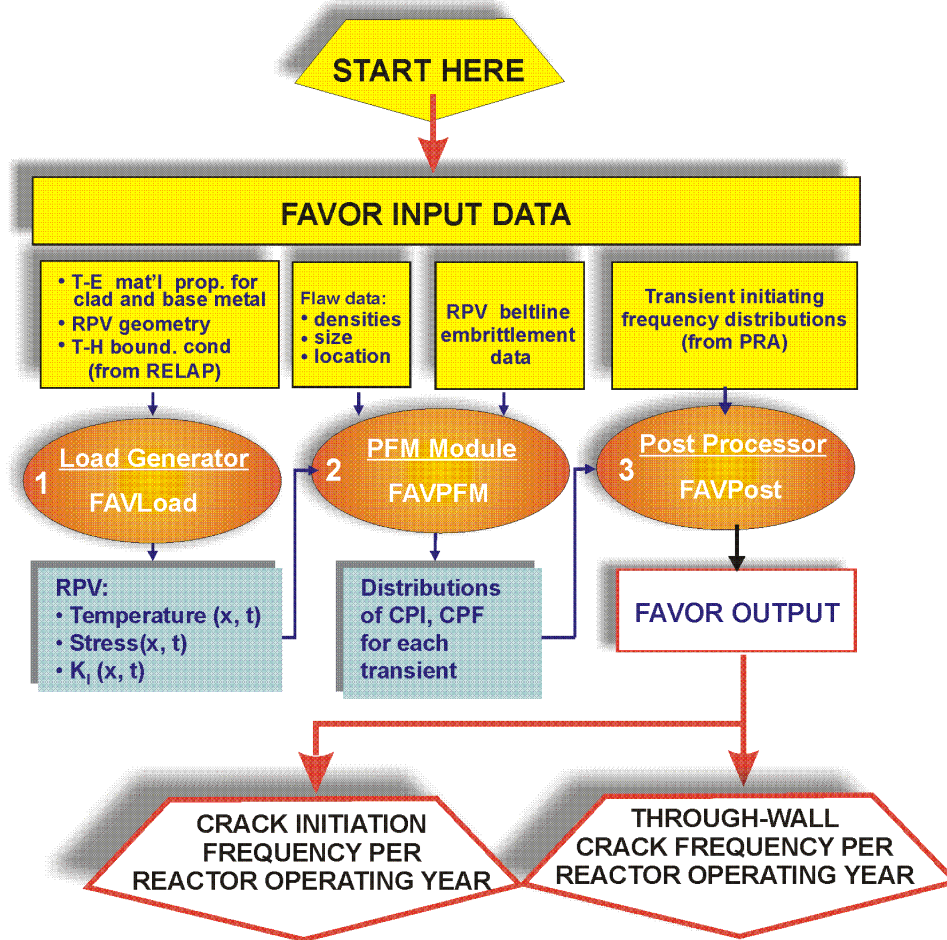


Figure 6-1: FAVOR data streams for (1) FAVLoad, (2) FAVPFM, and (3) FAVPost.

The FAVLoad, FAVPFM, and FAVPost codes have been designed to analyze reactor vessels in commercial pressurized-water reactors (PWR) and boiling-water reactors (BWR).

Over the years of development at Oak Ridge National Labs, the focus has been on developing FAVOR to be robust and easy to use. FAVOR's ultimate goal is to provide the user with an estimate of the conditional probabilities of reactor vessel crack initiation and/or failure if the RPV is subjected to the transient load being analyzed with FAVOR. The FAVPost module then applies annual probability transients determined by PRA analyses to determine the annual Through-Wall Cracking Frequency, which is calculated as a product of the CPF and a matrix defining the sequence (or event) frequency of the loading transients. Calculating a mean TWCF for RPVs subjected to pressure and temperature curves requires a statistical representation of the possible transients and their frequencies of occurrence.

Based on [1], prior releases of FAVOR and its predecessors were developed primarily to address the Pressurized Thermal Shock (PTS) issue. Therefore, they were limited to applications involving PWR

reactor vessels subjected to cool-down transients with thermal and pressure loading applied to the inner surface of the RPV wall. These earlier versions of FAVOR were applied in the PTS Re-evaluation Project to establish a technical basis to inform the revision of the original PTS Rule (Title 10 of the Code of Federal Regulations, Chapter I, Part 50, Section 50.61, 10CFR50.61). The FAVOR code continued to evolve and to be extensively applied by analysts from the nuclear industry and by regulators at the NRC, to ensure that the structural integrity of aging RPVs is maintained throughout the plant's operational service life including life extension. The v12.1 release of FAVOR represented a significant generalization over previous releases insofar as it included the ability to encompass a broader range of transients (i.e., both heat-up and cool-down) and vessel geometries, including both PWR and BWR RPVs. FAVOR v15.3, included improvements in the consistency and accuracy used for the calculation of K_I for internal surface-breaking flaws. FAVOR, v16.1, includes updates to the flaw-accounting logic in the FAVPFM module and corrections to some cladding influence coefficients for finite internal surface-breaking flaws.

As stated in Appendix G of the FAVOR Theory Manual (Reference [1]), the FAVOR code was subjected to both internal ORNL and external independent verification and validation studies throughout its development lifecycle. At the time of its initial release in 2001, FAVOR was being developed under the Software Quality Assurance (SQA) program at Oak Ridge National Laboratories (ORNL). Subsequent releases of FAVOR were subjected to periodic internal SQA audits; in all cases, the FAVOR code was judged compliant with ORNL SQA procedures and requirements. As the ORNL consensus standard, the ORNL SQA Program is registered to and compliant with the ISO 9001:2008 standard. In 2012, a formal ORNL SQA exemption was granted to FAVOR because the FAVOR software was being developed and maintained with funding from the NRC. The NRC support required that FAVOR be compliant with the terms and conditions of NRC Management Directive 11.7, which requires that all software development, modification, or maintenance follow the general guidance provided in NUREG/BR-0167. ASME Guides and Standards for Verification and Validation (V&V) studies and other references provided more specific guidance (specific to scientific computing applications) during the development of FAVOR. A recent effort to assess the FAVOR SQA against the ASME Code SQA standards [5] and [6] has identified some gaps in the documentation as outlined below. However, NRC has determined that the extensive independent verification and validation studies performed throughout the FAVOR lifecycle provide reasonable assurance that the FAVOR code results are sufficiently accurate and trust-worthy, such that FAVOR may be used to risk-inform regulatory decisions (Reference [7]).

Some of the elements of the updated technologies and computational methodology that have been incorporated into FAVOR (from v01.1 to the v16.1) are as follows:

1. Ability to incorporate new detailed flaw-characterization distributions from NRC research (with Pacific Northwest National Laboratory, PNNL).
2. Ability to incorporate detailed neutron fluence maps.
3. Ability to incorporate warm-prestressing effects into the analysis.
4. Ability to include temperature-dependencies in the thermo-elastic properties of base and cladding.

5. Ability to include crack-face pressure loading for surface-breaking flaws.
6. Addition of a new ductile-fracture model simulating stable and unstable ductile tearing.
7. Addition of a new embrittlement correlation.
8. Ability to include multiple transients in one execution of FAVOR.
9. Ability to include input from the Reactor Vessel Integrity Database, Revision 2, (RVID2) of relevant RPV material properties.
10. Addition of new fracture-toughness models based on extended databases and improved statistical distributions.
11. Addition of a variable failure criterion, i.e., how far must a flaw propagate into the RPV wall for the vessel simulation to be considered as “failed”?
12. Addition of semi-elliptic surface-breaking and embedded-flaw models.
13. Addition of through-wall weld stresses.
14. Addition of base material SIFIC(s) from ASME code, Section XI, Appendix A, Article A-3000, *Method of KI Determination*, for (a) finite semi-elliptical axial and circumferential inside surface flaws and (b) infinite axial and 360° continuous circumferential inside surface flaws into the FAVOR SIFIC database; and
15. Implementation of an improved PFM methodology that incorporates modern PRA procedures for the classification and propagation of input uncertainties and the characterization of output uncertainties as statistical distributions.

A list of key inputs to FAVOR, the important functions and algorithms used in FAVOR, and the FAVOR outputs used in critical decisions are listed in Table 6-1. Some key calculated outputs of FAVOR are K_I (applied stress-intensity factor) time history, through-wall temperature time history, and RT_{NDT} (Reference Nil-Ductility Transition Temperature) at the crack tip. These FAVOR outputs are further used in determining flaw propagation and determining CPI (Conditional Probability of crack Initiation) and CPF (Conditional Probability of Failure).

The current version of FAVOR, with the Table 6-1 inputs from the user, processes them through intermediate data flows to support the various models within the three modules. These inputs are based on the beltline region of a reactor vessel. Figure 6-2 illustrates a PWR example.

One objective of the modernization of FAVOR is to not impact the results of the fundamental models and algorithms in Table 6-1. The current FAVOR models and algorithms have been tested and validated against ABAQUS and used widely in the industry (Ref [7]). Maintaining consistency with the existing models and algorithms provides the foundation of the software requirements discussed in the next section.

Table 6-1: FAVOR Critical Inputs, Functions, and Outputs

Type	Description
Key Inputs	<ul style="list-style-type: none"> • Thermo-Mechanical Material Properties for clad and base metal of the RPV (i.e., thermal conductivity, specific heat, density, Young's Elastic Modulus, thermal expansion coefficient, Poisson's ratio) • RPV geometry • Thermal Hydraulic boundary conditions (from RELAP or similar Transient T-H code) • Fast Neutron fluence maps (entered as f_o on Embrittlement Data, described below) • Flaw densities, size, and location (plates, welds, and forgings) • Embrittlement Data (i.e., Cu, Ni, P, Mn, f_o, RT_{NDT0}) • Transient Initiating Frequency distributions (from PRA) • Probability distributions (aleatory and epistemic)
Important Functions and Algorithms	<ul style="list-style-type: none"> • FAVLoad Deterministic analyses <ul style="list-style-type: none"> ○ Thermal analysis ○ Stress analysis ○ Linear-Elastic Fracture Mechanics (LEFM) ○ Handling of residual stresses in welds ○ Handling of crack-face pressure for surface breaking flaws • Calculation of Nil-Ductility Transition Temperature, RT_{NDT} • Radiation embrittlement correlations • Fast neutron fluence attenuation and sampling • Handling of K_{IC} and K_{Ia} Databases and calculations of K_{IC} and K_{Ia} • Sampling of RT_{NDT} and RT_{Arrest} • Sampling of Material Chemistry • Flaw characterizations and uncertainty • FAVPFM algorithms and models <ul style="list-style-type: none"> ○ Warm prestressing logic ○ Truncation for probability distributions ○ Conditional Probability of Initiation (CPI) and Failure (CPF) ○ Post initiation flaw geometries and orientation ○ Ductile tearing models ○ Initiation-Growth-Arrest (IGA) model • FAVPost algorithm using FAVPFM distributions of conditional probabilities of initiation and failure with input transient initiating frequencies to create fracture and failure frequencies
Critical Outputs	<ul style="list-style-type: none"> • Temperature as a function of time throughout vessel wall location • Stress as a function of time throughout vessel wall (circumferential and axial) • K_I as a function of time throughout vessel wall • Probability distributions of crack initiation and vessel failure • Crack initiation frequency per reactor operating year • Through-wall crack frequency per reactor operating year

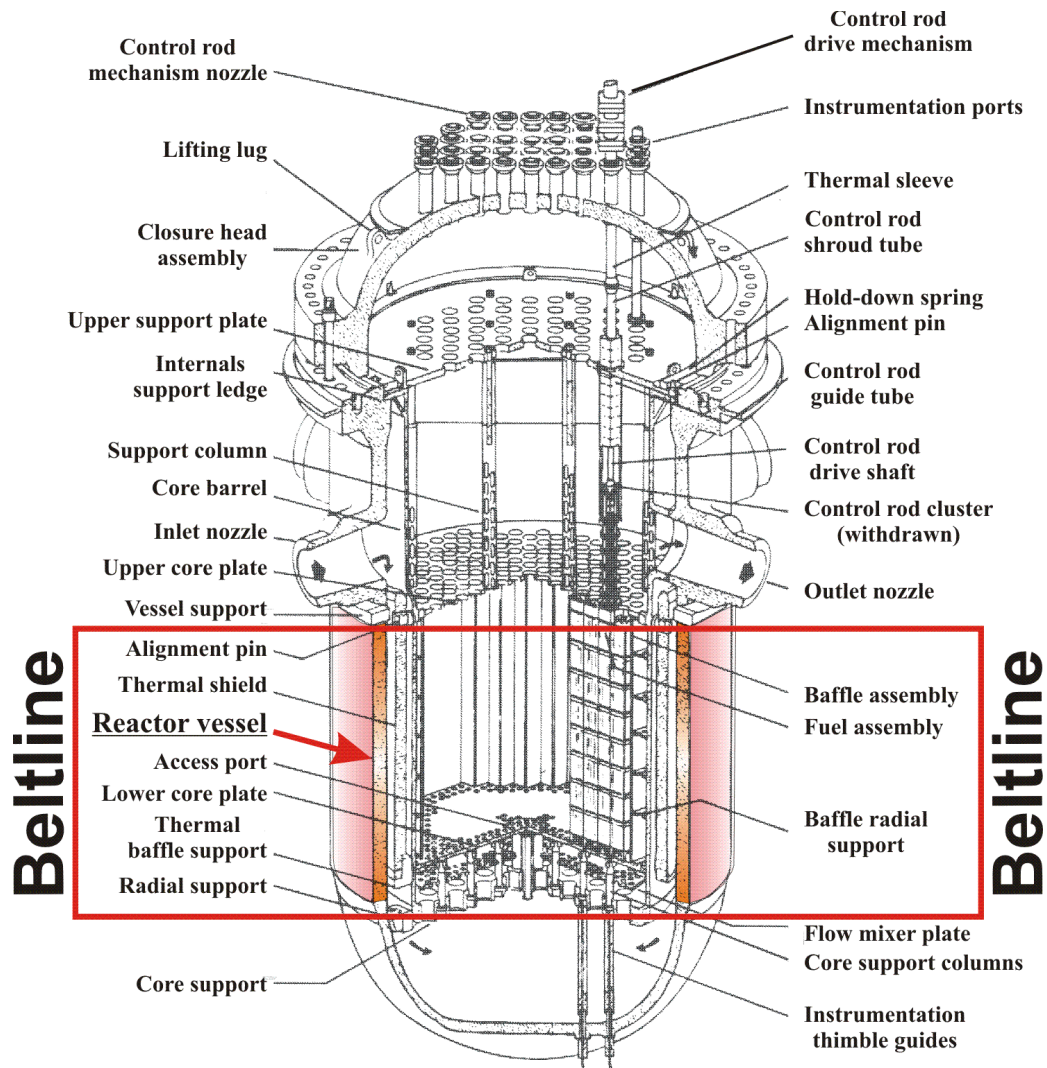


Figure 6-2: The beltline region of the reactor pressure vessel wall extends from approximately one foot above the active reactor core to one foot below the core for a pressurized water reactor (PWR).

