Technical Letter Report

TLR-RES/DE/REB-2022-03

FAVOR Software Design Document for v20.1.12

Date:

April 22, 2022

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 Design Document
Project Number	Subtask 1.2 of task order 31310020D0005 / 31310020F0103
Internal Project Organization	NRC/RES/DE/REB

Revision History

Revision	Date	Comments
0	04/22/2022	Original

Signatures

Role	Name	Signature	Date
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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: 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 Software Design 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 report is the Software Design Document (SDD) for FAVLoad, FAVPFM, and FAVPost.

Consistent with the FAVOR Software Quality Assurance Plan (Reference [3]) , the Software Design Document (SDD) covers the computational and logical sequence necessary to meet the software requirements for v20.1.12 (Reference [4]). Consistent with the FAVOR SQA plan, applicable software architecture, numerical methods, mathematical models, physical models, control flow, control logic, data model, data flow, process flow, data structures, process structures, and the applicable relationships between data structures and process structures are addressed. The design of the user interface and design of interfaces with other software are also specified. The software design considers FAVOR's current program's operating environment. Measures are also discussed to mitigate the consequences of problems. These potential problems include external and internal abnormal conditions and events that can affect the computer program critical outputs or functionality. Sufficient information in the design has been provided such that the code description can be passed to a competent programmer for implementation. The Software Design Description Criteria Form FAVOR-SQA-5 (Appendix E of Reference [3]) are used as an aide in developing this SDD.

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3 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 1, and a list of key documents that the project team creates during the life cycle of FAVOR development are shown in Table 2. This report focuses on the green highlighted document shown in these tables.

Table 1: Functional Responsibility Matrix[1]

P=Prepare/Perform A=Approve I=Input R=Review S=Surveillance OD=Own & Distribute **Documents/Actions**	NRC PM	Contractor PM	Code Custodian	Records Custodian	Software Developer	Software Tester	SQE[2]	QA Manager[2]
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		
Softwarel Test Plans[3] (STPs)		A	I, R[4]		I, R	P		

[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 **Documents/Actions**	NRC PM	Contractor PM	Code Custodian	Records Custodian	Software Developer	Software Tester	SQE[2]	QA Manager[2]
V&V Plan (SVVP)	I, R, A	I, R, A	R[4]	OD	I, R	P	I, R[4]	R, A
Software Tests and Results Reports[2] (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
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 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
Implementation Documentation   **1. FAVLoad, FAVPFM, FAVPost source code and executables**   **2. User's Manual**   **3. FAVOR Theory Manual**   **4. Acceptance Test Problems**

4 Software Description

The **F**racture **A**nalysis of **V**essels – **O**ak **R**idge (**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, then 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 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.

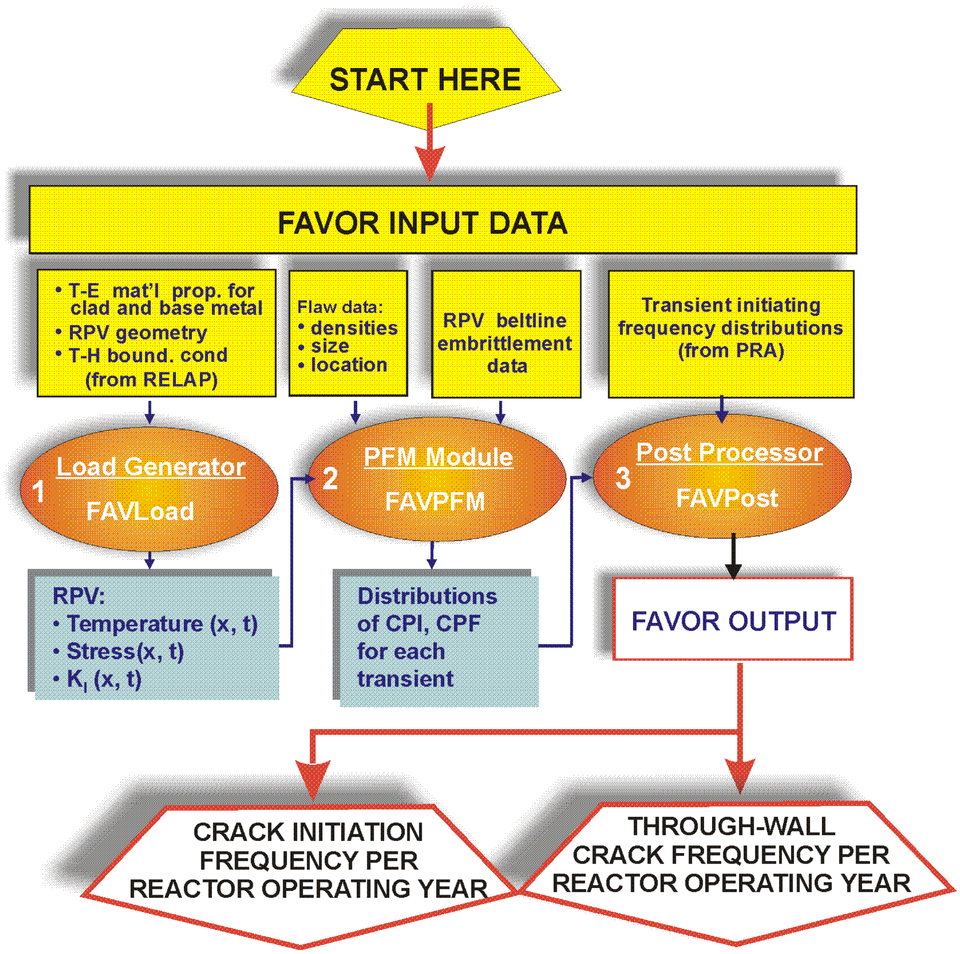


Figure 1: FAVOR data streams for (1) FAVLoad, (2) FAVPFM, and (3) FAVPost.

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 and 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-elliptical 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 3. 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 (v20.1.12) of FAVOR processes the Table 3 inputs from the user 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 2 illustrates a PWR example.

One objective of the modernization of FAVOR is to <u>not impact</u> the results of the fundamental models and algorithms in Table 3. 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 3: FAVOR Critical Inputs, Functions, and Outputs

Type	Description
Key Inputs	• 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 characteristics: density (if sampling approach is used), size, orientation, 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	• FAVLoad Deterministic analyses
	  ○ 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
	  ○ Warm prestressing logic
	  ○ Truncation for probability distributions
	  ○ Conditional Probability of Initiation (CPI) and Failure (CPF)
	  ○ Post initiation of 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	• 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

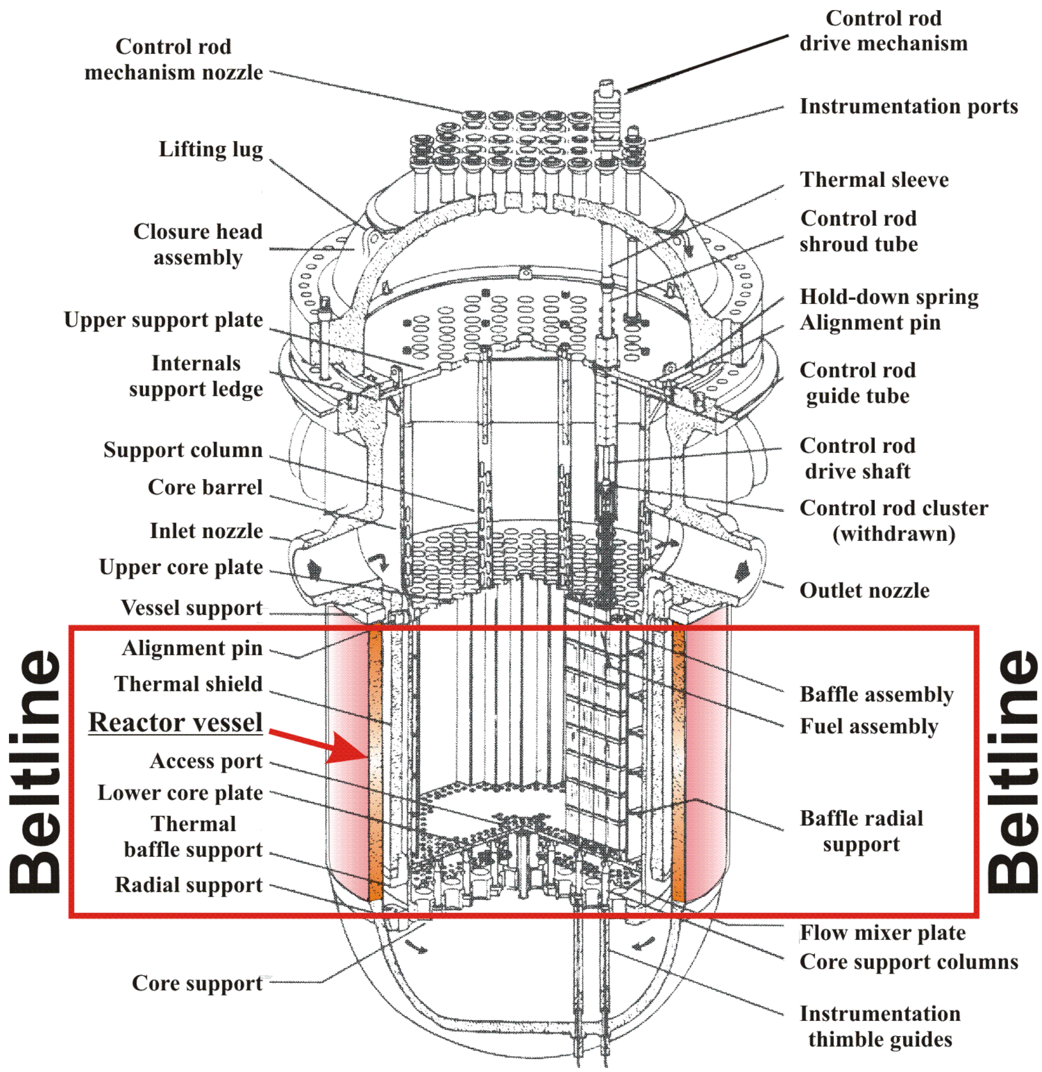


Figure 2: The beltline region of the reactor pressure vessel wall extends from approximately one foot above the active reactor core to one foot below the core for a pressurized water reactor (PWR).

5 Software Design

Due to the history of FAVLoad, FAVPFM, and FAVPost, the past software design is referenced from the code description documents (References [1] and [8]). FAVLoad, FAVPFM, and FAVPost are written in Fortran and should remain that way for new development.

The design of the new FAVOR software modifications is focused on satisfying the software requirements specified in the following:

- The Software Design Document details how the software shall be structured to satisfy the software requirements.
- Instructions for users to compile the code on a Windows PC, MAC OS, and LINUX OS are included with the release of the code.
- 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 public release of the code from GitHub.
- New design features are described in the next revision of the FAVOR Theory and or User's Manual, as applicable.

This remainder of this section defines the computational sequence necessary to meet the software requirements. Although the FAVOR Theory Manual [1] currently contains the SDD, this section complements that Theory manual by providing the additional control flow and logic required to meet the SRD requirements for the as-found flaw input. The design of the user interface and design of interfaces with other software is unaltered other than providing an as-found flaw file versus providing three VFLAW based flaw files. The design also maintains the same operating environment as v16.1 (i.e., MS Windows based). The software requirements and the design within this section incorporate measures to identify problems in user input that can affect the computer program critical outputs or functionality.

The design documentation in this section contains enough information so that the design can be passed to a competent programmer for implementation.

In order to meet software quality assurance requirements, the Software Design Description Criteria Form FAVOR-SQA-5 (see FAVOR SQAP [3]) is used as an aide.

45 design steps comprise the incorporation of the various Software Requirements stated in Reference [4]. Table 4 provides a summary and cross reference between the primary design step and the implemented software requirement(s). Note that the table only provides the most fundamental and most relevant cross reference. When taken in whole, all design elements are required to meet the software requirements. For instance, the modules or common blocks are required for most of the Software Requirements since it contains data that will be used across multiple routines. The intent of the table is to show major design logic. Although a design step may be involved in a minor way for some software requirement, it will not be shown in the table, as this would not focus on the most important design step for that software requirement. References are provided within each design step to the relevant Fortran source routines. All the Fortran source routines for v20.1.12 can be found on the NRC's FAVPRO GitHub repository (NOTE: Access to this GitHub repository is limited to NRC and its contractors).