7 Software Requirements

This Section provides a description of the software features/requirements for the modernized version of FAVOR which covers the change from v20.1 (as-found flaw version) to v20.1.12. The overall goal is to modernize the three FAVOR modules to bring the Fortran source code up to Fortran 2018 standards so parallel processing can improve run-time performance and also allow for better portability between compilers and operating systems. The software requirements are then organized into four types. The first set is related to input requirements, which are focused on ensuring that user enters the appropriate data, and that the software appropriately processes it. The second set of requirements are functional in nature. These include changes to models, functions, processes, or algorithms, which are required to process the user input data. As previously noted, the current FAVOR code has been extensively tested and benchmarked so the functional requirements will focus on not making significant changes to these models, functions, processes, and algorithms, except for the modernization techniques described herein. The third set of requirements are output based, which focus on displaying key results and descriptive characterization of flaw analyses. Finally, a performance requirement is specified to ensure run time is not significantly impacted by the software modifications. Modernization should drastically improve performance.

Consistent with FAVOR SQAP [3] GitHub shall be used to establish the software requirements based on all the assertion unit tests performed for the FAVOR code(s). Due to the detailed nature of the assertion tests, only key assertion tests relevant to a typical FAVOR attribute, identified in Table 6-1, will establish the software requirement that is described within this document and the next revision of the FAVOR Theory and User's Code manuals, as applicable. As each requirement is embedded in the FAVOR code repository (via assertion test), then by its very nature of being treated as code the complete history of each requirement is tracked at all times. The FAVOR repository and contents employ a continuous integration strategy using Continuous Integration for Verification, Enhancement, and Testing. Test documentation is available at the following link: [FAVOR/tests at main NRC-Research/FAVOR \(github.com\)](https://github.com/NRC-Research/FAVOR)

7.1 General Requirement: Implement modernization standards.

From Issue 7 | GitHub ("Draft list of improvements to source code", [Draft list of improvements to source code · Issue #7 · NRC-Research/FAVPRO \(github.com\)](https://github.com/NRC-Research/FAVPRO/issues/7)), the following improvements were made to modernize FAVOR:

7.1.1 Replace non-standard features.

Non-standard Feature	Occurrences (lines)
real*	696

7.1.2 Replace deleted features.

Deleted Feature	Occurrences (lines)
<i>arithmetic-if-stmt</i>	11

7.1.3 Replace obsolescent features.

Obsolescent Feature	Occurrences (lines)
Fixed source form	51,946
<i>common-stmt</i>	154
<i>block-data-stmt</i>	1
<i>equivalence-stmt</i>	3
<i>entry-stmt</i>	8
<i>character*</i>	75
<i>alternate-return</i>	26
Specific names for intrinsic functions	Example: <i>DSQRT</i> -> <i>SQRT</i>

7.1.4 Replace non-portable features.

Non-portable Feature	Occurrences (lines)
<i>double precision</i>	206

7.1.5 Recommendations for clarity and robustness

7.1.5.1 Test in Fortran.

Current tests examine the results in output files using an external tool: *numdiff*. This imposes limitations on the logic that can be incorporated. We recommend writing Fortran tests to allow for more sophisticated test logic.

7.1.5.2 Delete all trailing whitespace.

- FAVPost: issue #8
- FAVLoad: issue #9
- FAVPFM: issue #10

7.1.5.3 *Create like beginning/ending statements.*

- Replace continue-stmt as a terminating statement for do-construct with end-do-stmt.

7.1.5.4 *Improve string handling.*

- Replace fixed character string lengths with allocatable character string lengths.

7.1.5.5 *Prefer the use of variables over repetitive usage of literals.*

- Replace integer literals when referring to file unit numbers.

7.1.5.6 *Prefer explicit typing*

- Add implicit-none and add explicit types.

7.1.5.7 *Prefer the usage of intent **attributes for arguments.***

- Wherever possible, add intent-spec.

7.1.5.8 *Reformat comments.*

- Update the format of comments to improve the generation of Ford documentation.

7.1.5.9 *Remove change logs and revisions.*

- Removal change logs and revisions information from the source code
- Create a wiki to capture all change logs and revisions information.

7.1.5.10 *Improve readability.*

- Replace upper-case with lower-case (for example, INTEGER -> integer).
- Use consistent indentation practices.
- Consider changing the names of subroutines and functions to more comprehensible names.

7.1.5.11 *Avoid repeated code.*

- Add new functions when appropriate to avoid repeated code.
- Look for comments such as the following to check whether adding functions would be preferred.
 - *! USING THE SAME LOGIC AS ABOVE, WRITE RESULTS TO THE SCREEN*
 - *! EXTRACTED FROM SUBROUTINE _____*
 - *! FALLING TO HERE REQUIRES EXTRAPOLATION FROM LAST 2 POINTS - code following these comments is very similar.*

7.1.6 Design a Defensive Build System.

7.1.6.1 *General strategy*

- Set a compiler flags to
 - Enforce the Fortran 2018 standard.
 - Turn on all warnings, including warnings about obsolescent features.
- Create a -DSTRICT build option that treats warning messages as errors.
- Define a continuous integration (CI) test that fails when a strict build fails to compile.

7.1.6.2 *Representative list of warning messages to be addressed to comply with above strategy.*

gfortran warnings

Compiler flag	Warning Message	Frequency	Example line location
-Wconversion	Possible change of value in conversion from REAL(4) to INTEGER(4)	High	FAVPost.f:6706:18
-Wunused-label	Label *** defined but not used	High	FAVPost.f:2369:3
-Wunused-variable	Unused variable '***'	High	FAVPost.f:2888:53
Compiler flag	Warning Message	Frequency	Example line location
-Wunused-dummyargument	Unused dummy argument '***'	High	FAVPost.f:1800:24
n/a	Array reference out of bounds (2 > 1) in loop	~3 times	FAVLoad.f:7758:19
-Wmaybe-uninitialized	'***' may be used uninitialized in this function	~3 times	FAVPost.f:4963:0
-Wtabs	Nonconforming tab character	1 time	FAVPFM.f:11000:8
-Wintrinsic-shadow	'***' is also the name of an intrinsic. It can only be called via an explicit interface or if declared EXTERNAL	1 time	FAVPFM.f:18394:6
-Wsurprising	Array '***' is larger than limit set by '-fmax-stack-var-size=', moved from stack to static storage. This makes the procedure unsafe when called recursively, or concurrently from multiple threads. Consider using '-frecursive', or increase the '-fmaxstack-var-size=' limit, or change the code to use an ALLOCATABLE array.	1 time	FAVPFM.f:6627:48

7.1.6.3 *Prevent the introduction of obsolescent features.*

Obsolescent Feature	Occurrences (lines)
<i>computed-goto-stmt</i>	0
<i>stmt-function-stmt</i>	0
<i>label-do-stmt</i>	0
<i>forall-construct</i> & <i>forall-construct-stmt</i>	0
Assumed character length functions	0
<i>data-stmt</i> amongst executable statements	0

7.1.6.4 *Prevent the introduction of deleted features.*

Deleted Feature	Occurrences (lines)
<i>pause-stmt</i>	0
<i>assign-stmt</i>	0
<i>assigned-goto-stmt</i>	0
<i>assigned-format-specifier</i>	0
<i>hollerith-literal-constant</i>	0
<i>nonblock-do-construct</i>	~0
<i>real</i> and <i>double precision do</i> variables	0
vertical format control	~0
Branching to an <i>end-if-stmt</i> from outside its block	~0

Notes:

- *hollerith-literal-constant* is the *H* edit descriptor
- *nonblock-do-construct* appears to not be used in code but further inspection is required to be certain.

7.1.6.5 *Expose the modularity in the file/directory structure.*

- Separate each modules into its own file.
- Move the external procedure definitions to submodules in separate files.

7.1.6.6 *Eliminate redundant procedure copies.*

Potentially redundant subroutines:

Pattern	Subroutine name	Copies (file)
<i>*ch*</i>	<i>pchim, pchfe, chfev</i>	FAVLoad, FAVPFM
<i>get*</i>	<i>get_line, get_real</i>	FAVLoad, FAVPFM, FAVPost
<i>xget*</i>	<i>xgetf, xgetua</i>	FAVLoad, FAVPFM, FAVPost
<i>xset*</i>	<i>xsetf, xsetua</i>	FAVLoad, FAVPFM, FAVPost
<i>xer*</i>	<i>xerabt, xerclr, xercnt, xerctl</i>	FAVLoad, FAVPFM, FAVPost
	<i>xerdmp, xerhlt, xermax, xermsg</i>	FAVLoad, FAVPFM, FAVPost
	<i>xerprt, xerrwv, xersav</i>	FAVLoad, FAVPFM, FAVPost
(N.A.)	<i>erprn, fdump, FILE_INIT, check_alloc</i>	FAVLoad, FAVPFM, FAVPost

Potentially Redundant Functions:

Function name	Copies (file)
<i>pchst</i>	FAVLoad, FAVPFM
<i>i1mach</i>	FAVLoad, FAVPFM
<i>j4save</i>	FAVLoad, FAVPFM, FAVPost
<i>rndu</i>	FAVLoad, FAVPFM, FAVPost

Notes:

- The above tables were constructed manually from the output of grep.
- The two instances of pchim were verified to be identical by performing a diff of their respective parse trees.
- The identical nature of all redundant copies should be checked in an automated way.

7.1.6.7 Eliminate or enable dead code.

Tested code is trusted code. Dead code is untested code.

Examples of dead code:

- Commented code.
- Unreachable code, e.g., *if (.false.) then call dead_code*

Strategy:

- Eliminate dead code or

- Embed dead code in a conditional branch (e.g., *if* or *select case*) that can be reached by setting an input parameter.

Dead procedure names	File
TINT_old, SCOEFF_old, STRCAL_old	FAVLOAD

- Refactor currently dead subroutines that are meant for possible debugging purposes by adding logical parameters that allow caller to enable debugging or not.

"Dead" debuggers	File
MARKCPI	FAVPFM
MARKCPF	FAVPFM

7.1.6.8 Enforce structured programming.

- Replace *goto* with executable constructs that contain blocks.

7.1.6.9 Clarify the data dependencies.

Introduce functional programming by:

- Replacing subroutines with *pure* functions, encapsulating results in objects where necessary.
- Making function results objects where necessary.
- Making functions *elemental* where useful.
- Replacing local variables with immutable state via *associate-name => expr*.

7.1.6.10 Exploit intrinsic procedures.

Advantages:

- All intrinsic functions are *pure*, which facilitates concurrency and clarifies data dependencies.
- Compiler/library implementations sometimes outperform user implementations.
- Compactness.

Intrinsic procedure	Possible use
<i>transpose</i>	FAVLoad_v16.1.f(8072): COMPUTE BI=B(TRANSPPOSE)*D FAVLoad_v16.1.f(8210): COMPUTE BI=B(TRANSPPOSE)*D FAVLoad_v16.1.f(11882): FORM PRODUCT INVERSE(R) WITH ITS TRANSPPOSE FAVLoad_v16.1.f(11903): APPLY TRANSPPOSE(Q) TO QWB
<i>dot_product.</i>	FAVLoad_v16.1.f(7557): inner product of the basis vector and temperature vector

7.1.6.11 Employ higher-level abstractions.

Introduce object-oriented programming (OOP) by:

- Representing useful abstractions as extensible derived types (classes).
 - Define classes that capture file input/output data to enable more sophisticated results-checking and eliminate the need for *numdiff*.
 - Employing object-oriented design (OOD) patterns.

7.1.6.12 Exploit available parallelism.

1. Parallelize across independent runs (.e.g., parametric studies) using non-coarray parallel features:
 - Synchronization: *sync all, sync images*
 - Error termination: *error stop*
 - Image enumeration: *this_image, num_images*
 - Collective subroutines: *co_sum, co_max, co_min, co_reduce*
2. Parallelize individual runs using coarrays:
 - Write parallel algorithms, as necessary.
3. Express loop-level concurrency:
 - *do concurrent*
 - Array statements
 - *elemental* procedures

7.2 Input Requirements

7.2.1 Overall General Requirement: User Input Remains the Same as v20.1.1

The modernization of FAVOR will not impact the user input ensuring backward compatibility for the test suite of cases.

Consistent with v16.1 of FAVOR, ASCII text files either created by the user or created by previous executions of the FAVOR modules are used as input. User-created input files are organized by a sequence of keyword records with *fixed-field format* for the placement of parameter data located on the same line record as the keyword or on data lines following the keyword record. The data must be input exactly in the sequence and order prescribed in the sections below. Omission of data fields is not allowed. The 4-letter keywords always begin in column 1. Comment lines are designated by an asterisk, "*", in column 1. The user is encouraged to take full advantage of including comments in the input files as a method for internal documentation of the model. It has proven beneficial by the developers of FAVOR to use the input files (included in the example cases in the distribution package) as templates for the creation of new input datasets. In developing input datasets, the user should pay careful attention to the required units for each data record. FAVOR carries out conversions internally to ensure a consistent set of units for all analyses, however, the input data must be entered in the units specified per the user manual.

7.2.2 Input Requirement 1: FAVLoad User Input will remain unaffected or enhanced by modernization changes.

The following FAVLoad twelve User Inputs will be unaffected:

Record 1 – GEOM Record No. 1 inputs vessel geometry data, specifically the internal radius, IRAD, in inches, the wall thickness (inclusive of cladding), W, in inches, and the cladding thickness, CLTH, in inches. The thickness of the base metal is, therefore, $W - CLTH$.

Records 2 and 3 – BASE and CLAD Records 2 and 3 input thermo-elastic property data for the base (typically a ferritic steel) and cladding (typically an austenitic stainless steel), respectively: thermal conductivity, K, in Btu/hr-ft-°F, C, mass-specific heat capacity in Btu/lbm-°F, mass density, RHO, in lbm/ft³, Young's modulus of elasticity, E, in ksi, coefficient of thermal expansion, ALPHA, in °F⁻¹, and Poisson's ratio, NU. All property data are assumed to be independent of temperature if NTE = 0. If NTE = 1 on Records 2 or 3, then tables of temperature-dependent properties will be input.

Record 4 inputs the thermal stress-free temperature for both the base and cladding in °F. In addition, crack-face pressure loading on surface-breaking flaws can be applied with CFP = 1. If CFP = 0, then no crack-face pressure loading will be applied.

Records 5 and 6 – RESA and RESC Records 5 and 6 set weld residual stress flags, NRAX and NRCR, for axial and circumferential welds, respectively. If NRAX or NRCR are set to a value of 101, then weld residual stresses will be included in the FAVLoad output file. If NRAX or NRCR are set to a value of 0, then weld residual stresses will not be included in the FAVLoad output file.

Record 7 – TIME Record 7 inputs the total elapsed time, TIME, in minutes for which the transient analysis is to be performed and the time increment, DT, also in minutes, to be used when outputting results in FAVPFM. Internally, the FAVLoad module uses a constant time step of 1.0 second to perform finite-element through-wall heat-conduction analyses (1D axisymmetric). DT is the time-step size for which load results (temperatures, stresses, etc.) are saved during execution of the FAVLoad module; therefore, DT is the time-step size that will be used for all fracture analyses in subsequent FAVPFM executions. Note that there is no internal limit to the size of the time step; however, the computational time required to perform a PFM analysis is inversely proportional to DT. Furthermore, DT (in minutes) must be equal to an integer number of seconds, thus the smallest possible input for DT is 0.05 minutes (=3 seconds), and DT must be a multiple of 0.05 minutes.

Record 8 – NPRA Record 8 inputs the number of thermal-hydraulic transients, NTRAN, to be defined for this case. Records 9 through 12 are repeated for each of the NTRAN transients defined.

Record 9 – TRAN Record 9 provides a mechanism for cross-indexing the internal FAVOR transient numbering system with the initiating-event sequence numbering system used in the thermal-hydraulic analyses that were performed to develop input to FAVOR. The internal FAVOR transient number, ITRAN, is linked with the thermal-hydraulic initiating-event sequence number, ISEQ, with this record. Whereas the value of ITRAN will depend upon the arbitrary ordering of transients in the FAVLoad transient input stack, the value of ISEQ is a unique identifier for each transient. ITRAN begins with 1 and is incremented by 1 up to NTRAN transients.

Record 10 – NHTH Record 10 inputs the time history table for the convective film coefficient boundary conditions. There are NC data pairs of time, t , in minutes and film coefficient, h , in Btu/hr-ft² -°F entered following the NHTH keyword record line. The number of data pairs is limited only by the memory capacity of the computer. The film coefficient, $h(\tau)$, is used in imposing a Robin forced-convection boundary condition at the inner vessel wall, R_i , defined by,

$$q(R, \tau) = h(\tau)[T_{\infty}(\tau) - T_{wall}(R, \tau)] \text{ for } R = R_i, \tau \geq 0$$

where $q(R, t)$ is the heat flux in Btu/hr-ft², $T_{\infty}(\tau)$ is the coolant temperature near the RPV wall in °F, and $T_{wall}(R, \tau)$ is the wall temperature in °F.

Record 11 – NTHH Record 11 inputs the time history definition for the coolant temperature, $T_{\infty}(\tau)$, which is applied in the Robin boundary condition discussed above. The time history can take two forms depending on the value of the NT parameter. If NT is equal to an integer other than 101, then an ordered table with NT lines of time, τ , in minutes and temperature, T , in °F data pairs will follow the NTHH keyword record. The number of data pairs is limited only by the memory capacity of the computer. If NT = 101, then a stylized exponentially decaying time history will be used where the parameters are the initial coolant temperature, TINIT, in °F, the asymptote for the coolant temperature, TFINAL, decay curve in °F, and the decay time constant, BETA, in minutes⁻¹. These parameters define the time history of the coolant temperature by the following equation:

$$T_{\infty}(\tau) = T_{\infty-FINAL} + (T_{\infty-INIT} - T_{\infty-FINAL}) \exp(-\beta\tau)$$

Record 12 – NPTH Record 12 inputs the time history table for the internal coolant pressure boundary condition. There are NP data pairs of time, t , in minutes and internal coolant pressure, p , in kilo-pounds force per square inch (ksi) entered following the NPTH keyword record line. The number of data pairs is limited only by the memory capacity of the computer.

7.2.3 Input Requirement 2: FAVPFM User Input will remain unaffected or enhanced by modernization changes.

The modernization of FAVOR will not impact the user input ensuring backward compatibility for the test suite of cases. FAVPFM contains a total of 11 records plus the embrittlement map based on the number of weld and plate(forge) subregions specified.

The following FAVPFM User Inputs will be unaffected:

Record 1 – CNT1 inputs the number of simulations, NSIM, for the plant-specific analysis of this RPV, the number of trials/realizations. The IPFLAW flag sets the distributions of surface-breaking and embedded flaws within the RPV wall that are assumed for this analysis. IPFLAW = 1: surface-breaking flaws are internal (reside on the inside surface of the RPV) and embedded flaws are uniformly distributed within the inner 3/8ths of the RPV base metal; IPFLAW = 2: surface-breaking flaws are external (reside on the outside surface of the RPV) and embedded flaws are uniformly distributed in the outer 3/8ths of RPV base metal; IPFLAW = 3: surface-breaking flaws are both internal and external with 50% external surface-breaking and 50% internal surface-breaking flaws; Embedded flaws are distributed uniformly throughout the entire RPV base metal thickness; and IPFLAW = 4: As-found flaw option.

The IGATR flag (where IGATR is bounded from 100 to 1000, i.e., $100 \leq \text{IGATR} \leq 1000$.), is applied per flaw in the *Initiation-Growth-Arrest* (IGA) model,

WPS_OPTION sets the warm prestressing option (WPS_OPT=1|2|3) on or off (WPS_OPT=0).

WPS_OPTION = 0 do not include warm prestressing in analysis

WPS_OPTION = { 1|2|3 } – enter into WPS state when $dK/dt < 0$

Three options are available for recovery from a WPS state.

WPS_OPTION = 1 exit WPS and be available for initiation when applied- K_I exceeds maximum K_I determined from all previous discrete transient time steps i.e., $dK/dt > 0$ and $K_I > \alpha * K_{I_{max}}$ where $\alpha = 1$;

WPS_OPTION = 2 exit WPS and be available for initiation when $dK/dt > 0$ and $K_I > \alpha * K_{I_{max}}$ where $\alpha = 0$;

WPS_OPTION = 3 exit WPS and be available for initiation when applied K_I exceeds maximum K_I determined from all previous discrete transient time steps i.e., $dK/dt > 0$ and $K_I > \alpha * K_{I_{max}}$ where α is sampled from a log-logistic distribution as discussed in the *Theory Manual* [1] with location parameter = 0, scale parameter = 1.15643, and shape parameter = 20.12346.

The PC3_OPT flag sets the Category 3-flaws-in-plate-material option (PC3_OPT = 0 do not perform or = 1 do perform analysis). In a typical PFM analysis, a substantial fraction of the total flaws are Category 3 flaws in plate regions. Based on experience and some deterministic fracture analyses, these flaws rarely contribute to the *CPI* or *CPF* with the plate flaw size distributions typically used. Therefore, setting PC3_OPT = 0 can result in significantly shorter execution times without affecting the solution, unless there are unusual circumstances such as using a new flaw-size distribution for plate flaws. In either case, the Category 3 plate flaws are included in the bookkeeping reports.

The CHILD_OPT flag sets the child reports option (CHILD_OPT = 0 do not include child subregion reports or = 1 include child subregion reports in the FAVPFM output file). The discretization and organization of major regions and subregions in the beltline includes a special treatment of *weld-fusion lines*. These fusion lines can be visualized as approximate boundaries between the weld subregion and its neighboring plate or forging subregions. FAVOR checks for the possibility that the plate subregions adjacent to a weld subregion (termed *parent* subregions) could have a higher degree of radiation-induced embrittlement than the weld. The irradiated value of RT_{NDT} for the weld parent subregion of interest is compared to the corresponding values of the adjacent (i.e., nearest neighbor) plate subregions. Each parent weld subregion will

have at most two adjacent child plate subregions. The embrittlement-related properties of the most-limiting (either the weld or the adjacent plate subregion with the highest value of irradiated RT_{NDT}) material are used when evaluating the fracture toughness of the weld subregion. A given *parent* weld subregion will have either itself or an adjacent plate subregion as its *child* subregion from which it will draw its chemistry.

The flaw orientation, location, size, fast-neutron fluence, and category are not linked. A *parent* plate subregion always has no *child* subregion dependency. For each transient, the basic major region and flaw-distribution reports are given in terms of the *parent* weld subregions. By setting $CHILD_OPT = 1$, in addition to the *parent* reports, major region and flaw-distribution reports will also be output in terms of the *child* subregions (i.e., the subregions that control the allocation of embrittlement properties to weld subregions). If this option is set, additional data will be passed onto FAVPost where *child* subregion reports will also be generated.

With the older ductile-tearing model (see Record 2 – CNT2 for details on the ductile-tearing models) turned on ($IDT_OPTION=2$), a second independent set of parent/child relationships are established to determine the source for ductile-tearing property data including chemistry content and USE_i . For ductile tearing, the controlling property is the relative magnitude of the irradiated upper-shelf CVN energy, USE_i . FAVOR checks for the possibility that the plate subregions adjacent to a weld subregion (termed *parent* subregions) could have a lower level of ductility than the parent weld subregion. The irradiated value of the upper-shelf CVN energy (USE_i) for the weld parent subregion of interest is compared to the corresponding values of the adjacent (i.e., nearest-neighbor) plate subregions. Each weld subregion will have at most two adjacent plate subregions. The embrittlement-related properties of the most-limiting (either the weld or the adjacent plate subregion with the lowest value of USE_i) material are used when evaluating the ductile-fracture properties of the weld subregion. A given *parent* weld subregion will have either itself or an adjacent plate subregion as its *child* subregion from which it will inherit its chemistry and USE_i . This model has been superseded by a newer ductile-tearing model ($IDT_OPTION=1$) which is not based on the USE_i and does not require a second parent/child dependency structure.

A restart option is included in FAVPFM. If $RESTART_OPTION \leq 0$, the current execution is not based on a restart of a previous run. At user-selected checkpoints during FAVPFM execution, a binary restart file will be created (RESTART.BIN) which during a subsequent execution can be used to restart FAVPFM from the point in the solution at which the restart file was created. By default, this restart file is created at intervals of 200 RPV trials. The user can change this checkpoint interval by setting $RESTART_OPTION$ to a negative integer. For example, if $RESTART_OPTION = -500$, then the effect will be the same as $RESTART_OPTION = 0$, except that the restart checkpoint interval will be 500 RPV trials. If $RESTART_OPTION \geq 1$, then this

execution will be treated as a restart case, and the user will be prompted for the name of a binary restart file created during a previous execution. For this restart case, new restart files will be created at user-selected checkpoint intervals where, for `RESTART_OPTION = 1`, the default checkpoint interval is 200. For `RESTART_OPTION > 1`, then the checkpoint interval is equal to the value of the flag setting, (e.g., `RESTART_OPTION = 500` indicates a checkpoint interval of 500 RPV trials).

Due to performance improvements in runtime, requirements to have restart capability have been eliminated. Future development activities will not require that this capability exists and maybe deleted.

Record 2 – CNT2 inputs a flag, `IRTNDT`, that designates the correlation to be used for irradiation shift calculations, where:

`IRTNDT = 992` → use Regulatory Guide 1.99, Rev. 2, for irradiation shift in RT_{NDT}

`IRTNDT = 2000` → use Eason 2000 [¹, ²] correlation for irradiation shift in RT_{NDT}

`IRTNDT = 2006` → use the Eason 2006 [³] correlation for irradiation shift in RT_{NDT}

`IRTNDT = 20071` → use the Kirk 2007 correlation for irradiation shift in RT_{NDT}

`IRTNDT = 20072` → use the RADAMO 2007 correlation for irradiation shift in RT_{NDT}

`IRTNDT = 20073` → use the combined EasonKirk/RADAMO 2007 correlation for irradiation shift

the normal operating coolant temperature, TC , in °F, the plant operating time, EPY , to be assumed for this case in effective full-power years, and a flag `IDT_OPTION` to turn on (`IDT_OPTION ≥ 1`) or off (`IDT_OPTION = 0`) the ductile-tearing model in the *IGA* sub model.

¹. E. D. Eason, J. E. Wright, and G. R. Odette, "Improved Embrittlement Correlations for Reactor Pressure Vessel Steels," NUREG/CR-6551, U. S. Nuclear Regulatory Commission, Washington, DC, 1998.

². M. T. Kirk, C. S. Santos, E.D. Eason, J.E. Wright, and G. R. Odette, "Updated Embrittlement Trend Curve for Reactor Pressure Vessel Steels," Paper No. G01-5, *Transactions of the 17th International Conference on Structural Mechanics in Reactor Technology (SMiRT 17)*, Prague, Czech Republic, August 17-22, 2003.

³. E. D. Eason, G. R. Odette, R. K. Nanstad, and T. Yamamoto, "A Physically Based Correlation of Irradiation-Induced Transition Temperature Shifts for RPV Steels, Oak Ridge National Laboratory, ORNL/TM-2006/530, 2006.

If IDT_OPTION=2, the ductile-tearing model introduced in v03.1 can be activated; however, this model is no longer supported and is maintained in FAVOR for backward compatibility with v03.1 executions only. The newer ductile-tearing model (IDT_OPTION=1) is recommended when investigating the effects of ductile tearing. The flag IDT_INI provides additional reporting concerning flaw initiation due to ductile tearing. Currently, there is no model in FAVOR to determine the probability of flaw initiation by ductile tearing. The ductile-tearing model simulates re-initiation by tearing only after a flaw has arrested. The additional reporting when IDT_INI=1 provides a log of the number of potential ductile-tearing flaw initiations (when $J_{applied} > J_{Ic}$) that occurred during the analysis.

It should be noted that setting IDT_INI=1 has the potential of significantly increasing the computational time for a given run. When IDT_INI=0, the checks for ductile-tearing initiation are not carried out. When the ductile-tearing option is activated, however, checks for ductile-tearing re-initiation of an arrested flaw will always be performed.

The flag ILONG_OUT provides additional reporting concerning the contribution to the CPI and CPF from the major regions in the belt line for each transient. When ILONG_OUT=1, a series of files named *History_itran_iseq.out* (where itran is the FAVOR transient number and iseq is the associated thermal-hydraulic initiating-event sequence number from the RELAP5 cases) will be created during the execution that will contain results data for all of the RPV trials. The user should note that for long FAVPFM executions, these files could become quite large, and their creation may have an impact on run times. When ILONG_OUT=0, these files are not created.

Please note due to the current well validated and verified state of FAVOR, the original ILONG_OUT=1 setting which generates large files named *History_itran_iseq.out* will no longer be a requirement and maybe deleted in the future. Other generated files (e.g., Arrest.out and Trace.out) provide sufficient information to identify and determine cause of potential issues. See Record 7.

Record 3 – CNT3 inputs values for the flow stress, FLWSTR, in ksi to be used in the failure model of plastic collapse (ligament instability), the upper bound for K_{Ic} and K_{Ia} , USKIA, in $\text{ksi}\sqrt{\text{in.}}$, a flag K1a_Model to designate which arrest model (1 or 2) to use in checking for stable arrest, the weld layer resampling option, LAYER_OPT, (on or off), and the fraction of the total wall thickness, FAILCR, used in the vessel failure criterion. If a flaw, propagating from the inner surface of the vessel, grows to this depth into the wall (relative to the inner surface), then the event will be designated as a *vessel failure*, where $0.25 \leq \text{FAILCR} \leq 0.95$.

Record 4 – GENR 4 inputs the value of two multipliers, SIGFGL and SIGFLC, used to obtain the standard deviations of a global and local normal distribution for fluence

sampling, where the fluence at the inner surface, $\widehat{f(0)}$, is sampled from two normal distributions such that:

$$\sigma_{global} = SIGFGL \times fluence_{subregion}$$

$$\widehat{f} \leftarrow N(fluence_{subregion}, \sigma_{global})$$

$$\overline{\sigma_{local}} = SIGFLC \times \widehat{f}$$

$$\widehat{f(0)} \leftarrow N(\widehat{f}, \overline{\sigma_{local}})$$

where $fluence_{subregion}$ is the best-estimate for the subregion neutron fluence as input in the embrittlement map (to be described below).

Records 5 and 6 – SIGW AND SIGP input the values of the standard deviations of the initial normal sampling distributions for the weld and plate chemistries, respectively. On Record 5, the three data fields include the standard deviations for the weight % of copper, Cu, WSIGCU, nickel, Ni, WSIGNI, and phosphorous, P, WSIGP in welds. On Record 6, the three data fields include the standard deviations for the weight % of Cu, PSIGCU, Ni, PSIGNI, and P, PSIGP in plates and forgings. The heat estimates for Cu, Ni, and P given in the embrittlement map described below are used as the means of the normal sampling distributions for the weld and plate chemistries.