Table 4: Software Design Verification Against Software Requirements

Software Requirement	Design Step(s) implementing requirement
7.1 General Requirement: Implement modernization standards.	**Design 1**
7.2.1 Overall General Requirement: User Input Remains the Same as v20.1.1.	**Design 2**
7.2.2 Input Requirement 1: FAVLoad User Input will remain unaffected or enhanced by modernization changes.	**Design 2**
7.2.3 Input Requirement 2: FAVPFM User Input will remain unaffected or enhanced by modernization changes.	**Design 2**
7.2.4 Input Requirement 3: FAVPost User Input will remain unaffected or enhanced by modernization changes.	**Design 2**
7.2.5 Input Requirement 4: RPV flaw-characterization using the VFLAW based approach shall be unaffected.	**Design 2**
7.2.6 Input Requirement 5: For incorrect user inputs, ensure that FAVOR protects user from entering into an invalid or erroneous state.	**Design 3**
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.	**Design 4 thru Design 30**
7.3.2 Functional Requirement 1: Modernization Changes will not significantly impact v16.1 FAVLoad, FAVPFM, and FAVPost results.	**All Design #s**
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.	**Design 4**
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.	**Design 5**
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.	**Design 6**
7.3.6 Functional Requirement 5: Based on user selection, FAVOR shall have the ability to perform both deterministic and probabilistic fracture analyses.	**Design 7**
7.3.7 Functional Requirement 6: For deterministic fracture analyses, based on the prior functional requirements in 7.3.3, 7.3.4, and 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.	**Design 8**

Software Requirement	Design Step(s) implementing requirement
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.	**Design 9**
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).	**Design 10**
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.	**Design 11**
7.3.11 Functional Requirement 10: For probabilistic fracture analyses, the determination of conditional probability of crack initiation, CPI, shall be performed as described in the SRD.	**Design 12**
7.3.12 Functional Requirement 11: For probabilistic fracture analyses, a flaw propagation model shall be implemented with the assumptions described in the SRD.	**Design 13**
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.	**Design 14**
7.3.14 Functional Requirement 13: For probabilistic fracture analyses, the determination of conditional probability of vessel failure, CPF, shall be performed consistent with the approach described in the SRD.	**Design 15**
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.	**Design 16**
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, $\boldsymbol{F(I)}$.	**Design 17**
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 7.3.15 to generate discrete distributions of through-wall crack (i.e., vessel failure) per reactor operating year, $\boldsymbol{F(F)}$, similar to $\boldsymbol{F(I)}$ (Requirements 7.3.16).	**Design 18**
7.3.16 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.	**Design 19**

Software Requirement	Design Step(s) implementing requirement
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.	**Design 20**
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.	**Design 21**
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.	**Design 22**
7.4.4 Output Requirement 3: Provide error messages.	**Design 23**
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 flaw (or axial stress for circumferential flaw), applied stress intensity factor, K_I, for aspect ratios 2, 6, 10, and infinite.	**Design 24**
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.	**Design 25**
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.	**Design 26**
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.	**Design 27**
7.4.9 Output Requirement 8: For probabilistic LEFM analyses, the output values as listed in the FAVOR SRD shall be presented.	**Design 28**
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.	**Design 29**

Software Requirement	Design Step(s) implementing requirement
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), 95^{th} % CPI, and 99^{th} % CPI along with the corresponding conditional probability of failure (CPF) values and a ratio of (CPF/CPI) for all transients.	**Design 30**
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).	**Design 31**
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 (i.e., 7.4.12).	**Design 32**
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.	**Design 33**
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.	**Design 34**
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.	**Design 35**
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 tabular data as described in the FAVOR SRD.	**Design 36**
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 tabular data for each transient as described in the FAVOR SRD.	**Design 37**
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.	**Design 38**
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.	**Design 39**
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.	**Design 40**
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 information as described in the FAVOR SRD.	**Design 41**

Software Requirement	Design Step(s) implementing requirement
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 detailed information described in the FAVOR SRD shall be provided when the flaw tracking option is selected.	**Design 42**
7.4.23 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. Detail information, as described in the FAVOR SRD, shall be provided when the flaw tracking option is selected.	**Design 43**
7.5.1 Performance Requirement 1: Run times will not be significantly degraded.	**Design 44**
7.5.2 Performance Requirement 2: Capable to be run on MAC, LINUX, and Microsoft Windows operating systems.	**Design 45**

Design 1 Implement modernization standards (SR 6.1).

This design step is continuously being implemented and leverages GitHub through continous integration and testing. See github link (FAVOR/SourceCodeImprovementList.md at main · NRC-Research/FAVOR (github.com))

Design 2 Modifications are designed to ensure backward compatibility in reading input files.

Implements software requirements 1, 2, 3. The following tabulated main subroutines are used in reading user input:

Main Program	Subroutine	Description
FAVLoad	FILE_INIT_LOAD(FNAME1,FNAME2)	Queries for user input/output file names. Calls Banner_load routine.
FAVLoad	RDINPT(MTRAN,NTRVAR)	Main Routine for reading the FAVLoad input data file. Calls STRIP_LOAD and RD79 subroutines.
FAVLoad	STRIP_LOAD(I)	Subroutine strips comment from the user input dataset (file 78) of all keywords and creates a numeric file in file 79.

Main Program	Subroutine	Description
FAVLoad	RD79 (MTRAN,NTRVAR)	This subroutine reads numeric file 79 and stores data in module therm_h, such as vessel geometry data (including finite element node data), thermoelastic material properties of base and cladding, and transient definition. This subroutine also echoes the input data to an output file and generates the thermal transient data when the user has selected a stylized transient definition. RD79 calls subroutines get_fields, get_real, get_int, xermsg to parse user entered data, and print error messages in the case of user error. In addition, xsetua, check_alloc_load, pchim, pchfe, xerdmp, and xerabt.
FAVPFM	FILE_INIT_PFM (IQA, TC, FNAME1, FNAME2, FNAME3, FNAME4, FNAME5, FNAME6, FNAME8, MTRAN, THICK)	Queries user for input/output filenames and opens all files. Calls routines strip_comments, banner_pfm, echo_pfm, echo2, RDDET and RDPFM, and check_alloc_pfm.
FAVPFM	STRIP_COMMENTS	This subroutine strips out comment lines from file "ird=41" and writes remaining lines to file "iout=42”.
FAVPFM	RDDET (MTRAN,THICK)	Subroutine RDDET reads the user specified FAVLoad output dataset which contains the load data.
FAVPFM	RDPFM	Subroutine RDPFM performs the following tasks: 1. Reads the user-created FAVPFM input dataset from file 15. 2. Strips the comment cards (those cards having an * asterisk in column 1) and card type names and writes the comment-free dataset to file 16. 3. Writes cards of FAVPFM input dataset to file 17 as a numeric file which will later be read into memory. This subroutine calls subroutines RDBAL and RD17 to accomplish these tasks. 4. Reads numeric file 17 into memory
FAVPFM	RDSURF (ISMAX)	Reads data from the user specified VFLAW input file that characterizes surface-breaking flaws (category 1 flaws) and is applicable to both weld and plate regions.

Main Program	Subroutine	Description
FAVPFM	RDWELD (IWMAX)	Reads data from the user specified VFLAW input file that characterizes embedded flaws postulated to reside in weld regions.
FAVPFM	RDPLAT (THICK, IPMAX, RO, RI)	Reads data from the user specified VFLAW input file that characterizes embedded flaws postulated to reside in plate regions.
FAVPFM	RDFOUND (NWSUB, NTSUB, THICK, ISMAX, IWMAX, IPMAX)	Reads in the user-specified as-found flaw file containing unique flaw id, flaw type, subregion, flaw orientation, flaw depth, aspect ratio, and flaw radial location within vessel wall.
FAVPost	FAVPost	Main routine which performs the following reads: 1. Reads in the FAVPFM generated INITIATE.DAT (Unit 86) and FAILURE.DAT (Unit 87) files. 2. If the FAVPFM NSIM.DAT file exist, reads in the number of RPV simulations. 3. Reads in the user prompted response for number of RPV simulations and whether or not convergence tables are built. If convergence tables are being built, reads in user response for RPV Trial Increment. 4. Calls FILE_INIT_POST subroutine.
FAVPost	FILE_INIT_POST(FNAME1,FNAME2, FNAME3, FNAME4)	This subroutine queries user for input/output filenames and opens all files.
FAVPost	RDCPI(MTRAN,NSIM1,NSIM,PFMI, SMPCTI, SMPCTF_CL, SMPCTF_DT, SMPCTIA, SMPCTFA, SMPCTIC, SMPCTFC, SMPCTI_C, SMPCTF_CL_C, SMPCTF_DT_C, SMPCTIA_C, SMPCTFA_C, SMPCTIC_C, SMPCTFC_C, NTMAJ, IEND, ICHILD, WIPCTK1, WIPCTK2, WIPCTK3, WFPCTK1, WFPCTK2, WFPCTK3, PIPCTK1, PIPCTK2, PIPCTK3, PFPCTK1, PFPCTK2, PFPCTK3, IWMAX, IPMAX)	This subroutine reads the file containing the values of conditional probability of initiation (fracture) that is generated by the FAVPFM module. These values are stored in the PFMI (i,j) array, where the (i,j) value if the conditional probability that the jth vessel will experience cleavage fracture when subjected to the ith transient.

Main Program	Subroutine	Description
FAVPost	RDCPF(MTRAN, NSIM1, NSIM, ICHILD, write_to_output, PFMF, WIPCT, WFPCT, WIPCTA, WFPCTA, WIPCTC, WFPCTC, PIPCT, PFPCT, PIPCTA, PFPCTA, PIPCTC, PFPCTC, WIPCT_C, WFPCT_C, WIPCTA_C, WFPCTA_C, WIPCTC_C, WFPCTC_C, PIPCT_C, PFPCT_C, PIPCTA_C, PFPCTA_C, PIPCTC_C, PFPCTC_C)	This subroutine reads and stores the file containing the values of conditional probability of vessel failure that is generated by the FAVPFM module. These values are stored in the PFMF (i,j) array, where the (i,j) value is the conditional probability that the jth vessel will fail due to cleavage fracture when subjected to the i^{th} transient. Failure means that the flaw that initiated in cleavage fracture is predicted to propagate through the vessel wall to a distance corresponding to a user-specified fractional part of the wall thickness.
FAVPost	RDPRA	Reads the user-input file which contains the PRA data (the probability distribution functions (pdfs, also known as histograms). Also strips the file of all comment records (by calling the STRIP subroutine) that contain an asterisk in column 1 and writes the results to file 84. Then rewinds file 84 and strips it of all non-numeric characters and writes the all-numeric file to file 83 such that the data can be read into memory by subroutine PRA.
FAVPost	PRA(MTRAN, NHIST, ISEQI, TFREQ1, CDFQ, IPPFM, IPPOST)	Reads in user-specified probability distributions functions (pdfs) for the transient initiating frequencies.

Design 3 Check for incorrect user inputs and provide guidance to user on errors.

Main Program	Subroutine	Description
Common	SLATEC error handling routines (xsetua, xsetf, xermsg, xermax)	Routines that handle generic input errors.
Common	check_alloc(func_name, error, nerr, nf_out)	Checks for memory allocation errors that might be caused by input errors and protects user from entering into an invalid or erroneous state.
Common	FILE_INIT	Common to FAVLoad, FAVPFM, and FAVPOST, this subroutine checks for missing or duplicate input and output file names.
FAVLoad	RD79 (MTRAN,NTRVAR)	Following input errors are checked: 1. Reactor Vessel geometry entries, 2. Material Properties (e.g., thermal conductivity, specific heat, Young's modulus, coefficient of thermal expansion-alpha, and Nu) for base and clad, 3. Thermal stress-free temperature and crack-face pressure loading option, 4. Axial and circumferential weld residual

		stress options, 5. Total transient time and time increment, 6. Number of transients, 7. Transient identifiers, ITRAN and ISEQ, 8. Time history table for convective film coefficient, 9. Time history table for coolant temperature (tabular data but not exponentially decaying time history), and 10. Time history table for internal coolant pressure.
FAVPFM	RD17 (TC,IQA) in module read_data_s	Following input errors are checked: 1. The number of specified values on each control card are met, 2. FAILCR input value is between 0.25 and 0.95, 3. ITRAN is not greater than MTRAN, 4. Mismatch between ITRAN and ISEQ, 5. Weld subregion definitions, 6. Plate subregion definitions, 7. Consistency of Chemistry and RT_{NDT0} values in subregions within a major region, 8. Number of specified IGA trials less than maximum allowed, 9. Number of specified IGA trials more than minimum allowed.
FAVPFM	RDSURF, RDWELD, and RDPLAT	Checks user specified VFLAW files for version number and invalid data entry.
FAVPFM	RDFOUND	Following input errors are checked for user specified flaws in the as-found flaw file: 1. Incorrect version number, 2. Subregion number greater than total number of subregions, 3. Flaw orientation is different than axial or circumferential, 4. Outside allowable minimum and maximum depth for surface breaking flaws and/or embedded flaws, 5. Aspect ratio for surface breaking flaws is not either 2,6,10 or 99, 6. Aspect ratio for embedded flaws is not between 1 and 20, and 7. Duplicate flaw-ids.
FAVPOST	Main Program	Checks for version number in FAVPFM output files and for consistency in the number of specified transients and transient sequence number.

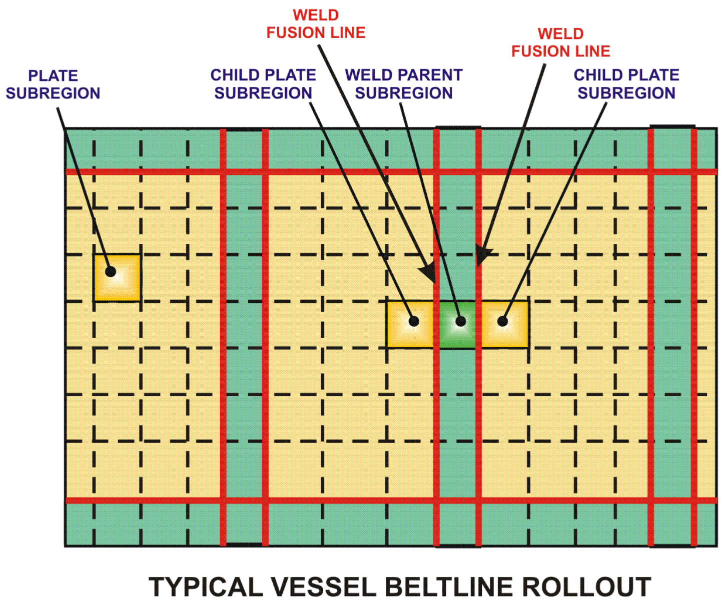
FAVPOST	PRA	Following input errors are checked for user specified flaws in the as-found flaw file: Inconsistent number of transients between PRA input file and FAVPFM output files used as input, Invalid histogram data, and Invalid TH sequence number.

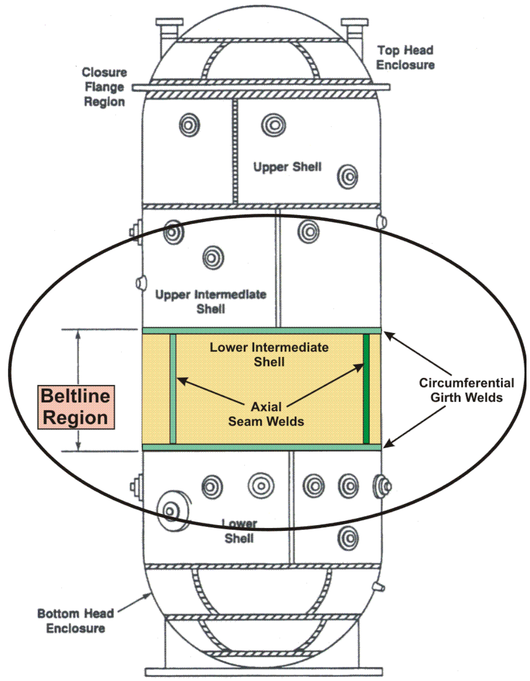
In order to ensure that all physical and empirical models represent the key attributes and characteristics identified in Table 3 to an industry acceptable standard, Design 4 through Design 41 steps are implemented.

Design 4 Model both Pressurized and Boiling Reactor Vessel Beltline walls so finite-element thermal analyses in a one-dimensional axisymmetric geometry can be performed.

The design in modeling both PWR and BWR vessel walls with a finite-element thermal analysis in a one-dimensional axisymmetric geometry is based on the following:

1. In order to solve finite-element equations consistent with a one-dimensional axisymmetric geometry (Reference [9]) for a cylindrical vessel with clad and base material, fundamental vessel geometry data, including vessel's inner radius, wall thickness, and cladding thickness are required. Temperature-dependent thermo-elastic properties are also required for the cladding and base materials. This design requirement is captured under Design 2 and 3 above for the FAVLoad input. An illustrative picture of a BWR below shows how specification of subregion in FAVPFM input can be used to resolve the variation in radiation damage in terms of plate, axial weld, and circumferential weld major regions. Note for purposes of calculating temperature, hoop stress, and axial stress time-history profiles, the specification of plate, axial weld, or circumferential weld regions are not required.





2. To perform a thermal analysis to determine the temperature time-history, $T(r,\tau)$, FAVLoad models the RPV wall as an axisymmetric one-dimensional structure with the temperature profile being dependent on the radial position, r, and elapsed time, τ, in the transient. In the absence of internal heat generation, the transient heat conduction equation is a second-order parabolic partial differential equation:

$$\rho\ c_p(T)\ \frac{\partial T}{\partial \tau} = \frac{1}{r}\frac{\partial}{\partial r}\left[k(T) r \frac{\partial T}{\partial r}\right]$$

where ρ is the mass density, $c_p(T)$ is the temperature-dependent mass-specific heat capacity, and k(T) is the temperature-dependent thermal conductivity. Note that any temperature dependencies in the mass density should be included in the characterization of the mass-specific heat capacity, leaving the mass density as a constant in the problem formulation. The above equation can be expressed in the following canonical form:

$$\frac{\partial \mathrm{T}}{\partial \tau} - \frac{1}{\mathrm{r}}\frac{\partial}{\partial \mathrm{r}}\left[\lambda(\mathrm{T})\ \mathrm{r}\ \frac{\partial \mathrm{T}}{\partial \mathrm{r}}\right] = 0 \text{ for } \mathrm{r} \in \mathbb{R}^1; \tau \in (0,\infty)$$

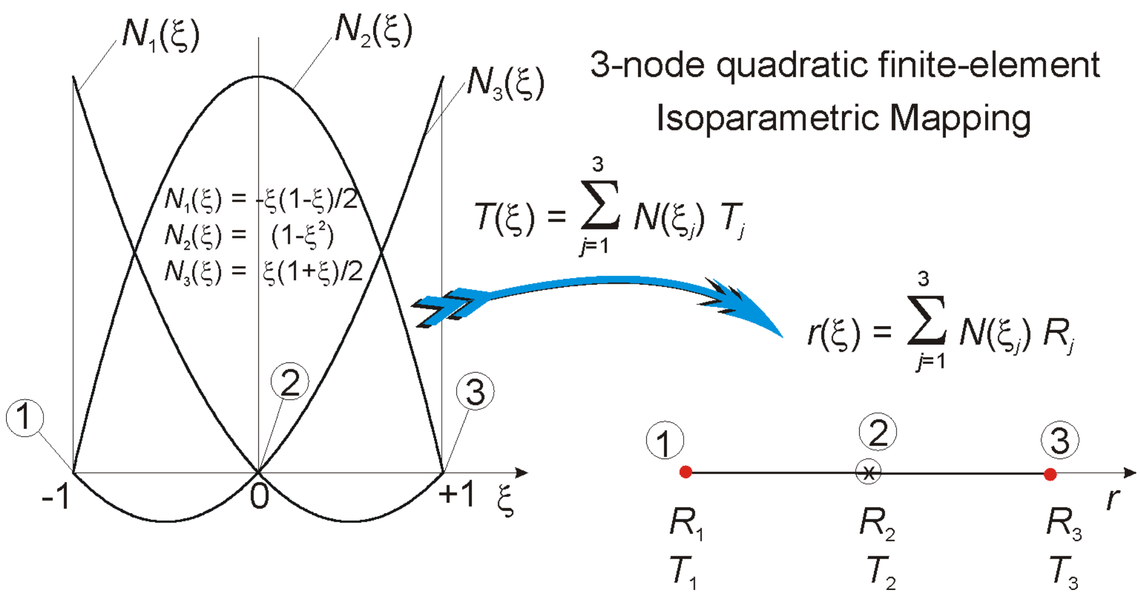
where the property grouping $\lambda(T) = \frac{k(T)}{\rho\ c_p}(T)$ is the temperature-dependent thermal diffusivity of the material. The initial and boundary conditions are then applied.

$$\underline{\text{Initial Condition}}$$
$$T(r,0) = T_{initial} \text{ for } R_i \le r \le R_o$$

$$\underline{\text{Boundary Conditions}}$$
$$q(R_i,\tau) = h(\tau)(T_\infty(\tau) - T(R_i,\tau)) \text{ at } r = R_i$$
$$q(R_o,\tau) = 0 \text{ at } r = R_o$$

where q is a prescribed boundary heat flux, $h(\tau)$ is the time-dependent convective film coefficient, $T_\infty(\tau)$ is the time-dependent bulk coolant temperature, and R_i and R_o are the inner and outer radii of the vessel wall, respectively. Input data to the thermal model include the mesh definition, property data, and prescribed time-histories for $h(\tau)$ and $T_\infty(\tau)$.

Isoparametric mapping is employed for the finite-element method [9], see figure below. To arrive at an axisymmetric $\mathbb{R}^1$ Euclidean space, the isoparametric mapping uses three-node quadratic basis functions.



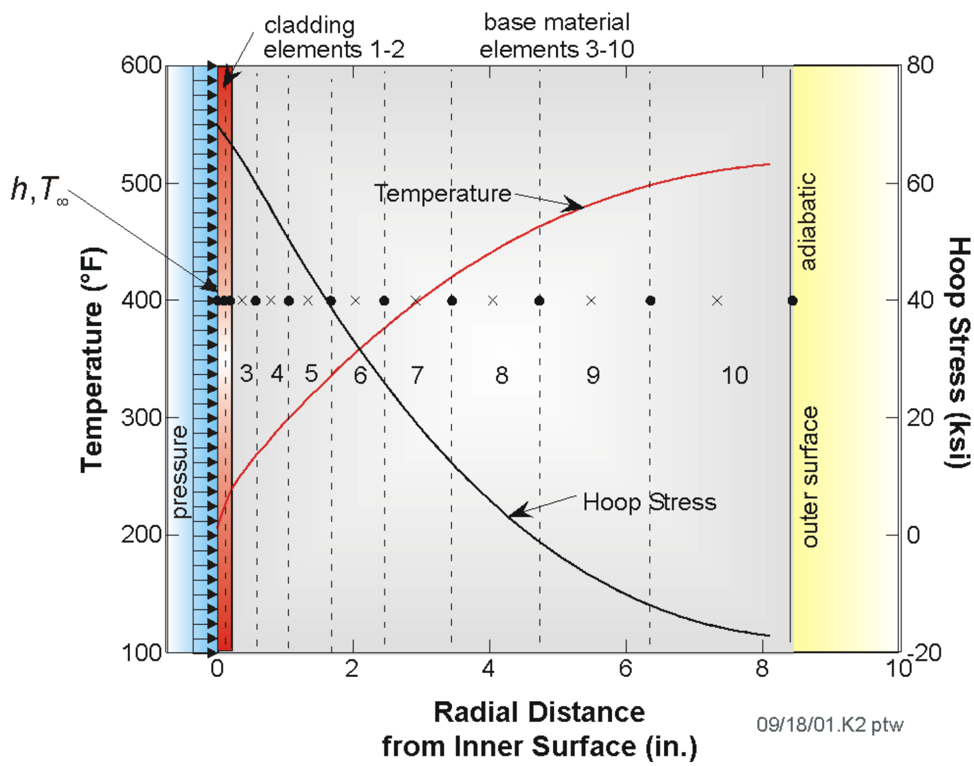
The temperature time history can be solved using the finite-element method, where the variational formulation for the transient heat conduction equation is given in [9]. The fundamental decisions required to implement the finite-element method are (1) choice of basis functions, (2) choice of mapping, and (3) choice of method for element integration. FAVLoad employs the use of the isoparametric mapping shown above with 3-node quadratic cardinal basis functions, specifically:

$$\{N(\xi)\} = \begin{Bmatrix} N_1(\xi) \\ N_2(\xi) \\ N_3(\xi) \end{Bmatrix} = \frac{1}{2}\begin{Bmatrix} -\xi(1-\xi) \\ 2(1-\xi^2) \\ \xi(1+\xi) \end{Bmatrix}; \left\{\frac{dN}{d\xi}\right\} = \begin{Bmatrix} \dfrac{dN_1}{d\xi} \\ \dfrac{dN_2}{d\xi} \\ \dfrac{dN_3}{d\xi} \end{Bmatrix} = \frac{1}{2}\begin{Bmatrix} (-1+2\xi) \\ -4\xi \\ (1+2\xi) \end{Bmatrix}$$

The elements of the thermal stiffness matrix [9], are calculated using a full-integration fourth-order Gauss-Legendre quadrature rule with the following weights, ω_i, and Gauss sampling points, ξ_i,

$$\int_{-1}^{+1} g(\xi)d\xi \approx \sum_{i=1}^{4} \omega_i g(\xi_i) \text{ where } \{\xi_i\} = \begin{Bmatrix} -\sqrt{\dfrac{3+2\sqrt{6/5}}{7}} \\ -\sqrt{\dfrac{3-2\sqrt{6/5}}{7}} \\ \sqrt{\dfrac{3-2\sqrt{6/5}}{7}} \\ \sqrt{\dfrac{3+2\sqrt{6/5}}{7}} \end{Bmatrix} ; \{\omega_i\} = \begin{Bmatrix} \dfrac{1}{2} - \dfrac{1}{6\sqrt{6/5}} \\ \dfrac{1}{2} + \dfrac{1}{6\sqrt{6/5}} \\ \dfrac{1}{2} + \dfrac{1}{6\sqrt{6/5}} \\ \dfrac{1}{2} - \dfrac{1}{6\sqrt{6/5}} \end{Bmatrix}$$

In FAVLoad, a graded mesh is generated through the wall thickness using ten three-node quadratic isoparametric axisymmetric elements (21 nodes). The first two elements represent the cladding, and the remaining eight elements model the base material. Explicit forward time integration is employed with a fixed time step of 1.0 second. For illustrative purposes, a temperature and hoop-stress profile is shown below for a fixed time in an example transient.