The weld chemistries are sampled using the following protocols:

$\overline{Cu} = Cu_{Heat} \times WSIGCU$ $\sigma_{Cu}^* = \min(0.0718 \times Cu_{Heat}, 0.0185)$ $\widehat{\sigma}_{Cu} \leftarrow N(\overline{Cu}, \sigma_{Cu}^*)$ $\widehat{Cu} \leftarrow N(Cu_{Heat}, \widehat{\sigma}_{Cu})$	<p style="text-align: center;"><i>For Ni-addition welds</i> <i>Heats 34B009 & W5214</i></p> $\widehat{Ni} \leftarrow N(Ni_{Heat}, WSIGNI)$ $; WSIGNI = 0.162 \quad ; \widehat{P} \leftarrow N(P_{Heat}, WSIGP)$ <p style="text-align: center;"><i>For other heats</i></p> $\widehat{\sigma}_{Ni} \leftarrow N(0.029, 0.0165)$ $\widehat{Ni} \leftarrow N(Ni_{Heat}, \widehat{\sigma}_{Ni})$
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The plate chemistries are sampled using the following protocols:

$$\widehat{Cu} \leftarrow N(Cu_{Heat}, PSIGCU) \quad ; \quad \widehat{Ni} \leftarrow N(Ni_{Heat}, PSIGNI) \quad ; \quad \widehat{P} \leftarrow N(P_{Heat}, PSIGP)$$

Record 7 – TRAC provides a mechanism for the user to put a trace on a particular flaw, KFLAW, in a specific simulation, IRPV, and for a specific transient, ITRAN. This

facility provides a Quality Assurance tool to verify the computational models(s) used to calculate values of *CPI* and *CPF*. Data describing the initiation, crack growth, and arrest check calculations are written to the files TRACE.OUT and ARREST.OUT. The variable ITRACK=1 creates flaw-tracking log tables to help identify values for (ITRAN, IRPV, KFLAW) to specify in later executions. These tables can be found in the file TRACE.OUT. An additional file is created called FLAW_TRACK.LOG which provides data for the first 10,000 flaws sampled during the execution.

Record 8 – LDQA provides a mechanism for the user to carry out, as a deterministic or diagnostic exercise, deterministic calculations for the transients received from the FAVLoad module. This utility allows the user to tailor output reports containing (1) time histories of load-related variables at a specific location in the RPV wall or (2) through-wall profiles of load-related variables at a specific transient time. There are eight parameters associated with this record appearing on a single data line.

- (1) IQA = 1 activates the deterministic analysis module; no PFM analysis will be performed.

IQA = 0 ignore the rest of the data on this data line and proceed with a PFM analysis.

- (2) IOPT = 1 generate time history results at a specific location in the RPV wall.

IOPT = 2 generate through-wall profiles of stress and applied K_I at a specific time.

- (3) IFLOR = 1 flaw orientation is axial.

IFLOR = 2 flaw orientation is circumferential.

- (4) IWELD = 0 do not include weld residual stresses.

IWELD = 1 include weld residual stresses.

- (5) IKIND = 1 inner surface-breaking flaw.

IKIND = 2 embedded flaw.

IKIND = 3 outer surface-breaking flaw.

- (6) XIN – only used if IKIND = 2 (otherwise ignored).

if IOPT = 1; XIN = location of inner crack tip from inner surface (in.).

if IOPT = 2; XIN = $2d$ = flaw depth (see Fig. 6 of FAVOR User Manual).

- (7) XVAR – meaning depends on the value of IOPT.

if IOPT = 1; XVAR = flaw depth (in.) (a for IKIND = 1; $2d$ for IKIND = 2 in Fig. 6 of FAVOR User Manual).

if IOPT = 2; XVAR = elapsed time in minutes

- (8) ASPECT - aspect ratio = L / a for IKIND = 1; aspect ratio = $L / 2d$ for IKIND = 2

if IKIND = 1 or 3; ASPECT = 2, 6, 10, or 999

if IKIND = 2; ASPECT > 0.0

Record 9 – DTRF provides a means to specify the starting and ending times for specific transients supplied in the FAVLoad output file. The variable NT sets the number of ISQ records that follow the DTRF record. The following NT records contain values for ITRAN (= the transient number in the transient stack supplied in the FAVLoad output file), ISEQ (= the corresponding identifying thermal-hydraulic sequence number), TSTART (= starting time in minutes), and TEND (= ending time in minutes). Only those transients in the FAVLoad transient stack for which the user wishes to set special values of TSTART and TEND need be identified by the DTRF records. All other transients in the stack, not explicitly specified in the DTRF records, will use the global transient start (always = 0.0) and ending times set by the execution of the FAVLoad module.

Records 10+NT and 11+NT give the number of major regions and subregions for welds and plates, respectively. The sum of the number of weld subregions, NWSUB, and the number of plate subregions, NPSUB, gives the total number of embrittlement map records to follow this keyword line. NWMAJ is the number of major weld regions, and NPMAJ is the number of major plate regions.

Records 12+NT through 11+NT+NWSUB+NPSUB contain the embrittlement map data. Following Record 11+NT, there will be NWSUB + NPSUB data lines (one record per subregion and one data line per record) that contain the embrittlement map for all of the weld and plate subregions. Note that the data records for the weld subregions must precede the data records for the plate subregions. There are 20 fields in each record.

- (1) subregion number – subregion numbers should start with 1 and then increment by 1 for the complete embrittlement map.

Flaws in welds have been observed to reside along the fusion line between the weld and adjacent plate; therefore, it is possible that the adjacent plate(s) could have a higher degree of embrittlement and/or less ductility than the weld. The embrittlement/ductility-related properties of the most limiting (of the weld or the adjacent plate) material shall be used when evaluating flaw advancement by cleavage propagation or ductile tearing. If this subregion is a weld region, FAVOR will determine if one of the adjacent plate(s), located in adjacent-plate subregions, is more limiting, i.e., has a higher RT_{NDT} for cleavage propagation and a lower value of USE_i for flaw advancement by ductile tearing (IDT_OPTION=2 only). If so, FAVOR will use the embrittlement/ductility properties of the more limiting subregion, where separate sets of parent/child relationships are determined for cleavage propagation and ductile tearing. The next two fields are valid only if the subregion designated in field 1 is a weld subregion. From a roll-out map of the RPV beltline, select the plate subregions that are adjacent to the weld subregion in field 1. If field 1 refers to a plate subregion, just repeat the subregion number from field 1 in fields 2 and 3.

- (2) left-adjacent plate subregion number
- (3) right-adjacent plate subregion
- (4) major region number
- (5) best estimate for fast-neutron fluence at inside surface of RPV wall (1019 neutrons/cm2)
- (6) heat estimate for copper content (wt% Cu), Cu_{Heat}
- (7) heat estimate for nickel content (wt% Ni), Ni_{Heat}
- (8) heat estimate for phosphorous content (wt% P), P_{Heat}
- (9) heat estimate for manganese content (wt% Mn), Mn_{Heat}
- (10) if field 1 is a weld subregion, select the method for determining the standard deviation for the normal distribution used to simulate the Ni content.

= 1 use the constant value given in the WSIGNI field on Record 5. (These are Ni-addition welds from heats 34B009 and W5214 in the RVID2 database.)

= 2 sample from a normal distribution with $\widehat{\sigma}_{Ni} \leftarrow N(0.029,0.0165)$ (all other heats).

- (10) If field 1 is a plate subregion with IRTNDT=2000 or 2006 on Record 2 (ignored if IRTNDT=992).
- = 1 Combustion Engineering (CE) plate
 - = 2 all other plates and forgings
- (11) Copper saturation flag when IRTNDT = 2000 or 2006 on Record 2 (ignored if IRTNDT=992)
- = 0 for plates and forgings
 - = 1 for Linde 80 and Linde 0091 weld fluxes
 - = 2 for all weld fluxes other than Linde 80, Linde 0091, or Linde 1092
 - = 3 for Linde 1092 weld flux
- (12) RVID2 heat estimate for unirradiated value of RTNDT (RTNDT0) (°F) (see Appendix A)
- (13) Standard deviation for RTNDT0 (°F). If the RTNDT(u) Method in Appendix A is either MTEB 5-2 or ASME NB-2331, enter a 0.0. If the RTNDT(u) Method in Appendix A is Generic, enter a best-estimate for the standard deviation.
- (14) Irradiation-shift-correlation flag when IRTNDT=2000 or 2006 on Record 2.
- = 11 → weld major region
 - = 21 → plate major region
 - = 31 → forging major region
- (14) Irradiation-shift-correlation flag when IRTNDT = 992 on Record 2.
- = 11 → weld major region; no chemistry-factor override
 - = 12 → weld major region; with chemistry-factor override
 - = 21 → plate major region; no chemistry-factor override
 - = 22 → plate major region; with chemistry-factor override
 - = 31 → forging major region

- (15) Angle of subregion element, $d\theta$ (degrees) (see Fig. 17 of the FAVOR User Manual).
- (16) Axial height of subregion element, dz (inches) (see Fig. 17 of the FAVOR User Manual).
- (17) Weld fusion area (=0.0 for plate subregions) (in²)
- (18) Weld orientation; =1 axial; =2 circumferential (ignored if Plate subregion)
- (19) Chemistry-factor override; (if IRTNDT=992 on Record 2 and irradiation shift correlation flag (field 13) = 12 or 22), otherwise set to 0.
- (20) Unirradiated upper-shelf CVN energy (USE0) in [ft-lbf] from RVID2, (used only if IDT_OPTION=2).

7.2.4 Input Requirement 3: FAVPost User Input will remain unaffected or enhanced by modernization changes.

The modernization of FAVOR will not impact the user input ensuring backward compatibility for the test suite of cases. FAVPost contains (2 x NTRAN) + 1 data records where each record may involve more than one line of data.

The following FAVPost User Inputs will be unaffected:

Record 1 – CNTL inputs the number of transients, NTRAN, for which initiating frequency probability density distributions (histograms) are being input.

Records 2 and 3 are repeated for each of the NTRAN transients.

Record 2 inputs the FAVOR transient number, ITRAN, the number of lines, NHIST, in Record 3 which contains the initiating frequency histogram (in terms of relative frequency), and the initiating- sequence event number, ISEQ, from the thermal-hydraulic studies that supplied the transient for input to FAVOR.

Record 3 contains the initiating Event Sequence Probability Density Functions (Histograms)

Input NHIST lines containing one histogram data pair per line, where the first field is the value of the transient initiating frequency in *events per reactor-operating year* and the second field is the probability density (as a relative frequency in percent).

7.2.5 Input Requirement 4: RPV flaw-characterization using the VFLAW based approach shall be unaffected.

The ability to incorporate detailed flaw-characterization distributions for surface breaking flaws, embedded flaws in welds, and embedded flaws in plates or forgings shall be maintained. [8]

7.2.6 Input Requirement 5: For incorrect user inputs, ensure that FAVOR protects user from entering into an invalid or erroneous state.

FAVOR shall display error messages to the user in the output file when a user enters an invalid entry in the user input file. These messages shall be clear and understandable enough for the user to quickly identify and understand the entry error and provide possible solutions.

FAVOR shall also display error messages to the user on the file entry screen when user specifies an incorrect file name or duplicate file name for an output file.

7.3 Functional Requirements

7.3.1 Overall Functional Requirement: All physical and empirical models shall represent the key attributes and characteristics of the phenomena being modeled to an industry acceptable standard.

The modernization of FAVOR shall not impact the results of the physical and empirical models. These have been extensively benchmarked in previous versions of FAVOR [7]. A summary of the models is shown in Table 6-1.

7.3.2 Functional Requirement 1: Modernization Changes will not significantly impact v16.1 FAVLoad, FAVPFM, and FAVPost results

The key outputs as identified in Table 6-1 shall not be adversely impacted and should provide reasonable agreement within tolerance of compiler accuracies. Differences greater than 1% are not acceptable unless there is a valid reason for the difference (e.g., correction of an error).

7.3.3 Functional Requirement 2: Both Pressurized and Boiling Reactor Vessel walls shall be adequately modeled to perform finite-element analyses in a one-dimensional axisymmetric geometry.

7.3.3.1 Fundamental vessel geometry data for the vessel beltline (where the fuel resides), including the vessel's inner radius, wall thickness, and cladding thickness shall be represented.

7.3.3.2 The beltline of the RPV shall be defined by the input data and cover the axial distance from one foot below the reactor core to one foot above the reactor core.

- 7.3.3.2.1 FAVOR shall provide the ability for the RPV beltline to be divided into major regions such as axial welds, circumferential welds, and plates or forgings that may have their own embrittlement-sensitive chemistries.
- 7.3.3.2.2 In addition, FAVOR shall provide the ability to further discretize the major regions into subregions to accommodate detailed neutron fluence maps that can include significant details regarding azimuthal and axial variations in neutron fluence.
- 7.3.3.3 *Temperature-dependent thermo-elastic properties shall be represented for the cladding and base materials.*
- 7.3.3.4 *Transient heat conduction equation with temperature-dependent properties shall be solved for the combined cladding and base materials to produce time-varying temperature profiles through the wall.*
- 7.3.4 **Functional Requirement 3: Finite-element stress analysis shall calculate radial displacements and then, through strain-displacement and linear-elastic stress-strain relationships, time-varying axial and hoop stress profiles are calculated.**
 - 7.3.4.1 *Stresses shall include the effects of thermal and mechanical loading (internal pressure applied to the inner vessel surface and exposed crack face) along with the option of superimposed weld-residual stress profiles developed by the HSST program.*
 - 7.3.4.2 *Finite-element stress model shall capture the steep stress gradient at the clad-base interface.*
 - 7.3.4.3 *Finite-element stress model shall include the Stress-free temperature by the user and consider the effects of an initial thermal-differential expansion between the cladding and base materials in the quasi-static load path.*
 - 7.3.4.4 *Finite-element thermal and stress models shall use the same quadratic elements and graded-mesh discretization.*
 - 7.3.4.5 *Applied stress-intensity factor, K_I , solutions as a function of transient elapsed time and radial position in the wall shall be calculated based on the finite-element method together with the definition of the thermal-hydraulic boundary conditions.*
 - 7.3.4.6 *Time-dependent stress-intensity factors for infinite and finite length, internal and external, surface-breaking flaws shall be calculated for a bounding range of flaw depths, sizes, and aspect ratios. These factors shall be based on valid benchmark Abaqus calculations, ASME based, or another benchmark.*
 - 7.3.4.7 *An embedded flaw model shall be implemented that bounds range of flaw lengths, sizes, and aspect ratios. The model shall be based on a valid benchmark calculation, ASME based, or another benchmark.*
- 7.3.5 **Functional Requirement 4: FAVOR shall have the capability to model internal surface breaking flaws, external surface breaking flaws, and embedded flaws that cover a wide range of aspect ratios, axial and circumferential orientations, and depths.**