The subroutines in FAVLoad and associated descriptions that implement the thermal analysis described above are shown in the table below.

FAVLoad Subroutine	Called by Subroutine(s)	Calls Subroutine(s)	Description
FAVLoad Main	NA	MODEL, MGAUSST, SCOEFF_T, TRANST, INTERP	Main driver routine for the FAVLoad Module to perform 1-D finite element thermal analysis to determine through-wall time dependent temperatures T(x,t) for each of the transient thermal-hydraulic boundary conditions imposed on the inner surface of the RPV.
ELEMNT_T	SCOEFF_T	pchfe, ONER	Forms Temperature-Dependent Element Thermal Conductivity and Heat Capacity Matrices.
INTERP	TRANST	None	Linearly interpolates for YOUT when X=XIN from the tabular values of Y(I) given at X(I) points I=1, NAR using the following passed values in the call INTERP(X, Y, NAR, XIN, MM, YOUT, ND, MTRAN) from subroutine TRANST.
MODEL	FAVLoad Main	None	Generates nodal connectivity for finite element model.
MGAUSST	FAVLoad Main, SCOEFF_T	None	Performs four-point Gaussian numerical integration.
MSB	TRANST	None	Calculates Thermal Vector Due to Thermal Capacity of the structure.
ONER	ELEMNT_T, SELEMNT_T	None	Calculates the shape functions and their Cartesian derivatives for the Gauss Point R for the one dimension, three-nodal Isoparametric Axisymmetric Bar Element.
SCOEFF_T	FAVLoad Main, TRANST	MGAUSST, MGAUSS	Assembles Temp-Dependent global thermal and stiffness matrices.
SELEMNT_T	SCOEFF_T	pchfe, ONER, TINT	Forms Mechanical Stiffness Matrix.
TRANST	FAVLoad Main	SYMSL1, SCOEFF_T, INTERP, MSB, SYMSL2	Driver routine for thermal finite element analysis.
SYMSL1	TRANST	None	Performs mathematical matrix reduction.
SYMSL2	TRANST	None	Performs mathematical vector reduction.

Design 5 Perform finite-element stress analysis by calculating radial displacements, and through the use of the strain-displacement and linear-elastic stress-strain relationships, calculate time-varying axial and hoop stress profiles.

FAVLoad carries out a displacement-based finite-element analysis of the vessel using a one-dimensional axisymmetric model of the vessel wall. The calculated displacements are converted into strains using strain-displacement relationships, and the associated stresses are then calculated using linear-elastic stress-strain relationships. At each time station during the transient, the structure is in a state of static equilibrium; thus, the load history is considered *quasi-static.*

Let (u, v, w) be the radial, circumferential, and axial displacements, respectively, of a material point in a cylindrical (r, θ, z) coordinate system. The general two-dimensional axisymmetric case requires the following:

$$v = 0; \tau_{r\theta} = \tau_{\theta z} = 0; \gamma_{r\theta} = \gamma_{\theta z} = 0$$

where $\tau_{r\theta}, \tau_{\theta z}$ are shear stresses and $\gamma_{r\theta}, \gamma_{\theta z}$ are shear strains. The strain-displacement relationships in matrix form for the two-dimensional case are as follows:

$$\begin{Bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \\ \gamma_{zr} \end{Bmatrix} = \begin{bmatrix} \frac{\partial}{\partial r} & 0 \\ \frac{1}{r} & 0 \\ 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & \frac{\partial}{\partial r} \end{bmatrix} \begin{Bmatrix} u \\ w \end{Bmatrix}$$

For the one-dimensional axisymmetric case, (r, θ, z) are principal directions, and $w = 0; \frac{\partial}{\partial z} = 0$; such that

$$\varepsilon_{rr} = \frac{\partial u}{\partial r}; \quad \varepsilon_{\theta\theta} = \frac{u}{r}; \quad \varepsilon_{zz} = \frac{\partial w}{\partial z} = 0; \quad \gamma_{zr} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial r} = 0$$

For the case of a long cylinder with free ends and no axial or circumferential variations in temperature or material properties and with no radial variation in material properties, the radial and circumferential stresses for the one-dimensional axisymmetric case are calculated from the strains by the following relationship:

$$\sigma_{rr} = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_{rr} + \nu\varepsilon_{\theta\theta}] - \frac{\alpha E}{1-2\nu}(T - T_{ref})$$
$$\sigma_{\theta\theta} = \frac{E}{(1+\nu)(1-2\nu)}[(1-\nu)\varepsilon_{\theta\theta} + \nu\varepsilon_{rr}] - \frac{\alpha E}{1-2\nu}(T - T_{ref})$$

where

$\sigma_{rr} =$ radial normal stress
$\sigma_{\theta\theta} =$ circumferential (hoop) normal stress
$\varepsilon_{rr} =$ radial normal strain
$\varepsilon_{\theta\theta} =$ circumferential (hoop) normal strain
$T =$ wall temperature as a function of r
$T_{ref} =$ thermal stress-free reference temperature
$r =$ radial position in wall
$E =$ Young's modulus of elasticity
$\nu =$ Poisson's ratio
$\alpha =$ linear coefficient of thermal expansion

For generalized plane-strain conditions, the stress in the axial direction, σ_{zz}^{PS}, is given by:

$$\sigma_{zz}^{PS} = \nu(\sigma_{rr} + \sigma_{\theta\theta}) - \alpha E(T - T_{ref})$$

To obtain the axial stresses with the ends free (assuming no cap load), it is necessary to remove the net end force associated with the plane-strain condition. This net load is given by:

$$f^{PS} = 2\pi \int_{R_i}^{R_o} \sigma_{zz}^{PS} r dr$$

where R_i and R_o are the inner and outer radii of the cylinder.

In FAVOR, the radial and hoop stresses are calculated using the finite-element method and applied to each finite element, and thus radial variations in the material properties E, α, and ν can be included by letting the properties vary from one element material group to another. To account for radial variations in properties when calculating the axial stresses, the following equation is applied to each element *j:*

$$\sigma_{zz-j}^{PS} = \nu_j(\sigma_{rr-j} + \sigma_{\theta\theta-j}) - \alpha_j E_j(T_j - T_{ref})$$

The axial stress in each element under plane-strain conditions is now known. To achieve a free-end condition, the force f_j^{PS} must be released in such a manner that the change in axial strain (displacement) is the same for each element, because it is assumed that initial planes remain in plane under load (GPS condition). If Δf_j is the reduction in the plane-strain force, f_j^{PS}, on element *j*, then

$$\frac{\Delta f_1}{A_1 E_1} = \frac{\Delta f_2}{A_2 E_2} = \cdots \frac{\Delta f_{nele}}{A_{nele} E_{nele}}$$

and

$$\sum_{j=1}^{nele} (f_j^{PS} + \Delta f_j) = 0$$

where

$$f_j^{PS} = A_j\left[\nu_j\left(\sigma_{rr-j} + \sigma_{\theta\theta-j}\right) - \alpha_j E_j(T_j - T_{ref})\right]$$

$$A_j = \pi(r_{o-j}^2 - r_{i-j}^2)$$

where r_o and r_i are the outer and inner radii of element *j*, respectively. Let f_{p-j} be the axial forces that are the result of adding internal pressure, *p*. Specifying that the axial displacements for each element be the same provides the following relationships:

$$\frac{f_{p-1}}{A_1 E_1} = \frac{f_{p-2}}{A_2 E_2} = \cdots \frac{f_{p-nele}}{A_{nele} E_{nele}}$$

and

$$\sum_{j=1}^{nele} f_{p-j} = \pi R_o^2 p$$

where

$$f_j = \Delta f_j + f_{p-j}$$

Recalling that the uniform change in axial strain has no effect on either σ_{rr} or $\sigma_{\theta\theta}$, the axial stress is calculated from the following:

$$\sigma_{zz-j} = \frac{\left(f_j^{PS} + f_j\right)}{A_j}$$

FAVOR uses a reduced-integration two-point Gauss-Legendre quadrature rule for the calculation of σ_{rr} and $\sigma_{\theta\theta}$ in each element. The Gauss sample points and weights for two-point quadrature are:

$$\int_{-1}^{+1} g(\xi)d\xi \approx \sum_{i=1}^{2} \omega_i g(\xi_i) \text{ where } \{\xi_i\} = \begin{Bmatrix} -\sqrt{\dfrac{1}{3}} \\ +\sqrt{\dfrac{1}{3}} \end{Bmatrix}; \{\omega_i\} = \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

For the calculation of the axial stresses, each of the elements is divided into two sub-elements, each containing one of the two Gauss points, and the axial stresses are calculated at each of the Gauss points. Stresses at the nodes of the finite-element mesh are obtained by interpolation and extrapolation using a cubic spline fit of the stresses at the Gauss points. The stress analysis uses the same mesh and quadratic elements that are applied in the thermal analysis described in the previous design description.

When temperature-dependency is included in the thermal stress analysis, FAVLoad requires expansion coefficient data to be input that define the total thermal expansion from a specified reference temperature, T_{ref}. With $\overline{\alpha}_{(T_{ref},T)}$ data from handbook sources, this reference temperature is typically at room temperature, and the thermal strains should then be calculated by

$$\varepsilon^{th} = \overline{\alpha}_{(T_{ref},T)}\left(T - T_{ref}\right) - \overline{\alpha}_{(T_{ref},T_{s-free})}\left(T_{s-free} - T_{ref}\right)$$

where the above second term represents the total thermal strain due to the difference between the reference temperature, T_{ref}, and RPV stress-free temperature, $T_{s\text{-}free}$. This term is necessary to enforce the assumption that there is no initial thermal strain at the RPV stress-free temperature.

(1) Thermal expansion coefficient data available in the ASME BPVC, Sect. II, Part D, include both the *instantaneous* coefficient of linear thermal expansion, α_T, (or *thermal expansivity*) at a specified temperature T and the *mean* coefficient of linear thermal expansion, $\overline{\alpha}_{(T_{ref},T)}$, where the two are related by:

$$\overline{\alpha}_{(T_{ref},T)} = \frac{1}{\left(T - T_{ref}\right)} \int_{T_{ref}}^{T} \alpha_T dT$$

For the implementation in FAVLoad, the correct data input should be the mean coefficient of linear thermal expansion. In verification studies, values for α_T and $\overline{\alpha}_{(T_{ref},T)}$ were obtained from Table TE-1 of the ASME Code, Sect. II, Part D, Material Group D (includes A533B) and High Alloy Steels (includes SS304).

(2) As noted in Reference [10], $\overline{\alpha}_{(T_{ref},T)}$ is based on a specified reference temperature, T_{ref} (typically $T_{ref} = 70\ °F$).

(3) For the thermal strain calculations in FAVLoad, it is assumed that there is no thermal strain at a user-input thermal stress-free temperature, T_{sfree}, where typically, $T_{ref} \neq T_{sfree}$. To ensure that the thermal strain is in fact zero at T_{sfree}, a mapping of $\overline{\alpha}_{(T_{ref},T)}$ to $\overline{\alpha}_{(T_{sfree},T)}$ is required.

$$\overline{\alpha}_{(T_{sfree},T)} = \frac{\overline{\alpha}_{(T_{ref},T)}(T - T_{ref}) - \overline{\alpha}_{(T_{ref},T_{sfree})}(T_{sfree} - T_{ref})}{(T - T_{ref})\left[1 + \overline{\alpha}_{(T_{ref},T_{sfree})}(T_{sfree} - T_{ref})\right]}$$

Internally, FAVLoad scales the input thermal expansion coefficient data, resulting in the following equation:

$$\alpha(T) = \frac{\overline{\alpha}_{(T_{ref},T)}(T - T_{ref}) - \overline{\alpha}_{(T_{ref},T_{sfree})}(T_{sfree} - T_{ref})}{(T - T_{ref})\left[1 + \overline{\alpha}_{(T_{ref},T_{sfree})}(T_{sfree} - T_{ref})\right]}$$

This relationship ensures that the correct total thermal strain is being calculated with respect to $T_{s\text{-}free}$.

FAVLoad Subroutine	**Called by Subroutine(s)**	**Calls Subroutine(s)**	**Description**
FAVLoad Main	NA	MODEL, MGAUSST, SCOEFF_T, SIGMA, SPLIN2, Stress_Profiles, TINT	Main driver routine for the FAVLoad Module to perform 1-D finite element stress analysis to determine through-wall time dependent circumferential and axial stresses - STRESS(x,t) for each of the transient hydraulic boundary conditions imposed on the inner surface of the RPV.
Function F5	SIGMA	None	Evaluates the value of the function F5 (x,xv,yv,C,n) given n original tabular values xv(n), yv(n)),and the cubic spline coefficients, C(3,n-1) using Horners method to evaluate the cubic polynomial in each panel xv(i) and xv(i+1).
MODEL	FAVLoad Main	None	Generates nodal connectivity for finite element model.
MGAUSS	FAVLoad Main, SCOEFF_T	None	Performs one-point Gaussian numerical integration.
ONER	SELEMNT_T	None	Calculates the shape functions and their Cartesian derivatives for the Gauss Point R for the one dimension, three-nodal Isoparametric Axisymmetric Bar Element.
SCOEFF_T	FAVLoad Main, SIGMA	MGAUSS	Assembles Temp-Dependent global stiffness matrices.
SELEMNT_T	SCOEFF_T	pchfe, ONER, TINT	Forms Element Stiffness Matrix.
SIGMA	FAVLoad Main	SCOEFF_T,	Calculates stress at Gauss points using Finite

FAVLoad Subroutine	Called by Subroutine(s)	Calls Subroutine(s)	Description
		SYMSL1, SYMSL2, STRCAL_T, SPLIN2, F5, TINT	Element Method. Contains two ENTRY routines called SIGMA1 and SIGMA2.
SPLIN2	SIGMA	None	SPLIN2 (F,X,N,C,WK,*) performs a cubic spline interpolation.
STRCAL_T	SIGMA	ONER, pchfe, SYMSL3, TINT	Calculate Stresses at Gauss Points.
Stress_Profiles	FAVLoad Main	SIGMA (SIGMA1 and SIGMA2), TINT	Calculates Hoop and Axial Stress Profiles.
SYMSL1	SIGMA	None	Performs mathematical matrix reduction.
SYMSL2	SIGMA	None	Performs mathematical vector reduction.
SYMSL3	STRCAL_T	xermsg	Solves linear system of equations Reduces Vector.
Function TINT	SELEMNT_T, SIGMA, STRCAL_T, Stress_Profile	FEM_Interp function	Interfaces to the FEM_Interp function, which interpolates using the basis functions of the parent element. Used to determine nodal temperatures.

Design 6 Provide 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 orientation, and depths.

The design of FAVOR is focused on the problem and transient being evaluated and the capability to model BWR vessel geometries as well as PWR geometries.

FAVOR was originally developed to perform deterministic and probabilistic fracture mechanics (PFM) analyses of reactor pressure vessels subjected to cool-down thermal hydraulic transients imposed on the inner (wetted) surface of the reactor such as those associated with accidental Pressurized Thermal Shock (PTS) conditions and normal transients associated with reactor shutdown.

For such cool-down transients, the flaw population of interest are those flaws on and/or near the inner surface of the reactor vessel wall, because at the inner surface, the temperature is at its minimum and the tensile stress and radiation-induced embrittlement are at their maximum. These tensile stresses tend to open existing cracks located on or near the internal surface of the RPV wall.

Therefore, earlier versions of FAVOR were limited to modeling internal surface-breaking flaws and/or embedded flaws that reside near the inner surface of the vessel wall. The embedded flaws (quantified in the embedded flaw characterization files) are assumed to be distributed uniformly throughout the entire vessel wall; however, for computational efficiency, only those postulated to reside in the first 3/8 of the base metal (wall thickness exclusive of clad thickness) were included in the analysis. For cool-down transients, the applied-K_I driving force for embedded flaws postulated to reside in the vessel wall beyond the inner 3/8 of the wall thickness is too small to have a conditional probability of initiating an embedded flaw in cleavage fracture.

For heat-up transients, such as normal transients associated with reactor start-up, flaws on or near the external surface of the reactor vessel are the most risk-significant because the tensile stresses are at their maximum there. The $FAVOR^{HT}$ code was designed to perform analyses of these heat-up transients; i.e., however, it was limited to the modeling of embedded flaws in the outer 3/8 of the RPV wall thickness. $FAVOR^{HT}$ did not have the capability of modeling external surface-breaking flaws.

6.1 Flaw Modeling Options and Classification

The current version of FAVOR has consolidated the capabilities of the previous versions of FAVOR as well as added additional capabilities. FAVOR now has the user-specified optional ability to model three different flaw populations as follows:

Flaw Population Option 1 – All surface-breaking flaws (quantified in the surface flaw characterization input file from VFLAW) are **internal** surface breaking flaws and only those **embedded flaws in the first 3/8** of the RPV wall thickness are included in the model. The primary application of this option is for modeling cool-down transients. Through-wall flaw propagation is included in this option.

Flaw Population Option 2 – All surface-breaking flaws (quantified in the surface flaw characterization input file from VFLAW) are **external** surface-breaking flaws and those **embedded flaws in the outer 3/8** of the RPV wall thickness are included in the model. The primary application of this option is for modeling heat-up transients. Through-wall flaw propagation is not included in this option because failure is assumed if crack growth initiation is predicted (i.e. probability of crack growth initiation = probability of failure). This is because an external surface crack would be growing into increasingly embrittled material, and is thus not assumed to be able to arrest.

Flaw Population Option 3 – This additional population includes **internal and external** surface-breaking flaws; all of the **embedded flaws are uniformly distributed through the RPV wall** (approximately 8/3 times the number of embedded flaws postulated in Options 1 and 2). The number of postulated surface breaking flaws is double that of Options 1 or 2; and they are evenly divided between internal and external surface breaking flaws. The application of Option 3 is for modeling transients in which the pressure-induced loading is dominant (e.g., hydro-testing, etc.), since the applied-K_I for all flaws has a smaller dependence on their respective locations. Through-wall flaw propagation is not yet included in this option for external surface breaking flaws or embedded flaws residing in the outer half of the vessel wall. These flaws are assumed to result in vessel failure upon initiation of cleavage fracture. Internal surface breaking flaws and embedded flaws within the inner half of the vessel wall will be propagated upon cleavage fracture initiation.

Flaw Population Options 1 and 2 are available for computational efficiency. If the dominant loading is thermally induced, only those populations of flaws on or near the relevant RPV surface would likely ever initiate (and subsequently fail), so the other flaws are excluded from the analysis because their presence would not change the PFM solution(s) but could dramatically increase the computational resources (memory and time) to complete a PFM analysis.

FAVOR coding is designed to model 16 surface-breaking flaw types for PWR and BWR geometries as shown in the table below.

Table 5: Surface Breaking Flaws

Flaw type	Aspect ratio	Surface breaking	Orientation
1	**2**	Internal	Axial
2	**6**	Internal	Axial
3	**10**	Internal	Axial
4	**Infinite**	Internal	Axial
5	**2**	Internal	Circumferential
6	**6**	Internal	Circumferential
7	**10**	Internal	Circumferential
8	**Infinite**	Internal	Circumferential
9	**2**	External	Axial
10	**6**	External	Axial
11	**10**	External	Axial
12	**Infinite**	External	Axial
13	**2**	External	Circumferential
14	**6**	External	Circumferential
15	**10**	External	Circumferential
16	**Infinite**	External	Circumferential

In order to evaluate these type of flaws, **Stress-Intensity-Factor Influence Coefficients (SIFICs) databases for BWR vessel geometry (R_i/t ~ 20) and PWR geometry ($R_i/t \approx 10$) are required.** Two SIFIC databases for each of the 16 surface breaking flaw types are in FAVOR; one each for PWR geometry $R_i/t \approx 10$ and BWR geometry $R_i/t \approx 20$. The capability to calculate applied-K_I's for all 16 axially- and circumferentially oriented internal and external surface breaking flaw types for both BWR and PWR required the creation, implementation, and verification of a total 32 SIFIC databases.

Regarding flaw orientation, all pre-existing inner-surface breaking flaws are assumed to be circumferentially oriented. Pre-existing external surface-breaking flaws in axial welds are axially oriented; external surface-breaking flaws in circumferential welds are circumferentially oriented; and external surface-breaking flaws in plates are evenly divided between axial and circumferential orientations. Embedded flaws in welds assume the orientation of the weld, i.e., embedded flaws in axial welds are axially oriented, and embedded flaws in circumferential welds are circumferentially oriented. Embedded flaws in plates are evenly divided between axial and circumferential orientations.

The flaw models shown in the figure below are included in the **three categories of flaws** identified by FAVOR.

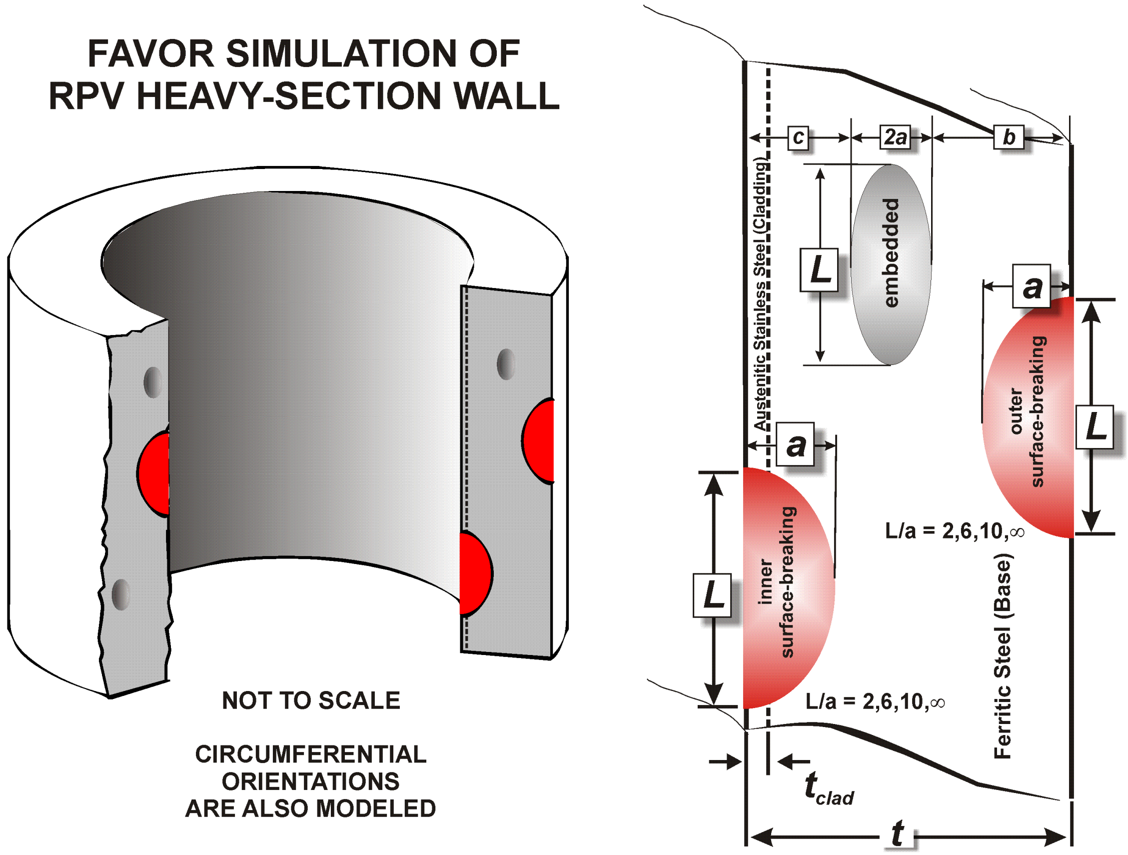


Figure 3: Flaw models implemented in FAVOR

Category 1: Surface-Breaking Flaws

Includes Flaw Population Option 1 – internal surface-breaking flaws only (flaw types 1-8)

Includes Flaw Population Option 2 – external surface-breaking flaws only (flaw types 9-16)

Includes Flaw Population Option 3 – internal and external surface-breaking flaws only (flaw types 1-16)

Category 2: Embedded Flaws Within 1/8th of the Thickness from Vessel Walls

Includes Flaw Population Option 1 with embedded flaws having fully elliptical geometry with the crack tip nearest the wetted inner surface located between the clad / base interface and the inner 1/8th of the base metal thickness.

Includes Flaw Population Option 2 with embedded flaws having fully elliptical geometry with crack tip nearest the external surface located in the outer 1/8th of the base metal thickness.

Includes Flaw Population Option 3 with embedded flaws having fully elliptical geometry with crack tip nearest the external surface located between the clad base interface and the outer half of the total wall thickness.

Note: base metal thickness = total vessel wall thickness – clad thickness.

Category 3: Embedded Flaws Between 1/8th and 3/8th of the Thickness from Vessel Walls

Includes Flaw Population Option 1 with embedded flaws having fully elliptical geometry with the crack tip nearest the wetted inner surface located between 1/8th and 3/8th of the base metal thickness.

Includes Flaw Population Option 2 with embedded flaws having fully elliptical geometry with crack tip nearest the external surface located between 1/8th and 3/8th of the outer base metal thickness.

Includes Flaw Population Option 3 with embedded flaws having fully elliptical geometry with crack tip nearest the external surface located in the outer half of the total wall thickness.

6.2 Stress Intensity Factor Influence Coefficients (SIFICs)

The common blocks in FAVLoad and associated descriptions that provide the SIFICs for all flaw specifications are shown in the table below. Note that FAVLoad also uses subroutines to provide SIFICS for some flaw specifications. These follow the common block table listing.