- 7.3.5.1 *Stress Intensity Factor-Influence Coefficients (SIFICs) used to calculate the applied K_i shall cover the range of PWR and BWR geometries (i.e., $10 < R/t < 20$).*
- 7.3.5.2 *SIFICs shall be applied to the deepest point of the flaw crack tip.*
- 7.3.5.3 *SIFICs shall be based on valid benchmark calculations, ASME based, or another benchmark.*
- 7.3.5.4 *FAVOR shall provide the capability for the crack face to be oriented normal to either of the two opening-mode principal directions, i.e., axial stresses opening circumferential flaws and hoop stresses opening axial flaws.*
- 7.3.5.5 *FAVOR shall include the combined states of mechanical loading due to internal pressure, thermal loading due to differential expansion between the cladding and base, crack-face pressure loading on surface-breaking flaws, and through-wall thermal stress loading due to temperature gradients in the cladding and base.*
- 7.3.5.6 *Based on user selection, FAVOR shall include the effects of residual stresses in axial and circumferential welds for all of the flaw models.*
- 7.3.6 **Functional Requirement 5: Based on user selection, FAVOR shall have the ability to perform both deterministic and probabilistic fracture analyses.**
- 7.3.7 **Functional Requirement 6: For deterministic fracture analyses, based on the prior functional requirements in 7.3.3, 7.3.4, 7.3.5, and user selection, FAVOR shall provide time histories of load-related variables at a specific location in the RPV wall or through-wall profiles of load-related variables at a specific transient time.**
- 7.3.7.1 *The FAVOR deterministic analyses shall be based on user specified flaw orientation, whether or not weld residual stresses are included, type of flaw (inner surface-breaking flaw, embedded flaw, or outer surface-breaking flaw), location of inner crack tip from inner surface, flaw depth, aspect ratio, and elapsed transient time (if a through-wall profile option is selected).*
- 7.3.8 **Functional Requirement 7: For probabilistic fracture analyses, FAVOR shall implement a Monte Carlo technique, where deterministic fracture analyses are performed on a large number of stochastically generated RPV trials or realizations.**
- 7.3.8.1 *Each stochastically generated RPV shall be based on perturbations in its chemistry and fluence properties along with uncertainties in postulated flaw population.*
- 7.3.8.1.1 When using VFLAW based files, each postulated flaw shall be positioned through sampling in a particular RPV beltline subregion having its own distinguishing embrittlement parameters. Sampling of flaw geometry (depth, length, aspect ratio, and location within the RPB wall) shall be performed.
- 7.3.8.1.2 When using as-found flaw file, each specified flaw shall have its own distinguishing embrittlement parameters.
- 7.3.8.2 *Global and Local Uncertainties in fast-neutron fluence attenuation shall be considered in determining the sampled fast-neutron fluence at the crack tip.*

7.3.8.2.1 The attenuation shall take the following form:

$$\overline{f_0(a)} = \widehat{f_0}(0) \times \exp(-0.24a)$$

where a is the position of the flaw tip (in inches) relative to the inner surface. The inner surface fluence is sampled from two normal distributions such that:

$$\sigma_{global} = SIGFGL \times fluence_{subregion}$$

$$\widehat{f}_{mean} \leftarrow N(fluence_{subregion}, \sigma_{global})$$

$$\overline{\sigma_{local}} = SIGFLC \times \widehat{f}_{mean}$$

$$\widehat{f_0}(0) \leftarrow N(\widehat{f}_{mean}, \overline{\sigma_{local}})$$

where the best estimate fluence, $fluence_{subregion}$, is input by the user at the subregion level. The global SIGFGL and local SIGFLC multipliers are supplied as input by the user.

7.3.8.3 *Plane-Strain Static Cleavage Initiation Toughness (K_{Ic}) and Plane-Strain Crack Arrest Toughness (K_{Ia}) correlations shall be based on measured data using ($T - RT_{NDT}$) as an index and industry standard statistical models.*

7.3.8.3.1 Data shall meet the validity requirements given in ASTM Standard E-399 to maintain consistency with the LEFM driving forces applied in the fracture model, and unirradiated RT_{NDT0} , determined according to the ASME Boiler and Pressure Vessel Code, Section III, NB-2331 shall be available.

7.3.8.4 *In the evaluation of RT_{NDT} , both epistemic and aleatory uncertainties shall be considered.*

7.3.8.5 *RT_{Arrest} shall be based on both an index temperature that defines the position of the plane-strain crack arrest toughness, K_{Ia} , transition curve on the temperature axis and a relationship between the index temperatures for the initiation and arrest fracture-toughness curves.*

7.3.8.6 *Plane-Strain Static Cleavage Initiation Toughness, K_{Ic} , as a function of ($T - RT_{NDT}$) shall be based on a Weibull statistical distribution and the use of a lower-bounding reference temperature (as established in 7.3.9.4) using fracture toughness data (as established in 7.3.9.3).*

7.3.8.7 *Plane-Strain Crack Arrest Toughness, K_{Ia} , as a function of ($T - RT_{NDT}$) shall be based on a Lognormal statistical distribution and the use of a normalized arrest reference temperature (as established in 7.3.9.5) using fracture toughness data (as established in 7.3.9.3).*

7.3.8.8 *Stochastically sampled methods shall be applied on material chemistry (i.e., Cu, Mn, Ni, and P) for plates, forgings, and welds used in the reactor vessel beltline model.*

- 7.3.8.8.1 The material chemistry sampling protocols shall distinguish between the first flaw simulated in a subregion and all subsequent flaws in the subregion. The plate, forging, or weld chemistry for the subsequent flaws shall be perturbations of the first sampled flaw chemistry for this subregion. This variation in chemistry shall simulate local variability in the subregion chemistry.
- 7.3.8.8.2 Initial sampling shall be based on a normal distribution and any uncertainties shall be based on well recognized and credible published data for plates, welds, and forgings.
- 7.3.8.8.3 When sampling either for the first flaw or subsequent flaws, negative chemistry values shall not be permitted and instead a truncation protocol shall be used to prescribe a 0.0 value.
- 7.3.8.8.4 When sampling a subregion for subsequent flaws, local variability shall be sampled using a logistic distribution for Cu, Ni, and P, and a Johnson S_B distribution for Mn.
- 7.3.8.8.5 Chemistry Resampling in plates and forgings shall not be performed as a flaw is propagated through the wall.
- 7.3.8.8.6 Chemistry Resampling in welds shall be performed once the flaw propagates from one $1/4t$ of the vessel wall thickness to an adjoining $1/4t$ region.
- 7.3.8.8.7 Despite the possibility that some embrittlement correlations will truncate chemistry values to a maximum value, the chemistry resampling protocols shall use non-truncated upper bound values when determining the local variability in chemistry.
- 7.3.8.8.8 Any resampled chemistry values that exceed the bounds of an embrittlement correlation shall be truncated back to the appropriate upper bound or saturation limit (e.g., Cu).
- 7.3.8.9 *FAVOR shall make available stochastic tools appropriate for the uncertainty that is being applied.***
- 7.3.8.9.1 FAVOR Stochastic tools shall include, at a minimum, the following:
1. Uniform,
 2. Weibull (3 parameter),
 3. Gaussian/normal,
 4. Truncated normal,
 5. Lognormal,
 6. Johnson S_B ,
 7. Logistic, and
 8. Log-Logistic distributions.
- 7.3.8.10 *Each RPV trial shall propagate the input uncertainties with their interactions through the model, thereby determining the probabilities of crack initiation and through-wall cracking for a set of postulated transient events at a selected time in the vessel's operating history.***

7.3.8.11 *A 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 shall be evaluated at each discrete transient time step for determining probability of crack initiation.*

7.3.8.12 *An optional warm prestress (WPS) model shall be available to ascertain whether crack initiation occurs. The model shall assume a flaw is in a state of WPS when the time-rate-of-change of the applied- K_I is negative.*

If a flaw is in a state of WPS, it is not eligible for initiation (or re-initiation if it has arrested) until it leaves the WPS state.

Three conditions must be met for a flaw to not be in a state of WPS and, thereby, to be eligible for initiation. These three conditions are:

Condition (1): the applied- K_I is greater than $K_{IC(\min)}$, where $K_{IC(\min)}$ is defined by the fracture toughness model ($a_{K_{IC}}$ of the Weibull distribution) for the temperature at the flaw tip;

Condition (2): a rising applied- K_I field – the time-rate-of-change of the applied- K_I is positive ($dK_I/d\tau > 0$);

Condition (3): in a rising applied- K_I field, the driving force at the flaw tip must exceed some portion of the previously established maximum applied- K_I (designated as $K_{I(\max)}$) experienced by the flaw during the transient up to the current point in time under consideration.

7.3.8.13 *Flaws that are postulated to be in a weld shall be assumed to reside on the fusion line between the weld and adjacent plate or forging.*

7.3.8.13.1 The higher value of RT_{NDT} between the plate (or forging) and weld subregion shall be used before entering the PF Monte Carlo loop.

7.3.8.14 *PFM output shall provide the ability to estimate uncertainties in its outputs in terms of discrete statistical distributions. By repeating the RPV trials a large number of times, the output values of conditional probability of initiation ($0 \leq CPI \leq 1$) and conditional probability of failure ($0 \leq CPF \leq 1$) by through-wall cracking constitute a random sample from the probability distribution over the output induced by the combined probability distributions over the several input variables.*

7.3.9 Functional Requirement 8: The assumed initial fracture mechanism shall be stress-controlled cleavage initiation (in the transition-temperature region of the vessel material) modeled under the assumptions of linear-elastic fracture mechanics (LEFM).

7.3.9.1 *The failure mechanism by through-wall cracking shall be based on the prediction of sufficient flaw growth either (1) to produce a net-section plastic collapse of the remaining ligament or (2) to advance the crack tip through a user-specified fraction of the wall thickness.*

- 7.3.9.1.1 Flaw growth shall be based on either cleavage propagation or stable ductile tearing.
- 7.3.9.1.2 If the conditions for unstable ductile tearing are satisfied, then vessel failure by through-wall cracking shall be assumed to occur.

7.3.10 Functional Requirement 9: When calculating the Plane-Strain Static Cleavage Initiation Toughness – K_{Ic} , radiation embrittlement shall be considered and be based on an industry acceptable standard or one that has been benchmarked to a valid standard.

- 7.3.10.1 *At a minimum, one model shall include an irradiated shift in Reference Nil-Ductility Transition Temperature, RT_{NDT} , based on 10CFR50.61 (Regulatory Guide 1.99, revision 2), where:*

$$\Delta RT_{NDT} = (CF)f_0(\delta)^{(0.28-0.10\log_{10}(f_0(\delta)))}$$

CF = chemistry factor, a continuous function of copper and nickel

$f_0(\delta)$ = best-estimate neutron fluence [10^{19} n/cm²; $E > 1$ MeV] attenuated from the inner surface to the clad/base metal interface

δ = distance from the inner surface to the clad/base metal interface [in.]

- 7.3.10.2 *Other implemented irradiated shift models in RT_{NDT} shall consider the effects of matrix hardening and age hardening and be benchmarked against measured reactor surveillance data.*

These model(s) shall be based on the physical relationship between basic material composition, irradiation-condition variables, and measurable quantities such as yield-strength increase, Charpy-transition-temperature shift, and toughness-transition-temperature shift (e.g., from the database of Charpy shift values, ΔT_{30} , generated in US commercial reactor surveillance programs).

- 7.3.10.3 *Due to epistemic uncertainty in sampled CVN transition shift values, $\widehat{\Delta T}_{30}$ as typically used in the irradiated shift models above, it is necessary to transform these $\widehat{\Delta T}_{30}$ values into shifts in the fracture-toughness transition temperature. The following correction factors shall be applied:*

$$\widehat{\Delta RT}_{NDT}(r, \dots) = \begin{cases} 0.99 \widehat{\Delta T}_{30}(r, \dots) & \text{welds} \\ 1.10 \widehat{\Delta T}_{30}(r, \dots) & \text{plates and forgings} \end{cases}$$

7.3.11 Functional Requirement 10: For probabilistic fracture analyses, the determination of conditional probability of crack initiation, CPI, shall be performed as follows:

$$CPI_{(l,j,k)} = \|\{cpi(\tau^m)\}_{(l,j,k)}\|_{\infty} \text{ for } 1 \leq m \leq n, \text{ where:}$$

$cpi(\tau^m)_{(i,j,k)}$ – instantaneous conditional probability of crack initiation at time, τ^m , for transient index, i , RPV trial index, j , and flaw index, k . m is the timestep and n is the maximum timestep for each transient.

The modeled thermal-hydraulic transients shall be assumed to occur such that the conditional probability of CPI is evaluated. For combining multiple flaws, the CPI for the i^{th} transient and j^{th} RPV trial shall be calculated as:

$$\begin{aligned} CPI_{RPV(i,j)} &= 1 - \prod_{k=1}^{nflaw} (1 - CPI_{(i,j,k)}) \\ &= 1 - \left[(1 - CPI_{(i,j,1)}) (1 - CPI_{(i,j,2)}) \dots (1 - CPI_{(i,j,nflaw)}) \right] \end{aligned}$$

7.3.12 Functional Requirement 11: For probabilistic fracture analyses, a flaw propagation model shall be implemented with the following assumptions:

7.3.12.1 *For the VFLAW based flaw input, initial flaw orientation shall be assigned as follows:*

Applied Flaw Orientations by Major Region

Major Region	Flaw Category 1	Flaw Category 2	Flaw Category 3
axial weld	circumferential	axial	axial
circumferential weld	circumferential	circumferential	circumferential
plate/forging	circumferential	axial/circumferential*	axial/circumferential*

Flaw Category 1 – surface-breaking flaw

Flaw Category 2 – embedded flaw in the base material between the clad/base interface and $\frac{1}{8}t$

Flaw Category 3 – embedded flaw in the base material between $\frac{1}{8}t$ and $\frac{3}{8}t$

*Flaw Categories 2 and 3 in plates/forgings shall be equally divided between axial and circumferential orientations.

7.3.12.2 *Following crack initiation in cleavage fracture, both internal surface-breaking flaws and embedded flaws become infinite axial or 360° circumferential flaws, depending on the initial orientation.*

7.3.12.3 *For VFLAW based flaw input, when crack initiation in cleavage fracture occurs, all internal surface breaking flaws are assumed to be 360° circumferentially oriented.*

7.3.12.4 *For as-found flaw input, when crack initiation in cleavage fracture occurs, all internal surface breaking flaws retain the initial orientation and become either infinite axial or 360° circumferentially oriented.*

7.3.12.5 *For any external surface-breaking flaws or embedded flaws in the outer half of the RPV wall upon initiating in cleavage fracture shall be assumed to propagate through the entire wall thickness causing RPV failure.*

7.3.12.6 Following crack initiation, flaw geometries shall be as follows:

Post-Initiation Flaw Geometries and Orientations

FLAW TYPE & GEOMETRY	LOCATION	ORIENTATION	AFTER INITIATION
surface-breaking (semi-elliptical)	RPV internal surface	<i>circumferential</i>	360° internal surface breaking flaw
surface-breaking (semi-elliptical)	RPV external surface	<i>axial</i>	failure of RPV
		<i>circumferential</i>	failure of RPV
embedded flaw (elliptical)	crack tip between $(0 - \lambda.t)$ where: $\lambda = 3/8$ for flaw population 1; $\lambda = 1/2$ for flaw population 3	<i>axial</i>	surface-breaking infinite length flaw with nearly same depth as original crack-tip
		<i>circumferential</i>	surface-breaking 360° flaw with nearly same depth as original crack-tip
embedded flaw (elliptical)	crack tip between $(\lambda.t - t)$ where: $\lambda = 5/8$ for flaw population 2 $\lambda = 1/2$ for flaw population 3	<i>axial</i>	failure of RPV
		<i>circumferential</i>	failure of RPV

Note that as-found flaw input shall not allow for external surface breaking flaws.