All base material SIFICs for inside surface-breaking flaws are calculated using curve fits from the ASME BPVC, Appendix A, Article A-3000 (see Appendix G of the Theory Manual (Reference [1]). The base material SIFICs in the FAVOR database are no longer used; however, the database SIFICs for the cladding and external surface-breaking flaws continue to be applied. *Note that during the development of this document, an issue was identified in the application of the ASME based SIFICs. The SIFICs for axial infinite aspect ratio flaws are not using the ASME based SIFICs for greater (a/t) flaw depths of 0.4, instead the SIFICs from the original base FAVLoad arrays are used. Similarly, the SIFICs for circumferential 360-degree aspect ratio flaws are not using the ASME based SIFICs for greater (a/t) flaw depths of 0.2, instead the SIFICs from the original base FAVLoad arrays are used. This was identified and corrected on the FAVPRO GitHub repository as Pull Request* #651.

Time-dependent stress-intensity factors for infinite- and finite-length, internal and external, surface-breaking flaws are calculated for a range of flaw depths, sizes, and aspect ratios. Due to its generality, the **embedded-flaw model was implemented in the FAVPFM module**, rather than FAVLoad.

Subroutine rt10_20ax is used to transform (by interpolation / extrapolation / curve fit) the axial flaw related SIFICs installed in FAVOR (in Table 6 below) to the specific RPV geometry (R / t and clad thickness) currently being analyzed, i.e., per the user input data in the FAVLOAD input file (Ri / t and clad thickness).

Subroutine rt10_20cir is used to transform (by interpolation / extrapolation / curve fit) the circumferential related SIFICs installed in FAVOR (in Table 6 below) to the specific RPV geometry (R / t and clad thickness) currently being analyzed, i.e., per the user input data in the FAVLOAD input file (Ri / t and clad thickness).

Both subroutines rt10_20ax and rt10_20cir use subroutine **SIFIC_INTERPOLATE** to interpolate on Ri/t for the actual problem. In addition, module **getKn_clad_h** containing multiple subroutines for K0 and K1 and clad thickness is used to calculate the curve fits for K0 and K1 for the actual cladding thickness entered by the user.

Table 6: SIFICs for Finite Length Internal and External-Surface-Breaking Flaws

FAVLoad Common Block	Subroutine(s) Using Common Block	Description of Common Block
KSTARAX10	rt10_20ax	Contains cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length axially oriented inner surface breaking flaws for RPVs with an internal radius to wall thickness ratio of 10, as well as for infinite axial flaw in base material.
KSTARAX20	rt10_20ax	Contains cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length axially oriented inner surface breaking flaws for RPVs with an internal radius to wall thickness ratio of 20, as well as for infinite axial flaw in base material.
KSTARCIR10	rt10_20cir	Contains cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length circumferentially oriented inner surface breaking flaws for RPVs with an internal radius to wall thickness ratio of 10, as well as for infinite circumferential flaw in base material.
KSTARCIR20	rt10_20cir	Contains cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length circumferentially oriented inner surface breaking flaws for RPVs with an internal radius to wall thickness ratio of 20, as well as for infinite circumferential flaw in base material.
EXKSTARAX10	rt10_20ax	SIFICs for external surface breaking finite length semi-elliptical (AR of 2, 6, and 10) for RPVs with Ri / t = 10 for base.
EXKSTARAX20	rt10_20ax	SIFICs for external surface breaking finite length semi-elliptical (AR of 2, 6, and 10) for RPVs with Ri / t = 20 for base.

Table 7: SIFICs for Infinite Length External-Surface-Breaking Flaws

FAVLoad Module Procedure / Data Blocks	Called by Submodule/Subroutine(s)	Description
KSTINF10AXext / ABAW10AXext(15,30), AKSTAX10ext(15,30)	stress_intensity_factor_m /FAVLoad Main	SIFICs for Infinite Length external-surface-breaking axially oriented flaws for a RPV with a Ri/t of 10.
KSTINF10CRext / ABAW10CRext(15,37), AKSTCR10ext(15,37)	stress_intensity_factor_m /FAVLoad Main	SIFICs for external-surface-breaking 360-degree circumferential flaws for a RPV with a Ri/t of 10.
KSTINF20AXext / ABAW20AXext(15,30), AKSTAX20ext(15,30)	stress_intensity_factor_m /FAVLoad Main	SIFICs for Infinite Length external-surface-breaking axially oriented flaws for a RPV with a Ri/t of 20.
KSTINF20CRext / ABAW20CRext(15,37), AKSTCR20ext(15,37)	stress_intensity_factor_m /FAVLoad Main	SIFICs for external-surface-breaking 360-degree circumferential flaws for a RPV with a Ri/t of 20.

See Tables B33 through B36 of Reference [1] for values of external SIFICs.

SIFICs for Base Material

Subroutine *get_A3000_SIFICs(axial, L_over_a, irow, jcol, kcol, R_over_t, twall, aw, sific, G0, G1, G2, G3)* contains closed-form curve fits for SIFICs for flaws in RPV base material. The curve fits were developed by the ASME Working Group on Flaw Evaluation and are contained in the ASME Boiler and Pressure Vessel Code, Section XI, Appendix A, Article A-3000 – Method of Determination KI Determination. The required inputs are the R / t ratio, aspect ratio L / a, flaw orientation, and normalized flaws depths a / t. The subroutine returns an array of SIFIC(s) corresponding to these inputs.

This subroutine is called from SUBROUTINES rt10_20ax and rt10_20cir to prepare SIFICs for:

AXIAL – infinite length and finite length (aspect ratios 2, 6, and 10)

CIRC – 360-degree and finite length (aspect ratios 2, 6, and 10)

These SIFICs are applied in modules KI_axial_calc and KI_circ_calc within submodule calculate_ki_s, with stress curve fit coefficients, using the method of superposition to calculate KI contribution for base material KI_{base}.

Also, in modules KI_axial_calc and KI_circ_calc, the total KI for each internal surface breaking flaw depth will be calculated as $KI_{total} = KI_{base} + KI_{clad}$

Input data to subroutine get_A3000_SIFICs is as follows:

- axial = logical (TRUE means axial, FALSE means circumferential).
- L_over_a = Aspect Ratio (2c/a as defined in Theory and User Manual).

- irow = number of flaw depths (15, 8, or 1).
- jcol = 4 – number of SIFICs.
- kcol = 1 or 10.
- R_over_t = vessel inner radius / wall thickness.
- twall = RPV wall thickness.
- aw = array holding a / t (flaw depth / twall) for each of the flaws.
- SIFIC – array of stress intensity factor influence coefficients that will be applied in the calculation of K_I.
- G0, G1, G2, and G3.

Note: G0, G1, G2, and G3 are not used outside of this subroutine.

SIFICs for External Surface-Breaking Flaw Models – Semi-Elliptical and Infinite Length

SIFICs are calculated to provide capabilities for the calculation of applied-K_I values using the weight-function technique for external surface breaking flaws for BWR and PWR geometries as required for the analysis of heat-up transients. Reference [11] describes the basis for the external surface-breaking SIFICs and the underlying equations and models used to calculate $K_{I,applied}$.

External Semi-Elliptical Finite Surface Flaws

Tables B23-B27 of the FAVOR Theory Manual (Reference [1]) provide SIFICs for axial external-surface semi-elliptical flaws for PWRs having R/t = 10. SIFICs for R/t = 10 are tabulated for these aspect ratios (2:1, 6:1, and 10:1) for a/t = 0.1, 0.2, 0.3, 0.4, and 0.5. For BWRs (R_i/t = 20), SIFIC(s) for an axial orientation and for relative flaw depths of a/t = 0.1, 0.2, 0.3, 0.4, and 0.5 (with aspect ratios 2:1, 6:1, and 10:1) are presented in Tables B28-B32 of Reference [1].

External Infinite-Length Surface Flaws

Table B33 in Reference [1] presents SIFICs for external axial infinite flaws for PWRs (Ri/t = 10). These SIFICs have been non-dimensionalized by multiplying by the factor ($0.1t^{1/2}$), where t is the wall thickness. Table B34 Reference [1] displays SIFIC(s) for external 360° circumferential surface flaws for PWRs, and these SIFIC(s) have been non-dimensionalized by multiplying by the factor ($10t^{3/2}$). For both orientations, the range of relative flaw depths are a/t = {0.01, 0.02, 0.03, 0.05, 0.075, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 0.95}. The non-dimensional SIFIC(s) make them applicable for all vessels with Ri/t = 10.

Table B35 Reference [1] presents SIFICs for external axial infinite flaws for BWRs (R_i/t = 20). These SIFICs have been non-dimensionalized by multiplying by the factor ($0.1t^{1/2}$), where t is the wall thickness. Table B36 displays SIFICs for external 360° circumferential surface flaws for BWRs, and the SIFICs have been non-dimensionalized by multiplying by the factor ($10t^{3/2}$). For both orientations, the range of relative flaw depths are a/t = {0.01, 0.02, 0.03, 0.05, 0.075, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 0.95}. The non-dimensional SIFIC(s) make them applicable for all vessels with R_i/t = 20.

Note that during the development of this document and modernization of FAVOR, an issue was identified in the application of external surface SIFICs for 360 deg circumferential flaws in FAVLoad. The interpolation for infinite external SIFICs scheme in FAVPFM was not totally correct. The intent was to interpolate between table for r/T of 10 and 20. However, these SIFIC tables have different number of entries for r/t of 10 and 20 and the a'/a values are not consistent/compatible. Note that the interpolation for external axial flaws was removed in 2009. ASME now provides formulas for external flaws and these tables will eventually be replaced with ASME formulas. The identified error does not impact the FAVPFM results because all external flaws are assumed to fail if they initiate so the external infinite SIFICs will not be used in a PFM analysis. This was identified on the FAVPRO GitHub repository as Pull Request #661.

Table 8: FAVLoad Common Blocks containing Final Interpolated SIFICs

FAVLoad Common Block	Subroutine(s) Using Common Block	Description of Common Block
SIFAX	rt10_20ax, calculate_ki_s, calculate_ki_m	Contains ABAQUS based final base and cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length axially oriented inner surface breaking flaws for user specified RPV radius to wall thickness ratio.
Ext_SIFAX	rt10_20ax, calculate_ki_s, calculate_ki_m	Contains base final SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) axially oriented external surface breaking flaws for user specified RPV radius to wall thickness ratio.
SIFCLADAX	rt10_20ax, calculate_ki_s, calculate_ki_m	Contains ABAQUS based cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length (i.e., 99) axially oriented inner surface breaking flaws for user specified RPV radius to wall thickness ratio and specified clad thickness.
SIFCIR_new	rt10_20cir, calculate_ki_s	Contains ASME A3000 model based SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) circumferentially oriented inner surface breaking flaws for user specified RPVs radius to wall thickness ratio.
SIFCIR	rt10_20cir, calculate_ki_s, calculate_ki.m	Contains ABAQUS based final base and cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length circumferentially oriented inner surface breaking flaws for user specified RPV radius to wall thickness ratio.
SIFCLADCIR	rt10_20cir, calculate_ki_s, calculate_ki.m	Contains ABAQUS based cladding SIFICs for finite length semi-elliptical (aspect ratios of 2, 6, and 10) and infinite length (i.e., 99) circumferentially oriented inner surface breaking flaws for user specified RPV radius to wall thickness ratio and specified clad thickness.

Design 7 Provide capability to perform both deterministic and probabilistic fracture analyses.

7.1 Overview

In order to implement this design feature, the FAVLoad output must provide FAVPFM $K_{I,applied}$ for all flaw types, as discussed in Design 6 , for all transients, timesteps, and flaw depths. Note that the embedded flaws are handled solely in FAVPFM, since these are closed-form solutions based on the EPRI NP-1181 approach (see below for further description). Also, Design 4 and Design 5 steps must be implemented to ensure that the heat conduction and thermo-elastic stress analyses have been completed. Table 9 provides a listing of the FAVLoad generated output for use in FAVPFM to perform both deterministic and probabilistic fracture analyses. The output of FAVLoad can be considered a thermal and stress database containing temperature, circumferential stress, axial stress, and $K_{I,applied}$ as a function of vessel wall position and time for each input transient. This file is saved as an ASCII output file designated by the user when executing FAVLoad.

Before calculating $K_{I,applied}$, FAVload performs the heat conduction and thermo-elastic stress analyses based on a 1-D axisymmetric finite element model of the RPV wall (Figure 4 and Design steps 4 and 5). Following these analyses and the development of the SIFICs from the previous Design step, $K_{I,applied}$ can now be calculated. Figure 5 provides the FAVLoad programming logic to generate $K_{I,applied}$.