7.3.12.7 The fraction of flaws that would fail the RPV shall be determined (at each time step for each flaw) by performing a Monte Carlo analysis of through-wall propagation of the infinite-length flaw.

- 7.3.12.7.1 This propagation sub model shall be an embedded Monte Carlo model that is repeated a user-set number of times using a different value of P_f each time. P_f shall be determined using a random number drawn from a uniform distribution on the open interval (0,1).
- 7.3.12.7.2 The nested-loop structure shall preclude the introduction of a bias in the results due to the arbitrary ordering of the transients. In other words, for a given RPV trial, flaw, and transient, the same value of CPI and CPF will be calculated irrespective of the position of the transient (or the number of transients) in the load-definition transient stack. This shall be accomplished by confining all random sampling to two sampling blocks, the first block at the top of the RPV Trial Loop and the second located at the top of the Flaw Loop. Any sampling required in the propagation sub model shall draw from sets of random number sequences created in the second sampling block. These set-aside random number sequences shall remain fixed for the current flaw and then are reset to the start of the sequence as each transient is incremented in the Transient Loop. New random number sequences are constructed (resampled) for each increment in the Flaw Loop.
- 7.3.12.8** *In each analysis, the infinite-length flaw shall be incrementally propagated through the RPV wall until it either fails the RPV or experiences a stable arrest.*
- 7.3.12.8.1 For the given flaw, subjected to the current transient, the change in cpi with respect to time shall be checked and if $dcpi/dt > 0$, then the flaw shall become a candidate for propagation through the wall.
- 7.3.12.8.2 Any flaw that is propagated shall assume that the propagation occurs instantaneously; i.e., the time station remains fixed during flaw growth. Time shall only advance only if the flaw is in a state of arrest.
- 7.3.12.9** *In each propagation, a K_{Ia} curve shall be sampled from the lognormal K_{Ia} distribution.*
- 7.3.12.10** *The applied K_I for the growing infinite-length flaw shall be compared to K_{Ia} as the flaw propagates through the wall. If crack arrest does not occur ($K_I \geq K_{Ia}$), the crack tip shall advance another small fixed increment, and again a check is made for arrest. If the crack does arrest ($K_I \leq K_{Ia}$), the simulation shall continue stepping through the transient time history checking for re-initiation of the arrested flaw. At the end of the Monte Carlo analysis, $P(F|I)$ shall be the number of flaws (that initiated at time τ^n) that propagated through the wall thickness causing RPV failure, divided by the total number of simulated flaws.*
- 7.3.13 Functional Requirement 12: If a ductile-tearing model is used, it shall not affect values of CPI produced by FAVOR. Counters maybe used to determine if ductile tearing maybe a potential issue for crack initiation.**
- 7.3.13.1 *Flaw growth (not CPI) shall be based on either cleavage propagation, stable ductile tearing, or if the conditions for unstable ductile tearing are satisfied, then vessel failure by through-wall cracking is assumed to occur.*

7.3.13.2 *Ductile-tearing model shall be based on measured surveillance data on RPVs such as Cu, Ni, Mn, and P content; the upper-shelf Charpy V-notch (CVN) energy, USE; and the unirradiated flow stress of the RPV steels.*

7.3.13.2.1 The ductile-tearing model shall correlate the variation of ductile crack initiation toughness, J_{IC} , with temperature and irradiation, and

7.3.13.2.2 Shall correlate the variation of ductile-tearing resistance as a function of temperature, irradiation, and accumulated ductile tearing, Δa .

7.3.13.2.3 ASTM E-1820 shall be used to develop a J_R curve in power-law model form.

$$J_R = C(\Delta a^m)$$

7.3.13.2.4 ASTM E-1820 shall also be used to establish the relationship between current flow stress, σ_f , the initiation toughness, J_{IC} , and local tearing modulus, T_R .

7.3.13.3 *If a ductile model is being used, a ductile tear shall be assumed to occur at the current time, if $J_{applied}$ is greater than or equal to the ductile-tearing initiation toughness, J_{IC} , or the current value of J_R^* , where J_R^* is the value of $J_{applied}$ corresponding to a previous time step at which a stable ductile tear occurred.*

7.3.13.3.1 $J_{applied}$ shall be determined by converting the known value of $K_{I-applied}$ using a plane-strain conversion.

$$J_{applied} = \frac{(1 - \nu^2)}{E} K_{I-applied}^2$$

7.3.13.4 *If ductile tearing occurs, the sub model shall advance the position of the flaw, a_0 , as follows:*

7.3.13.4.1 First by the amount of ductile crack extension, Δa , produced by the known value of $J_{applied}$. That is, new flaw depth is $a^* = a_0 + \Delta a$.

7.3.13.4.2 The flaw then shall be advanced to a depth a^{**} , which is the first nodal position deeper than a^* . The local material tearing modulus, T_R , and applied tearing modulus, $T_{applied}$, shall be calculated at the new nodal position.

$$T_R = \left(\frac{E}{\sigma_f^2} \right) \left(\frac{dJ_R}{da} \right) = \left(\frac{E}{\sigma_f^2} \right) \times m \times C \times \Delta a^{(m-1)}$$

where E is the elastic modulus, σ_f is the sampled irradiated flow stress, and the remaining three variables, J_R , C , and m , come from the ductile-tearing model which is dependent on temperature and level of irradiation damage.

Given a J_R curve in power-law model form and current flow stress, σ_f , the initiation toughness, J_{IC} , and local tearing modulus, T_R , shall be defined per ASTM E-1820.

7.3.13.5 *The variation of ductile-tearing initiation toughness, J_{Ic} , in both the transition regime and on the upper shelf shall be calculated based on the Wallin's Master Curve [9] using the relationship between the upper-shelf temperature, T_{US} , the Master Curve reference temperature, T_0 , and the upper-shelf Master Curve. The following steps shall be followed in determining J_{Ic} :*

[1] Estimate a value of T_0 using the following relationship:

$$\widehat{T}_0 = \frac{\left(\widehat{RT}_{NDT-DT} + 8.28 - \left\{ 100.43 \left[(-\ln(1 - P_{T_0}))^{\frac{1}{2.036}} \right] \right\} \right) - 32}{1.8} \quad [^{\circ}\text{C}]$$

where $\widehat{RT}_{NDT-DT} = \widehat{RT}_{NDT0} + \widehat{\Delta RT}_{NDT}$ with \widehat{RT}_{NDT0} equal to the sampled unirradiated value of RT_{NDT} , $\widehat{\Delta RT}_{NDT}$ equal to the shift due to radiation embrittlement, and $P_{T_0} = \Phi$ is the fractile drawn for the epistemic uncertainty in RT_{NDT} .

[2] Estimate a value of the Upper-Shelf Temperature, T_{US} :

$$\widehat{T}_{US} = 48.843 + (0.7985 \widehat{T}_0) \quad [^{\circ}\text{C}]$$

[3] Calculate the mean J_c based on the Master Curve at T_{US} using the plane strain conversion from K_{Ic} to J_c .

$$J_{c(med)} = \frac{1000\{30 + 70 \exp[0.019(T_{US} - T_0)]\}^2(1 - \nu^2)}{E} \quad \left[\frac{\text{kJ}}{\text{m}^2} \right]$$

where $E = 207200 - (57.1 T_{US})$ [MPa] and $\nu = 0.3$

[4] Calculate an Estimate for ΔJ_{Ic} at T_{US} using the following relationship of J_{Ic} with Upper-Shelf Temperature.

$$\Delta J_{Ic} = J_{Ic}^{meas} - J_{Ic}^{288^{\circ}\text{C}}$$

$$\Delta J_{Ic} = 1.75 \left\{ C_1 \exp[-C_2(T_{US} + 273.15)] + C_3(T_{US} + 273.15) \ln(\dot{\epsilon}) \right\} - \sigma_{ref}$$

$$C_1 = 1033 \text{ MPa}$$

$$\text{Where: } C_2 = 0.00698 \text{ K}^{-1} \quad \dot{\epsilon} = 0.0004 \text{ sec}^{-1}$$

$$C_3 = 0.000415 \text{ K}^{-1} \quad \sigma_{ref} = 3.3318 \text{ MPa}$$

- [5] Calculate an Estimated Mean and Standard Deviation for the Aleatory Uncertainty in J_{Ic} based on the following equation.

$$\begin{aligned} \overline{J_{Ic}} &= J_{c(\text{med})} - \Delta J_{Ic} + \\ &1.75 \{ C_1 \exp[-C_2(T_{\text{wall}} + 273.15)] + C_3(T_{\text{wall}} + 273.15) \ln(\dot{\epsilon}) \\ &\quad - \sigma_{\text{ref}} \} \left[\frac{\text{kJ}}{\text{m}^2} \right] \end{aligned}$$

where $T_{\text{wall}}(R, t)$ is a given wall temperature in [$^{\circ}\text{C}$]. The estimate for the standard deviation shall be:

$$\sigma_{J_{Ic}} = 51.199 \exp(-0.0056T_{\text{wall}}) \left[\frac{\text{kJ}}{\text{m}^2} \right]$$

- [6] A value for J_{Ic} shall be sampled from a Normal Distribution based on the above relationship which includes the aleatory uncertainty in J_{Ic} .

$$\widehat{J}_{Ic} \leftarrow N(\overline{J}_{Ic}, \sigma_{J_{Ic}}) \left[\frac{\text{kJ}}{\text{m}^2} \right]$$

where the sampled value shall be truncated at $\overline{J}_{Ic} - 2\sigma_{J_{Ic}} \leq \widehat{J}_{Ic} \leq \overline{J}_{Ic} + 2\sigma_{J_{Ic}}$

- [7] An estimate for the Power-Law Exponent, m , and Coefficient, C , in the J-R curve relationship ($J_R = C(\Delta a^m)$) shall be calculated based on the sampled value of \widehat{J}_{Ic} and the local value of the wall temperature, $T_{\text{wall}}(R, t)$ using the following equation.

$$\overline{m} = a + b \exp\left(\frac{T_{\text{wall}}[^{\circ}\text{C}]}{d}\right) + c(\widehat{J}_{Ic} [\text{kJ}/\text{m}^2])^3$$

Where:

$$\begin{aligned} a &= 0.1117 \\ b &= 0.4696 \\ c &= 5.8701 \times 10^{-09} \\ d &= -758.19 \end{aligned}$$

$$\sigma_{\text{std-error}} = 0.08425$$

$$R^2 = 0.2992$$

The J - R curve exponent m with aleatory uncertainty shall be sampled from the following normal distribution:

$$\hat{m} \leftarrow N(\bar{m}, 0.08425)$$

The J - R curve coefficient, C , shall be calculated as:

$$\hat{C} = \frac{\hat{J}_{Ic}(atT_{wall})}{\left(\frac{\hat{J}_{Ic}(atT_{wall})}{2\hat{\sigma}_f} + \Delta a_0 \right)^{\hat{m}}}$$

where $\hat{\sigma}_f$ is the sampled flow stress and $\Delta a_0 = 0.2$ mm.

7.3.14 Functional Requirement 13: For probabilistic fracture analyses, the determination of conditional probability of vessel failure, CPF, shall be performed as follows:

- 7.3.14.1 $\Delta cpi(\tau^n)$, which is the incremental change in instantaneous conditional probability of initiation between timesteps, shall be calculated based on requirement 7.3.12;
- 7.3.14.2 $P(F|I)$, the number of flaws that propagated through the wall thickness divided by the total number of initiated flaws, shall be determined;
- 7.3.14.3 $cpf(\tau^n) = \sum_{m=1}^{n_{max}} P(F|I) \times \Delta cpi(\tau^m) = \sum_{m=1}^{n_{max}} \Delta cpf(\tau^m)$, shall be determined, where n_{max} is the time step at which the current value of CPI occurred, i.e., the time at which the maximum value of $cpi(\tau)$ occurred; and
- 7.3.14.4 The sup-norm of the vector $\{cpf(\tau^n)\}$, CPF, shall occur at the same time step as the CPI.
- 7.3.14.5 Similar to CPI, the modeled thermal-hydraulic transients shall be assumed to occur such that the conditional probability of CPF is evaluated. In addition, CPF shall be calculated over many flaws as CPI is done in Requirement 7.3.12.

$$CPF_{RPV(i,j)} = 1 - \prod_{k=1}^{n_{flaw}} (1 - CPF_{(i,j,k)})$$

7.3.15 Functional Requirement 14: Output files shall be created based on values calculated in 7.3.11 and 7.3.14, one containing values of conditional probability of crack initiation (e.g., PFMI(i,j)), and the other containing values of the conditional probability of vessel failure for each modeled transient for each vessel simulation (e.g., PFMF(i,j)), respectively.

7.3.16 Functional Requirement 15: User input of the distribution of transient initiating frequencies (typically obtained from Probabilistic Risk Analyses) shall be combined with conditional probability of crack initiation from Requirement 7.3.15 to generate discrete distributions of crack initiation frequency per reactor operating year, $F(I)$.

7.3.16.1 *The following process shall be followed when combining frequencies;*

7.3.16.1.1 First for each vessel simulation, j , a sample initiating frequency (in events per reactor year) shall be generated based on the input discrete cumulative distribution function of the transient-initiating frequency for a transient.

7.3.16.1.2 $\overline{\varphi(E)}_{(i)} \leftarrow CDF_{(i,j)}$ of transient- i initiating frequency for j^{th} vessel simulation.

7.3.16.1.3 A vector of transient-initiating frequencies for this vessel simulation, $\{\overline{\varphi(E)}\}_{(1 \times N_{TRAN})}$ shall be determined by looping and using the above sampling approach for each transient, where N_{TRAN} is the total number of transients.

7.3.16.1.4 During the looping on simulated vessels, j , take the inner product of the transient initiating frequencies vector and the j^{th} column-vectors in the PFMI and PFMF matrices shall be taken.

$$\Phi(I)_{(j)} = \sum_{i=1}^{N_{TRAN}} \overline{\varphi(E)}_{(i)} PFMI(i, j)$$

7.3.17 Functional Requirement 16: User input of the distribution of transient initiating frequencies (typically obtained Risk Analyses) shall be combined with values of the conditional probability of vessel failure from Requirement 7.4 to generate discrete distributions of through-wall crack (i.e., vessel failure) per reactor operating year, $F(F)$, similar to $F(I)$ (Requirements 7.5 and 7.5.1.1).

$$(F)_{(j)} = \sum_{i=1}^{N_{TRAN}} \overline{\varphi(E)}_{(i)} PFMF(i, j)$$

7.3.18 Functional Requirement 17: Statistical data in the form of relative densities, cumulative probabilities, and estimated percentiles for vessel failure and crack initiation shall be developed and later presented in tabulated histograms and summary tables for the various discrete distributions using standard empirical distribution functions on ordinal data.