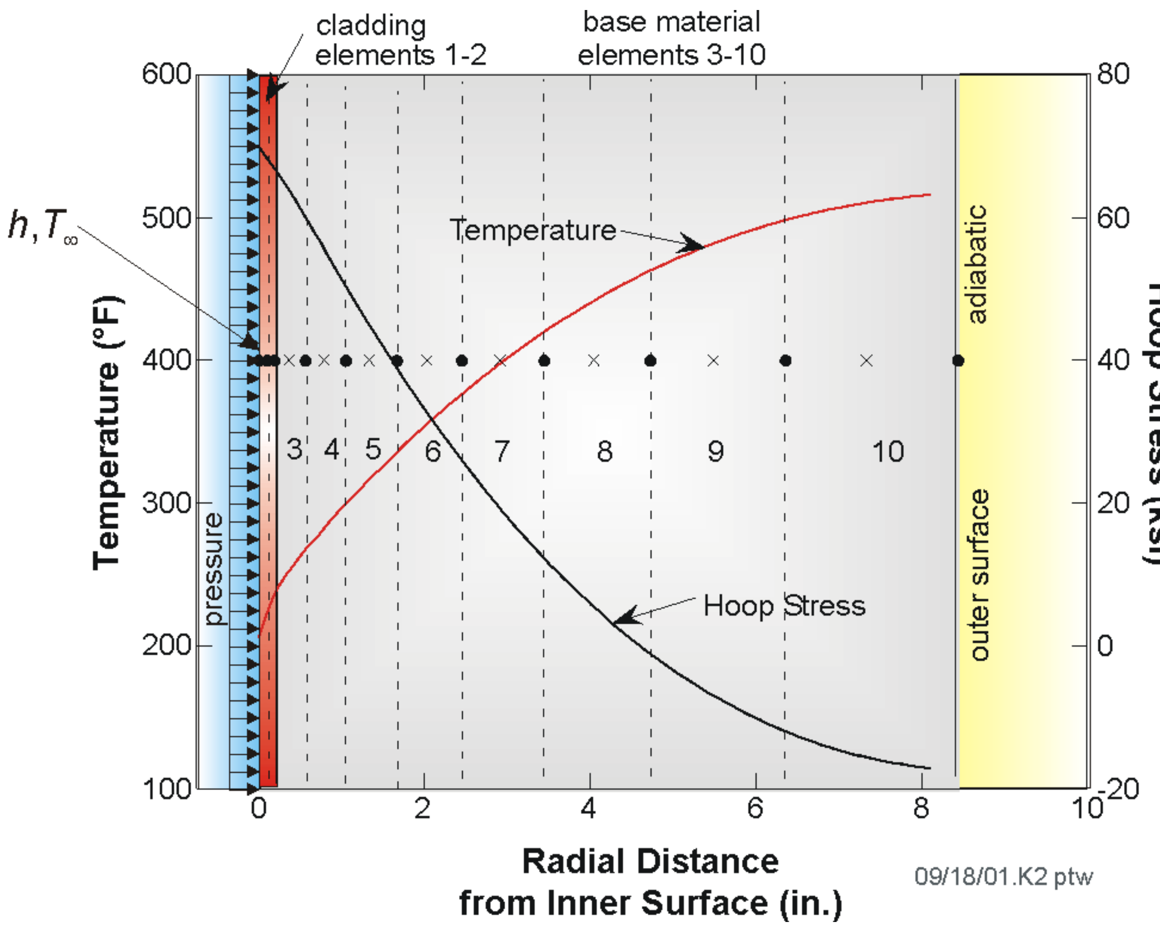
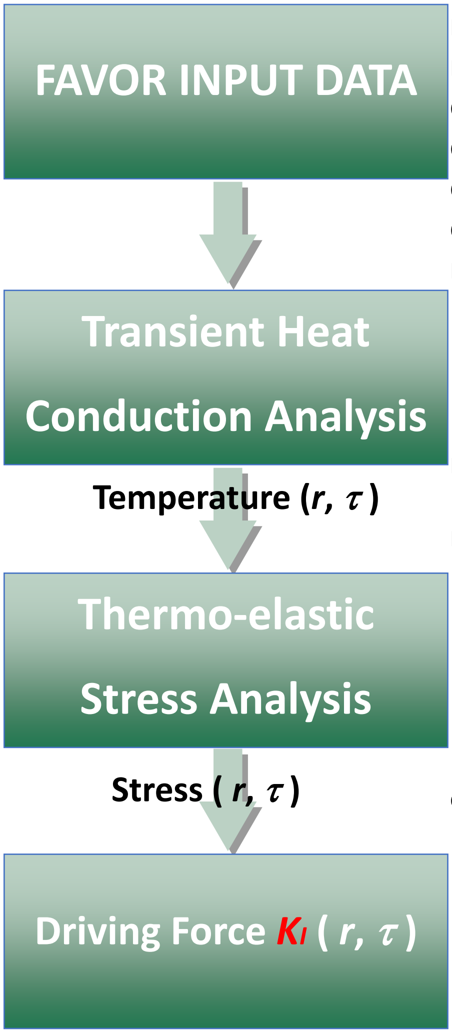


Figure 4: Mesh Points used in the Heat Conduction and Thermo-Elastic Stress Analyses based on a 1-D Axisymmetric Finite Element Model of the RPV Wall (No Flaw)



Loop on Transients

Do 888 ITRAN = 1,MTRAN

CALL MGAUSST – define gauss points for thermal analysis

CALL SCOEFF_T (assemble thermal conductivity matrix)

CALL TRANST (driver for thermal analysis)

CALL MGAUSS (define gauss points for stress analysis)

DO 891 ITSTP = 1, NTIMES

CALL INTERP

CALL SPLIN2 (spline coeff for thermal solutions)

CALL SIGMA (calculate stresses)

CALL CALKICRext (Creates EZKCR99 array - KI Infinite Circ. External)

CALL CALKIAXext (Creates EZKAX99 array - KI Infinite Axial External)

CALL STRESS_PROFILES (Calculates STRHCD and STAXCD (hoop and axial stresses, respectively))

CALL SEMAX (Calculates KI ISB & ESB Semi-Elliptical Axial at 9 depths)

CALL KI_axial_calc (Creates AKX*TOT arrays and EAK*TOT where * is either 2, 6, 10, or 99)

CALL SEMCIR (Calculates KI ISB & ESB Semi-Elliptical Circ. at 9 depths)

CALL KI_circ_calc (Creates CIRK*TOT arrays and ECIRK*TOT where * is either 2, 6, 10, or 99)

DO 893 J = 1, 16 (Call function TINT to apply cubic spline curve fit coefficients to determine temperature at r for time step (itstp) and transient (itran)

R = X(1) + HCD_int (J)

ZSURFT(J, IPOINT, ITSTP) = TINT(R)

893 CONTINUE (end flaw depth loop)

891 CONTINUE (end time loop)

888 CONTINUE (end transient loop)

CONSTRUCT organized FAVLoad Output File

INCLUDE Weld Residual stress and repeat loops

CONMPLETE FAVLoad organized Output File

***Note that submodule calculate_ki_s contains CALKIAXext, CALKICRext, , ki_axial_calc, ki_circ_calc, SEMAX, and SEMCIR.**

Figure 5: FAVLoad Calculational Flow and Subroutines Called to Generate FAVLoad Output file for use by FAVPFM

Table 9: FAVLoad Array Names Written in Order in FAVLoad Output File

Array Name	Description
zsurft (k, j, i)	Temperature
strhcd (k, j, i)	Hoop Stress
staxcd (k, j, i)	Axial Stress
axk99tot (k, j, i)	Axial KI; Internal Surface; Infinite
cirk99tot (k, j, i)	Circ KI; Internal Surface; Infinite
ezkax99 (k, j, i)	Axial KI; External Surface; Infinite
ezkcr99 (k, j, i)	Circ KI; External Surface; Infinite
cd3d(i), cd3d_ext(i)	Flaw Depths for Semi-Elliptical Flaw
axk2tot (k, j, i)	Axial KI; Internal Surface; Aspect = 2
axk6tot (k, j, i)	Axial KI; Internal Surface; Aspect = 6
axk10tot (k, j, i)	Axial KI; Internal Surface; Aspect = 10
cirk2tot (k, j, i)	Circ KI; Internal Surface; Aspect = 2
cirk6tot (k, j, i)	Circ KI; Internal Surface; Aspect = 6
cirk10tot (k, j, i)	Circ KI; Internal Surface; Aspect = 10
eaxk2tot (k, j, i)	Axial KI; External Surface; Aspect=2
eaxk6tot (k, j, i)	Axial KI; External Surface; Aspect=6
eaxk10tot (k, j, i)	Axial KI; External Surface; Aspect=10
ecirk2tot (k, j, i)	Circ KI; External Surface; Aspect = 2
ecirk6tot (k, j, i)	Circ KI; External Surface; Aspect = 6
ecirk10tot (k, j, i)	Circ KI; External Surface; Aspect = 10

Notes:
Prior to the above arrays being written out, the version number, number of transients (MTRAN), Transient Sequence Number (ISEQ), vessel geometry (RI, RO, and CLTH), number of time steps and mesh points (NTIMES and NCDH=16), Time Step Increments (DTIME(1:NTIMES), Mesh Discretization (HCD_int and HCD), and Pressure at each time step for each transient (PRESS(I,J)) are printed.
k = flaw depth index(1-16); j = transient number; and i = time step number
16 flaw depths (inclusive of zero) used for infinite length flaws and 9 flaw depths (inclusive of zero) used for finite length flaws.
The first call to SUBROUTINE STRESS_PROFILES does not include thru-wall residual stress whereas the 2nd call to SUBROUTINE STRESS_PROFILES does include residual stress. The same naming convention is used for both cases.
Note embedded flaws are handled within FAVPFM using the EPRI NP-1181 approach.

7.2 Embedded Flaw Model

The computational methodology implemented in FAVOR for calculating Mode I stress-intensity factors, K_I, for embedded flaws [12] is the EPRI NP-1181 analytical interpretation [13] of the ASME Section XI-Appendix A [14] model for embedded flaws and do not rely on SIFICs.

The procedure for calculating Mode I stress-intensity factors, K_I , is based on the resolution of nonlinear applied stresses through the RPV wall thickness into the linear superposition of approximate membrane and bending stress components. The K_I factor is thus computed from the following relation:

$$K_I = (M_m \sigma_m + M_b \sigma_b)\sqrt{\pi a/Q}$$

where:

$2a =$ the minor axis of the elliptical subsurface flaw
$Q =$ flaw shape parameter
$M_m =$ free-surface correction factor for membrane stresses
$M_b =$ free-surface correction factor for bending stresses
$\sigma_m =$ membrane stress
$\sigma_b =$ bending stress

The above equations are used in the FAVPFM subroutine, KEMB.

7.3 Cladding Effects on $K_{I,applied}$

Cladding has an effect on the $K_{I,applied}$ for shallow internal surface breaking flaws due to the difference of thermal expansion coefficients for cladding and base materials. The effects dissipate rapidly with increasing flaw depth. FAVLoad models this effect by combining the contributions to K_I from the clad and base, $K_{I,applied} = K_{I,clad} + K_{I,base}$. Figure 6 provides an illustration of the discontinuity at the clad-base interface and how the stresses are developed.

Subroutine SIGMA calculates the curve coefficients assuming linear distribution of hoop stresses in the clad region. These coefficients are then applied in Module Procedure KI_axial_calc to calculate $K_{I,clad}$. Similarly, curve coefficients assuming linear distribution of axial stresses in the clad region are calculated. The axial based coefficients are applied in subroutine KI_circ_calc to calculate $K_{I,clad}$ for circumferentially oriented flaws.

7.4 Data Transformations for Deterministic or Probabilistic Fracture Mechanics Analysis

FAVPFM input was designed to allow the user to select either a deterministic or probabilistic fracture mechanics analysis. An input parameter called IQA on the LDQA record was used to activate either option. IQA=1 to activate the deterministic analysis module within FAVPFM based on the FAVLoad output file containing the Table 9 array information. IQA=0 to activate the PFM analysis. The subroutines used to read in the user input, in particular IQA, are described in the above Design 2 requirement.