7.3.18.1 *The cumulative distribution function, CDF, $F(x)$, for $F(F)$ and $F(I)$, shall be defined by*

$$F(x) = \int_{-\infty}^x f(x) dx$$

where the estimator applied for $F(x)$ shall be based on the Kaplan-Meier estimate, $\hat{F}(x_{(i)}) = i/n$.⁴

7.3.18.2 Due to the poor fit in the true underlying distribution in the right/upper tail of the distribution based on the CDF using the above estimator, $\hat{F}(x_{(i)}) = i/n$, a shifted exponential distribution to represent the extreme right tail shall be used.

7.3.18.3 Due to Construction of Mixed Empirical/Exponential Distribution Functions, the following process shall be used.

7.3.18.3.1 Data shall be ordered by rank such that $X_1 \leq X_2 \leq \dots \leq X_n$

7.3.18.3.2 A piecewise linear CDF shall be fit to the first $n - k$ ordered data points and a shifted exponential CDF shall be fit to the k largest data points.

$$F(t) = \begin{cases} \frac{i}{n} + \frac{(t - X_{(i)})}{n(X_{(i+1)} - X_{(i)})} & \text{for } X_{(i)} \leq t \leq X_{(i+1)}, i = 0, 1, \dots, n - k - 1 \\ 1 - \left(\frac{k}{n}\right) \exp\left[-\frac{(t - X_{(n-k)})}{\theta}\right] & \text{for } t > X_{(n-k)} \end{cases}$$

Where:

$$\theta = \frac{\left[\left(\frac{1}{2} - k\right) X_{(n-k)} + \sum_{i=n-k+1}^n X_{(i)}\right]}{k}$$

7.3.18.3.3 The value of k shall be selected automatically such that only cumulative probabilities greater than 0.999 are estimated by the fitted shifted-exponential distribution.

7.3.18.3.4 The mean of this mixed distribution shall be $(X_{(1)} + X_{(2)} + \dots + X_{(n)})/n$ for $1 \leq k \leq n$, thus recovering the original sample mean.

7.3.18.3.5 The estimator for the variance shall be determined as follows:

$$\text{var}(X) = \frac{1}{3n} \left[2 \sum_{i=1}^{n-k-1} X_{(i)}^2 + \sum_{i=1}^{n-k-1} X_{(i)} X_{(i+1)} + X_{(n-k)}^2 \right] + \frac{k}{n} \left[(\theta + X_{(n-k)})^2 + \theta^2 \right] - \left[\frac{1}{n} \sum_{i=1}^n X_{(i)} \right]^2$$

⁴ Other estimators are also in common use, including the *mean rank* $\hat{F}(x_{(i)}) = i/(n+1)$ and *median rank* $\hat{F}(x_{(i)}) = (i-0.3)/(n+0.4)$ estimators.

7.3.18.3.6 Given a specified probability $0 < P_i < 1$, then the corresponding percentile (quantile) shall be calculated by:

(1) If $P_i > 1 - \frac{k}{n}$, then estimate from the fitted exponential right tail

$$X_{P_i} = X_{n-k} - \theta \ln \left[\frac{n(1 - P_i)}{k} \right]$$

(2) Else if $P_i \leq 1 - \frac{k}{n}$, then estimate from a piecewise linear interpolation within the empirical distribution.

$$X_{P_i} = \left(P_i - \frac{I}{n} \right) (X_{I+1} - X_I) + X_I$$

where I satisfies the relation $I \leq nP_i < I + 1$

7.4 Output Requirements

7.4.1 Overall Output Requirement: All important and critical input and output values shall be printed to an output file(s) for the user to assess and evaluate reactor vessel integrity.

All input shall be echoed or in the case of VFLAW based files or As-Found flaw files, only the file names need to be echoed. The important and critical outputs are temperature as a function of time throughout vessel wall location, both circumferential and axial stress with and without residual stresses as a function of time throughout vessel wall, K_I as a function of time throughout vessel wall, probability distributions of crack initiation and vessel failure, and crack initiation frequency per reactor operating year (Table 6-1).

7.4.2 Output Requirement 1: Sufficient verifiable information shall be provided in output file(s) that reference the FAVOR version number that was used to execute the case(s) along with date/time stamps of execution.

7.4.3 Output Requirement 2: Tabular results shall be printed to the output file(s), which assist the user in sorting which flaws (and flaw category), transients, material composition, vessel region, and vessel subregion have the greater or greatest impact on irradiated RT_{NDT} , CPI, and CPF.

7.4.4 Output Requirement 3: Provide error messages.

Error messages shall be provided to the user for possible user entry errors as generally described in Table 6-1. In addition, provide guidance on how to correct the user entry error.

7.4.5 Output Requirement 4: For deterministic analyses for surface breaking flaws, where a time history is selected by the user, results shall be provided in the form of tabular data

- containing time step, transient time, coolant temperature, reactor pressure, hoop stress components of membrane bending for axial flow (or axial stress for circumferential flow), applied stress intensity factor, K_I , for aspect ratios 2, 6, 10, and infinite.
- 7.4.6 **Output Requirement 5:** For deterministic analyses for embedded flaws, where a time history is selected by the user, results shall be provided in the form of tabular data containing time step, transient time, coolant temperature, reactor pressure, membrane and bending stresses, flaw shape parameter, free-surface correction factor for membrane and bending stresses, and applied stress intensity factor, K_I .
- 7.4.7 **Output Requirement 6:** For deterministic analyses where a through-wall analysis is selected by the user, results shall be in the form of those in Output Requirement 4 (surface breaking flaw) or in the form of Output Requirement 5 (embedded flaw). The tabular data contain time step, transient time, coolant temperature, and reactor pressure shall be replaced with the user selected timestep, incremental depth, temperature at that depth, and pressure at that depth. Remaining tabular stays the same except the data is reported out as a function of reactor vessel wall depth instead of time.
- 7.4.8 **Output Requirement 7:** For probabilistic LEFM analyses, user options shall be echoed in either output file (and/or "echo" type files) such that an independent reviewer can reconstruct the input without seeing the actual input file with the exception of the VFLAW flaw files.
- 7.4.9 **Output Requirement 8:** For probabilistic LEFM analyses, the following output values shall be presented:
- 7.4.9.1 *Initial random seeds used in the analysis,*
 - 7.4.9.2 *Mean value of CPI for all RPV simulations,*
 - 7.4.9.3 *Mean value of CPF for all RPV simulations,*
 - 7.4.9.4 *Tabular data showing maximum RT_{NDT} , % of flaws, number of simulated flaws, and number of flaws with $CPI > 0$, $CPF > 0$ (due to cleavage), $CPF > 0$ (due to ductile tearing) by parent subregion with totals shown for each column,*
 - 7.4.9.5 *Mean value of RT_{NDT} at crack tip,*
 - 7.4.9.6 *Tabular data showing maximum RT_{NDT} , % of flaws, number of simulated flaws, and number of flaws with $CPI > 0$, $CPF > 0$ (due to cleavage), $CPF > 0$ (due to ductile tearing) by child subregion with totals shown for each column,*
 - 7.4.9.7 *Tabular data showing number of simulated flaws, number of flaws with $CPI > 0$, % of total CPI, number of $CPF > 0$, and % of total CPF by category 1, 2, and 3 flaws for Weld and Plate for all the parent subregions with totals shown for each column,*
 - 7.4.9.8 *Tabular data showing number of simulated flaws, number of flaws with $CPI > 0$, % of total CPI, number of $CPF > 0$, and % of total CPF by category 1, 2, and 3 flaws for Weld and Plate for all the child subregions with totals shown for each column,*

- 7.4.9.9 *Tabular data showing number of simulated flaws, number of flaws with CPI > 0, % of total CPI, number of CPF > 0, and % of total CPF by category 1, 2, and 3 flaws for Weld and Plate by flaw orientation for all the parent subregions with totals shown for each column,*
- 7.4.9.10 *Tabular data showing number of simulated flaws, number of flaws with CPI > 0, % of total CPI, number of CPF > 0, and % of total CPF by category 1, 2, and 3 flaws for Weld and Plate by flaw orientation for all the child subregions with totals shown for each column,*
- 7.4.9.11 *Tabular data showing flaw depth, number of simulated category 1 flaws, number of flaws with CPI > 0 (for cat 1), % of total CPI (for cat 1), number of simulated category 2 flaws, number of flaws with CPI > 0 (for cat 2), % of total CPI (for cat 2), number of simulated category 3 flaws, number of flaws with CPI > 0 (for cat 3), and % of total CPI (for cat 3) for Weld and Plate,*
- 7.4.9.12 *Tabular data showing flaw depth, number of simulated category 1 flaws, number of flaws with CPF > 0 (for cat 1), % of total CPF (for cat 1), number of simulated category 2 flaws, number of flaws with CPF > 0 (for cat 2), % of total CPF (for cat 2), number of simulated category 3 flaws, number of flaws with CPF > 0 (for cat 3), and % of total CPF (for cat 3) for Weld and Plate,*
- 7.4.9.13 *Tabular data showing time step, transient time, % of total Cumulative Delta CPI (CDCPI), Cumulative Delta CPI of total CDCPI, % of total Cumulative Delta CPF (CDCPF), and Cumulative Delta CPF of total CDCPF.*
- 7.4.9.14 *Tabular data showing histogram of the relative density and cumulative density for initiating driving force KI for each transient.*
- 7.4.9.15 *A Failure mechanism summary for each transient which lists the number of trials where vessel failure occurred and % of total failure trials for the following failure modes:*
- 7.4.9.15.1 *Unstable ductile tearing,*
- 7.4.9.15.2 *Stable ductile tear to plastic instability,*
- 7.4.9.15.3 *Cleavage propagation to plastic instability,*
- 7.4.9.15.4 *Stable ductile tear exceeds wall depth failure criteria, and*
- 7.4.9.15.5 *Cleavage propagation exceeds wall depth failure criteria.*
- 7.4.9.16 *A cumulative summary report on multiple flaw statistics that shows the number of flaws incremented by one, the number of occasions that had that number of flaws with CPI > 0, % of total CPI that number of flaws contributed to CPI, the number of occasions that had that number of flaws with CPF > 0, and % of total CPF that number of flaws contributed to CPF. Summary totals shall be provided.*
- 7.4.10 Output Requirement 9: An array of values of conditional probability of crack initiation and the values of conditional probability of through-wall cracking (vessel failure) shall be reported in output files for each transient and RPV simulation, respectively.**
- 7.4.10.1 *A set of data reported shall be the source code version number, the number of transients, and the number of RPV simulations.*

- 7.4.10.2** *A block of data shall contain the transient sequence number and the user provided unique transient number.*
- 7.4.10.3** *Another block of data shall contain conditional probability of either crack initiation or through-wall cracking array by RPV simulation and transient.*
- 7.4.10.4** *For the output file containing the conditional probability of crack initiation, the following data blocks shall be provided:*
- 7.4.10.4.1 A data block shall contain the number of major regions and a flag indicating whether child subregions are included in the report.
 - 7.4.10.4.2 A data block shall contain an array of maximum RT_{NDT} and number of flaws by major region.
 - 7.4.10.4.3 A data block shall contain the maximum integer flaw depth in weld from weld flaw file that contains a flaw density greater than 0 and the maximum Integer Flaw depth in plate from plate flaw file that contains a flaw density greater than 0.
 - 7.4.10.4.4 A series of array data shall first contain the transient sequential number and unique user identified transient number, and then followed by an array of % of total CPI, % of total CPF due to cleavage, and % of total CPF due to ductile failure by major region for that transient.
 - 7.4.10.4.5 If the child subregion report was selected, an addition series of array data shall be provided that mimics the previous sub requirement, 7.4.10.4.4.
 - 7.4.10.4.6 The next series of data shall provide an array of percentage of total CPI for weld region for category 1, category 2, and category 3 flaws for both axial and circumferential flaws, followed by category 1, category 2, and category 3 flaws for axial flaws, and then followed by category 1, category 2, and category 3 flaws for circumferential flaws by depth of flaw for the specified transient in sub requirement 7.4.10.4.4.
 - 7.4.10.4.7 The next series shall provide data similar to the previous sub requirement, 7.4.10.4.6, except for plate material.
 - 7.4.10.4.8 CPF related data shall be provided in similar fashion as sub requirements 7.4.10.4.4 through 7.4.10.4.8, except that percentage of total CPI is replaced with percentage of total CPF.
- 7.4.10.5** *For the output file containing the conditional probability of through-wall cracking (vessel failure), the next series of array data shall first contain the transient sequential number and unique user identified transient number, and then following data results:*

- 7.4.10.5.1 % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material,
- 7.4.10.5.2 % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material,
- 7.4.10.5.3 % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material,
- 7.4.10.5.4 % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material,
- 7.4.10.5.5 % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material,
- 7.4.10.5.6 % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material,
- 7.4.10.5.7 % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Child Subregion,
- 7.4.10.5.8 % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Child Subregion,
- 7.4.10.5.9 % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Child Subregion,
- 7.4.10.5.10 % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Child Subregion,
- 7.4.10.5.11 % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Child Subregion,
- 7.4.10.5.12 % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Child Subregion,
- 7.4.10.5.13 % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Axial Flaws,
- 7.4.10.5.14 % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Axial Flaws,
- 7.4.10.5.15 % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Axial Flaws,
- 7.4.10.5.16 % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Circumferential Flaws,
- 7.4.10.5.17 % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Circumferential Flaws,
- 7.4.10.5.18 % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Circumferential Flaws,
- 7.4.10.5.19 % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Axial Flaws,
- 7.4.10.5.20 % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Axial Flaws,
- 7.4.10.5.21 % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Axial Flaws,

- 7.4.10.5.22 % of total CP and % of total CPF attributable to Category 1 Flaws in Plate Material for Circumferential Flaws,
- 7.4.10.5.23 % of total CP and % of total CPF attributable to Category 2 Flaws in Plate Material for Circumferential Flaws,
- 7.4.10.5.24 % of total CP and % of total CPF attributable to Category 3 Flaws in Plate Material for Circumferential Flaws,
- 7.4.10.5.25 % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Child Subregion for Axial Flaws,
- 7.4.10.5.26 % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Child Subregion for Axial Flaws,
- 7.4.10.5.27 % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Child Subregion for Axial Flaws,
- 7.4.10.5.28 % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Child Subregion for Circumferential Flaws,
- 7.4.10.5.29 % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Child Subregion for Circumferential Flaws,
- 7.4.10.5.30 % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Child Subregion for Circumferential Flaws,
- 7.4.10.5.31 % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Child Subregion for Axial Flaws,
- 7.4.10.5.32 % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Child Subregion for Axial Flaws,
- 7.4.10.5.33 % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Child Subregion for Axial Flaws,
- 7.4.10.5.34 % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Child Subregion for Circumferential Flaws,
- 7.4.10.5.35 % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Child Subregion for Circumferential Flaws,
- 7.4.10.5.36 % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Child Subregion for Circumferential Flaws,

7.4.11 Output Requirement 10: Final meaningful PFM statistics shall be presented to allow for statistical breakdown of mean conditional probability of crack initiation (CPI), 95th % CPI, and 99th % CPI along with the corresponding conditional probability of failure (CPF) values and a ratio of (CPF/CPI) for all transients.

- 7.4.11.1 *Probability distribution function in the form of a histogram for the frequency of crack initiation per reactor-operating year shall be provided showing both relative density and cumulative distributions.*

7.4.11.2 Summary descriptive statistics for the conditional probability of crack initiation per reactor-operating year shall be presented showing the following:

- 7.4.11.2.1 Minimum value,
- 7.4.11.2.2 Maximum value,
- 7.4.11.2.3 Range of values,
- 7.4.11.2.4 Number of RPV simulations used in the analysis,
- 7.4.11.2.5 5th percentile,
- 7.4.11.2.6 Median,
- 7.4.11.2.7 95.0th percentile,
- 7.4.11.2.8 99.0th percentile,
- 7.4.11.2.9 99.9th percentile,
- 7.4.11.2.10 Mean,
- 7.4.11.2.11 Standard deviation,
- 7.4.11.2.12 Standard error,
- 7.4.11.2.13 Variance (unbiased),
- 7.4.11.2.14 Variance (biased),
- 7.4.11.2.15 Moment Coefficient of Skewness,
- 7.4.11.2.16 Pearson's 2nd Coefficient of Skewness, and
- 7.4.11.2.17 Kurtosis.

7.4.11.3 Probability distribution function in the form of a histogram for the frequency for through-wall (vessel failure) cracking per reactor-operating year shall be provided showing both relative density and cumulative distributions.

7.4.11.4 Similar summary descriptive statistics as described in requirement 7.12.6.2 shall be presented for through-wall cracking per reactor-operating year.

7.4.12 Output Requirement 11: Breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency shall be presented by RPV beltline major region (parent).

7.4.12.1 The breakdown shall be presented in tabular form containing the following column data:

- 7.4.12.1.1 Major region,
- 7.4.12.1.2 Maximum RT_{NDT} ,
- 7.4.12.1.3 % of total flaws,
- 7.4.12.1.4 % of total frequency of crack initiation,
- 7.4.12.1.5 % of total through-wall crack frequency due to cleavage,
- 7.4.12.1.6 % of total through-wall crack frequency due to ductile,
- 7.4.12.1.7 % of total through-wall crack frequency due to both cleavage and ductile failure, and
- 7.4.12.1.8 Summary totals shall be provided, except for Major region and RT_{NDT} .

7.4.13 Output Requirement 12: Breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency shall be presented by RPV beltline major region (child), similar to the previous requirement for parent region (7.4.12 and 7.4.12.1).

7.4.14 Output Requirement 13: Breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency shall be presented by material, flaw category, and flaw depth.

7.4.14.1 A weld and then a plate breakdown shall be presented in tabular form containing the following column data:

- 7.4.14.1.1 Flaw depth,
- 7.4.14.1.2 % of total frequency of crack initiation for category 1 type flaws,
- 7.4.14.1.3 % of total frequency of crack initiation for category 2 type flaws,
- 7.4.14.1.4 % of total frequency of crack initiation for category 3 type flaws,
- 7.4.14.1.5 % of total through-wall crack frequency for category 1 type flaws,
- 7.4.14.1.6 % of total through-wall crack frequency for category 2 type flaws,
- 7.4.14.1.7 % of total through-wall crack frequency for category 3 type flaws, and
- 7.4.14.1.8 Summary totals shall be provided, except for Flaw depth.

7.4.15 Output Requirement 14: Breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency shall be presented by material, flaw category, and flaw depth for axial orientated flaws.

7.4.15.1 A weld and then a plate breakdown shall be presented in tabular form containing the same column data in the above requirement 7.12.9.1.

7.4.16 Output Requirement 15: Breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency shall be presented by material, flaw category, and flaw depth for circumferential orientated flaws.

7.4.16.1 A weld and then a plate breakdown shall be presented in tabular form containing the same column data in the above requirement 7.12.9.1.

7.4.17 Output Requirement 16: In order to assess convergence of the frequency of crack initiation and through-wall cracking frequency (per reactor-year), two output files (i.e., CPI and CPF) shall be made available to the user that contain the following tabular data:

7.4.17.1 *The trial number for both files,*

7.4.17.2 *The mean conditional probability of crack initiation per reactor-operating year in one file and mean conditional probability of through-wall cracking per reactor-operating year in the other file, respectively,*

7.4.17.3 *The 95th Percentile of the two frequencies, respectively,*

7.4.17.4 *The 99th Percentile of the two frequencies, respectively,*

7.4.17.5 *The 99.9th Percentile of the two frequencies, respectively,*

7.4.17.6 *The covariant mean of the two frequencies, respectively,*

7.4.17.7 *The 95th Percentile of the two frequencies covariance, respectively,*

7.4.17.8 *The 99th Percentile of the two frequencies covariance, respectively,*

7.4.17.9 *The 99.9th Percentile of the two frequencies covariance, respectively,*

7.4.18 Output Requirement 17: In order to assess transient impact on frequency of crack initiation and through-wall cracking frequency (per reactor-year), two output files (i.e., one for CPI and one for CPF) shall be made available to the user that contain the following tabular data for each transient:

7.4.18.1 *Probability distribution function in the form of a histogram for the frequency of crack initiation per reactor-operating year (or through-wall cracking frequency per reactor-year in the second file) shall be provided showing both relative density and cumulative distributions.*

7.4.18.2 *Summary descriptive statistics for the conditional probability of crack initiation per reactor-operating year (or through-wall cracking frequency per reactor-year in the second file) shall be presented showing the following:*

7.4.18.2.1 Minimum value,

7.4.18.2.2 Maximum value,

7.4.18.2.3 Range of values,

7.4.18.2.4 Number of RPV simulations used in the analysis,

7.4.18.2.5 5th percentile,

7.4.18.2.6 Median,

7.4.18.2.7 95.0th percentile,

7.4.18.2.8 99.0th percentile,

- 7.4.18.2.9 99.9th percentile,
- 7.4.18.2.10 Mean,
- 7.4.18.2.11 Standard deviation,
- 7.4.18.2.12 Standard error,
- 7.4.18.2.13 Variance (unbiased),
- 7.4.18.2.14 Variance (biased),
- 7.4.18.2.15 Moment Coefficient of Skewness,
- 7.4.18.2.16 Pearson's 2nd Coefficient of Skewness, and
- 7.4.18.2.17 Kurtosis.

7.4.19 Output Requirement 18: An output file shall be generated that provides the flaw arithmetic within each vessel region when using the VFLAW based flaw files.

- 7.4.19.1 Column data of major region and RPV inner surface area used in establishing the number of surface breaking flaws for each major region shall be provided.*
- 7.4.19.2 Column data of major weld region, user-input weld fusion line area, Category 2 Flaw weld fusion line area, and Category 3 weld fusion line area for each major region shall be provided.*
- 7.4.19.3 Column data of major region and plate volume for each major plate region shall be provided.*
- 7.4.19.4 Tabular data of number of flaws in each major region fractionalized by flaw category shall be provided for the 1st set of 1000 sets of flaw characterization files, such as:*
 - 7.4.19.4.1 By major weld region, # of Category 1 flaws, # of Category 2 flaws, # of Category 3 flaws, and # of total flaws, with a summary total under each column,
 - 7.4.19.4.2 By major plate region, # of Category 1 flaws, # of Category 2 flaws, # of Category 3 flaws, and # of total flaws, with a summary total under each column,
- 7.4.19.5 A breakdown of total number of flaws for the 1000 sets of flaw characterization files fractionalized by product from and category, such as:*
 - 7.4.19.5.1 The # of the flaw set (1 to 1000), # of weld Category 1 flaws, # of weld Category 2 flaws, # of weld Category 3 flaws, # of total weld flaws, # of plate Category 1 flaws, # of plate Category 2 flaws, # of plate Category 3 flaws, # of total plate flaws, and # of total plate and weld flaws for each flaw set.
 - 7.4.19.5.2 Following this breakdown, average values over the 1000 flaw characterization files of each column data provided in the previous requirement (7.12.14.6) shall be provided.
 - 7.4.19.5.3 In addition, a percentage breakdown over the 1000 flaw characterization files of each column data provided in the previous requirement (7.12.14.6) shall be provided.

- 7.4.19.5.4 Finally, an aspect ratio check for input flaw densities shall be done for weld and plate flaw specification files by selecting one row of one set of 1000 sets of flaw characterization files and printing a cumulative distribution by aspect ratio.
- 7.4.20 Output Requirement 19: FLAW_TRAC.log file shall be generated that provides the flaw arithmetic within each vessel region when using the VFLAW based flaw files.**
- 7.4.21 Output Requirement 20: CPI_History and CPF_History files shall be generated containing the running average (mean) of CPI and CPF, respectively, for the purposes of evaluating convergence.**
- 7.4.21.1 These files shall contain tabular data of trial #, mean CPI (or CPF) for transient i , $i + 1$, through the last transient.*
- 7.4.22 Output Requirement 21: An RTNDT.out file shall be generated that contains meaningful and descriptive output for crack tip RT_{NDT} distribution within the vessel. The file shall contain the following information:**
- 7.4.22.1 A table showing major region #, product, subregion # with the controlling $RT_{NDT}(max)$ for that major region and actual subregion #, and the $RT_{NDT}(max)$ value.*
- 7.4.22.2 An ascending ordered table by major region and RT_{NDT} for each major region that shows major region #, value of RT_{NDT} , # of flaws, cumulative total # of flaws, # of flaws with $CPI > 0$, cumulative total # of flaws with $CPI > 0$, summation total # of flaws over all regions, and summation total # of flaws with $CPI > 0$ over all regions.*
- 7.4.22.3 An ascending ordered table by RT_{NDT} which summarizes all major regions showing RT_{NDT} value, # of flaws, % of all flaws, % cumulative of all flaws, # of flaws with $CPI > 0$, % of all flaws with $CPI > 0$, and % cumulative of flaws with $CPI > 0$.*
- 7.4.23 Output Requirement 22: ARREST.out file shall be generated that provides detailed information on a particular flaw, transient, and vessel simulation that assists in QA verification of flaw propagation when flaw tracking option used (i.e., ITRAN, IRPV, and KFLAW specified). Otherwise, summary statistics are provided for stable arrest and histogram of stable arrest by depth of flaw shall be generated for each transient and for all transients. In addition to the summary statistics, the following detailed information shall be provided when the flaw tracking option is selected:**
- 7.4.23.1 Arrest trial # (trial number in IGA model), PF value, Parent region #, Child region #, depth of flaw, inner crack tip location (relative to inside vessel surface), flaw category #, and aspect ratio,*
- 7.4.23.2 The flaw status (e.g., initiate, propagate, arrest, reinitiate, stable), NFLAW (flaw #), TIME (elapsed time in transient), L (vessel wall internal node number in IGA model mesh), ZSURF (position of crack tip relative to inner surface), TEMP (crack tip temperature), P (scaled quantile in K_{Ia} statistical model), sampled DT30 (sampled $\overline{\Delta T}_{30}$ shift due to irradiation), sampled RT_{NDT0} , -DTEPA (sampled $-\overline{\Delta RT}_{epistemic-arrest}$ epistemic uncertainty term in RT_{Arrest}), DTARR (sampled $-\overline{\Delta RT}_{Arrest}$), DRTNDX (ΔRT_{NDT} irradiation shift), RTNDTA (RT_{Arrest} arrest reference temperature used in K_{Ia} lognormal model), RTNDT (RT_{NDT}*

irradiated reference temperature used in K_{IC} Weibull model), $TADJA$ ($\Delta T_{RELATIVE}$, temperature used in K_{Ia} lognormal model), $TADJI$ ($\Delta T_{RELATIVE}$, temperature used in K_{IC} Weibull model), KI (applied K_I [$ksi\sqrt{in.}$]) for driving force for crack, KIC (current value of K_{IC} [$ksi\sqrt{in.}$]), KIa (current value of K_{Ia} [$ksi\sqrt{in.}$]), $KJIC$ (current value of J_{IC} converted to K_{JIC} [$ksi\sqrt{in.}$]), KJR^* (current value of J_R^* converted to K_{JR^*} [$ksi\sqrt{in.}$]), $USEI$ (current value of irradiated upper-shelf CVN energy (ft-lbf), C_{DT} (coefficient for sampled J_R curve where $J_R = C_{DT}(\Delta\alpha^{m_{DT}})$), m_{DT} (exponent for sampled J_R curve where $J_R = C_{DT}(\Delta\alpha^{m_{DT}})$), $da0$ (accumulated flaw advancement under stable ductile tearing), P_{T0} (cumulative probability used in sampling $T0$), P_{JIC} (cumulative probability used in sampling for J_{IC}), P_m (cumulative probability used in sampling m_{DT} , and $sflow$ (sampled flow stress).

7.4.23.3 If a trial results in chemistry being resampled, the following values shall be reported:

7.4.23.3.1 SCU (sampled copper content), SNI (sampled nickel content), SPHOS (sampled phosphorous), and SMN (sampled manganese content),

7.4.24 **Output Requirement 23: TRACE.out file shall be generated that provides verification data for CPI and CPF calculations when Flaw tracking option is used (i.e., ITRAN, IRPV, and KFLAW specified). Otherwise, Summary of Category 1,2, and 3 Flaws that experience vessel failure, stable arrest, reinitiated, stable ductile tearing, or unstable ductile tearing by material type and flaw orientation are provided. If the Tracking option is used, the following detailed information shall be provided:**

7.4.24.1 *ITRAN* (transient #), *IRPV* (RPV Simulation), *FLAW*(Flaw #), *Subregion #s* (associated with Parent and Child), *IPASS* (number of flaws in the parent subregion), *SCU* (sampled \widehat{Cu} content), *SNI* (sampled \widehat{Ni} content), *SPHOS* (sampled \widehat{P} content), *SMN* (sampled \widehat{Mn} content), *SFID* (sampled/attenuated fluence $\widehat{f}_0(r) \times 10^{19}$ neutrons/cm² at the crack tip), *RTNDT0* (sampled unirradiated \widehat{RT}_{NDT0}), *DRTEPI* (sampled $\widehat{\Delta RT}_{epistemic}$ epistemic uncertainty term in \widehat{RT}_{NDT0}), *DRTNDT* (sampled $\widehat{\Delta T}_{30}$ CVN shift term from Eason and Wright model), *SDRTNDT* (sampled $\widehat{\Delta RT}_{NDT}$), *RTNDT* (sampled irradiated at crack tip), *FLAW CAT* (flaw category), *DEPTH* (flaw depth), *XINNER* (inner crack tip position for embedded flaws), *ASPECT* (flaw aspect ratio), *IORIENT* (axial=1 or circumferential=2 flaw orientation), *IHEAT* (inner surface=1 or outer surface=2 flaw), *I* (time increment counter), *TIME*(elapsed time in transient), *KI* (applied K_I [$ksi\sqrt{in.}$]). *TEMP* (temperature at crack tip), *CPI* (current conditional probability of initiation), *CDCPI* (current Δ_{cpi}), *FAIL CL* (number of trials failing the vessel at this time increment due to cleavage), *FAIL DT* (number of trials failing the vessel at this time increment due to ductile tearing), *CDCPF* (current Δ_{cpf} at this time), and *CPFTOT* (conditional probability of failure).

7.5 Performance Requirements

7.5.1 Performance Requirement 1: Run times will not be significantly degraded.

Runtimes are expected to be improved based on the result of modernization, particularly for those routines where parallel computations can be implemented.

7.5.2 Performance Requirement 2: Capable to be run on MAC, LINUX, and Microsoft Windows operating systems.

Executables based on the same source code shall be able to be run on MAC, LINUX, and Microsoft Windows operating systems and shall produce equivalent results within the tolerance of compilers.

Here ends the Software Requirements Document.