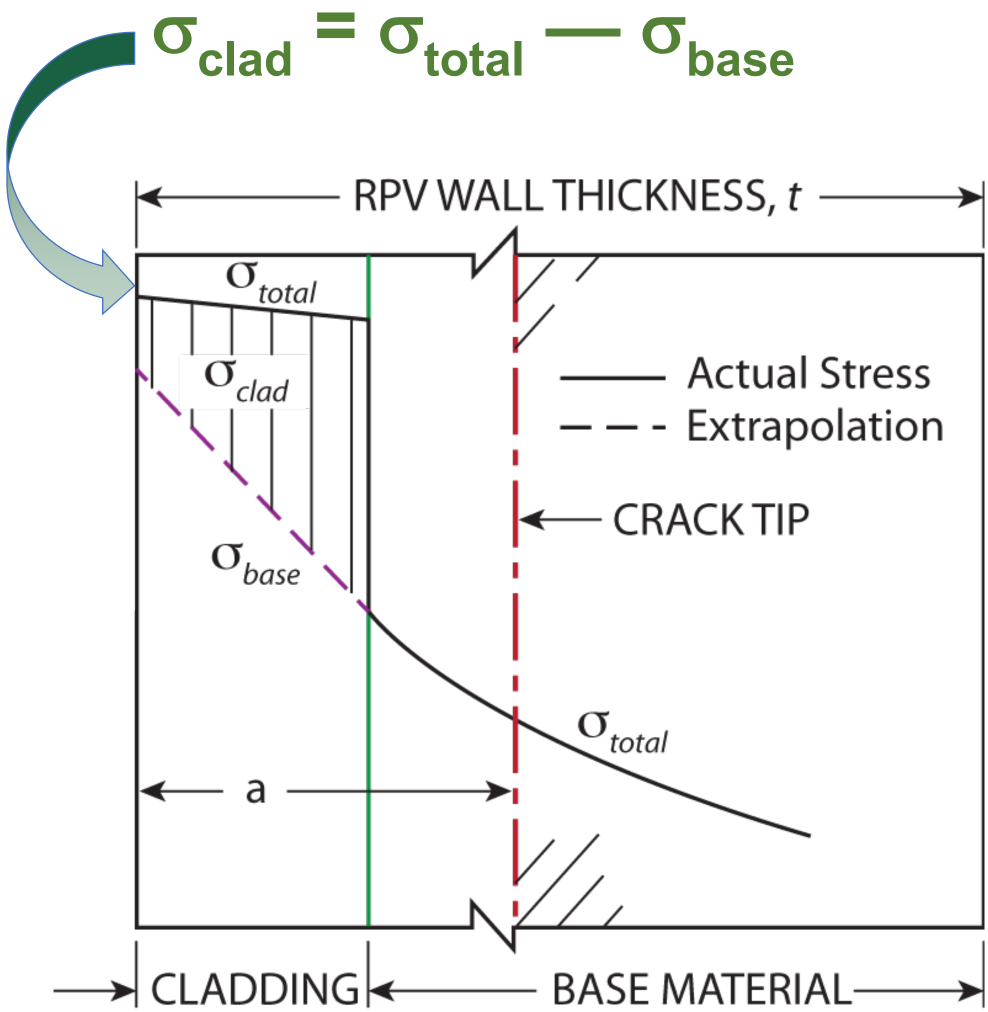


Figure 6: Illustration of Clad and Base Material Stresses at the RPV Interior Surface

Table 10: FAVLoad Clad Based SIFICs Arrays

R / t	Clad Thickness (inch)	FAVLoad internal arrays containing Clad Based SIFICs for Axial Flaws - Derived at ORNL using ABAQUS models Aspect Ratio			
		2	6	10	Infinite
10	0.156	a10cl1562 (8,2,10)	a10cl1566(8,2,10)	a10cl15610 (8,2,10)	a10cl15699 (15,2,1)
20	0.156	a20cl1562 (8,2,10)	a20cl1566 (8,2,10)	a20cl15610(8,2,10)	a20cl15699 (15,2,1)
10	0.25	a10cl252 (8,2,10)	a10cl256 (8,2,10)	a10cl2510 (8,2,10)	a10cl2599 (15,2,1)
20	0.25	a20cl252 (8,2,10)	a20cl256 (8,2,10)	a20cl2510 (8,2,10)	a20cl2599 (15,2,1)

R / t	Clad Thickness (inch)	FAVLoad internal arrays containing Clad Based SIFICs for Circumferential Flaws - Derived at ORNL using ABAQUS models - Note: SIFICs are identical (ORNL/NRC/LTR-94-8) to those for axial for the first 7 flaw depths. Aspect Ratio			
		2	6	10	Infinite
10	0.156	c10cl1562 (1,2,10)	c10cl1566(1,2,10)	c10cl15610 (1,2,10)	c10cl15699 (15,2,1)
20	0.156	c20cl1562 (1,2,10)	c20cl1566 (1,2,10)	c20cl15610(1,2,10)	c20cl15699 (15,2,1)
10	0.25	c10cl252 (1,2,10)	c10cl256 (1,2,10)	c10cl2510 (1,2,10)	c10cl2599 (15,2,1)
20	0.25	c20cl252 (1,2,10)	c20cl256 (1,2,10)	c20cl2510 (1,2,10)	c20cl2599 (15,2,1)

In order to perform the probabilistic fracture mechanics analysis, the FAVLoad output file is required in addition to the flaw characterization files. This section provides the software design to prepare the temperature, stress, K_I, and flaw profiles in a finite element mesh consistent with the FAVPFM analysis structure. The first part consists of reading the flaw files necessary to characterize surface breaking flaws, embedded flaws in welds, and embedded flaws in plate material. As previously discussed, Design 2 provides the software design on reading the various flaw files.

Subroutine RDSURF reads the user-named file that contains data regarding the density of surface breaking flaws (flaw per square foot of RPV internal surface area) and the probabilistic distribution of the aspect ratios. Subroutine RDWELD reads the user-named file that contains the data regarding the density of embedded flaws in weld material (flaws per fusion area) and the probabilistic distribution of their aspect ratios. Subroutine RDPLATE reads the user-named file that contains the data regarding the density of embedded flaws in plate material (flaws per in^3 of plate material) and the probabilistic distribution of their aspect ratios.

The format of the flaw data in the three files discussed above is compatible with the format of VFLAW computer code. A USNRC specification for the development of FAVOR was that it be compatible with the VFLAW computer code.

For the as-found flaw approach, subroutine RDFOUND reads in the user specified flaw geometries.

In order to proceed, FAVPFM needs to create the finite element mesh used in the analysis. This is done through the call to SFMESH. RI, RO, NPCRK, ASIZE, NCDP, and ZSURF are passed through the call to subroutine SFMESH. NDCP is an integer index in the mesh that corresponds to 95% of the RPV wall thickness. RI is the vessel internal radius and RO is the vessel external radius. NPCRK is set to 25 in subroutine RDDET which reads the FAVLoad output file. This is essentially the mesh size. ZSURF is the one-dimensional array of crack tip positions relative to inner surface in inches. The first 25 positions are set equal to ASIZE (25% of RPV thickness). Positions 26 to 60 are sequentially incremented by 0.25 inches. Once the boundary of the failure criterion is reached, the ZSURF upper bound is defined (i.e., array index NCDP is set <60). ASIZE is a one-dimensional array which defines the mesh in inches by increments of (0.01*RPV wall thickness) and its length is NPCRK long (i.e., 25 values). Therefore, ASIZE covers 25% of RPV wall.

```
CALL SFMESH
! Creates RPV thru-wall mesh to be used in PFM analysis.

ZSURFT(1-NPCRK) = ASIZE(I)
! = 0.01t, 0.02t, 0.03t, 0.04t…… (NPCRK=25)
UPPCD = 0.95 * THICK
do J = NPCRK+1, 60
        ZSURF(J) = ZSURF(J-1) + 0.25
        if (ZSURF(J).GE.UPPCD) then
                NCDP = J
                ZSURF(J) = UPPCD
                exit
        endif
end do
NCDP = J
```

Six subroutine calls are then made to prepare the necessary temperature, stresses, and K_I arrays corresponding to the mesh for PFM analysis.

(1) **Call TMPINT2D** – Transforms the thru-wall temperature distribution from the mesh written out by FAVLoad and read into FAVPFM (by subroutine RDDET) for each time step for each transient to the mesh generated by the subroutine SFMESH – as will be used when performing the probabilistic fracture mechanics analysis.

Figure 7 is an illustration of a transformation of the thru-wall temperature distribution at a single time step for a single transient. The large blue circles represent the temperatures at 16 thru-wall locations as was written out by FAVLoad and subsequently read into FAVPFM by subroutine RDDET. The small red dots represent the transformed temperature distribution to a mesh is generated by the subroutine SFMESH that is used during PFM or deterministic fracture analyses. This mesh is spaced in 0.01t increments for the first ¼ thickness of the RPV and spaced at a 0.25-inch increment thru the remainder of the wall thickness.

Similar transformations are performed at each user-specified time step for each transient included in the analysis. Recall that the user specifies a TIME record in the FAVLoad input file as follows: TIME TOTAL=250 DT=1.0.

Resulting MATRIX: TEMP (60, MTRAN, NTIMES)

(2) **CALL KAX99** – Transforms thru-wall K_I for internal surface breaking axially oriented infinite length flaws without and with thru-wall weld residual stress.

FAVLoad input matrices: ZKAX99 (16,MTRAN,NTIMES) and RZKAX99 (16,MTRAN,NTIMES)
Resulting FAVPFM matrices: AKAX99 (60, MTRAN, NTIMES) and RAKAX99 (60, MTRAN, NTIMES)

(3) **CALL KCR99** – Transforms thru-wall K_I for internal surface breaking circumferentially oriented infinite 360-degree flaws without and with thru-wall weld residual stress.

FAVLoad input matrices: ZKCRX99(16,MTRAN,NTIMES) and RZKCR99(16,MTRAN,NTIMES)
Resulting FAVPFM matrices: AKCR99(60, MTRAN, NTIMES) and RAKCR99(60,MTRAN,NTIMES)

(4) **CALL KAX99ext** – Transforms thru-wall K_I for external surface breaking axially oriented infinite length flaws without and with thru-wall weld residual stress.

FAVLoad input matrices: EZKAX99(16,MTRAN,NTIMES) and REZKAX99(16,MTRAN,NTIMES)
Resulting FAVPFM matrices: AKAX99ext(60, MTRAN, NTIMES) and RAKAX99ext(60,MTRAN,NTIMES)

(5) **CALL KCR99ext** – Transforms thru-wall K_I for external surface breaking circumferentially oriented infinite 360-degree flaws without and with thru-wall residual stresses.

FAVLoad input matrices: EZKCR99(16,MTRAN,NTIMES) and REZKCR99(16,MTRAN,NTIMES)
Resulting FAVPFM matrices: ECIRK99(60,MTRAN,NTIMES) and RECIRK99(60,MTRAN,NTIMES)

(6) **CALL SURFK3D** – Transforms thru-wall K_I for finite length semi-elliptical (aspect ratio 2, 6, and 10) internal and external surface breaking axially or circumferentially oriented flaws. Subroutine SPLINE performs each of the transformations.

(a) FAVLoad input matrix: AXK2TOT(9,MTRAN,NTIMES)
Resulting FAVPFM matrix: AXK2NEW (50,MTRAN,NTIMES)

(b) FAVLoad input matrix: AXK6TOT(9,MTRAN,NTIMES)
Resulting FAVPFM matrix: AXK6NEW(50,MTRAN,NTIMES)

(c) FAVLoad input matrix: AXK10TOT(9,MTRAN,NTIMES)
Resulting FAVPFM matrix: AXK10NEW(50,MTRAN,NTIMES)

(d) FAVLoad input matrix: CIRK2TOT(9,MTRAN,NTIMES)
Resulting FAVPFM matrix: CIRK2NEW (50,MTRAN,NTIMES)

(e) FAVLoad input matrix: CIRK6TOT(9,MTRAN,NTIMES)
Resulting FAVPFM matrix: CIRK6NEW (50,MTRAN,NTIMES)

(f) FAVLoad input matrix: CIRK10TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: CIRK10NEW (50,MTRAN,NTIMES)

(g) FAVLoad input matrix: RAXK2TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: RAXK2NEW (50,MTRAN,NTIMES)

(h) FAVLoad input matrix: RAXK6TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: AXK6NEW (50,MTRAN,NTIMES)

(i) FAVLoad input matrix: RAXK10TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: RAXK10NEW (50,MTRAN,NTIMES)

(j) FAVLoad input matrix: EAXK2TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: EAXK2NEW (50,MTRAN,NTIMES)

(k) FAVLoad input matrix: EAXK6TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: EAXK6NEW (50,MTRAN,NTIMES)

(l) FAVLoad input matrix: EAXK10TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: EAXK10NEW (50,MTRAN,NTIMES)

(m) FAVLoad input matrix: ECIRK2TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: ECIRK2NEW (50,MTRAN,NTIMES)

(n) FAVLoad input matrix: ECIRK6TOT (9,MTRAN,NTIMES)
ECIRK6NEW (50,MTRAN,NTIMES)

(o) FAVLoad input matrix: ECIRK10TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: ECIRK10NEW (50,MTRAN,NTIMES)

(p) FAVLoad input matrix: REAXK2TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: REAXK2NEW (50,MTRAN,NTIMES)

(q) FAVLoad input matrix: REAXK6TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: REAXK6NEW (50,MTRAN,NTIMES)

(r) FAVLoad input matrix: REAXK10TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: REAXK10NEW (50,MTRAN,NTIMES)

(s) FAVLoad input matrix: RECIRK2TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: RECIRK2NEW(50,MTRAN,NTIMES)

(t) FAVLoad input matrix: RECIRK6TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: RECIRK6NEW (50,MTRAN,NTIMES

(u) FAVLoad input matrix: RECIRK10TOT (9,MTRAN,NTIMES)
Resulting FAVPFM matrix: RECIRK10NEW (50,MTRAN,NTIMES)

NOTE: Any K_I array that begins with the letter R means the values of K_I in this array include the thru-wall weld residual stress.

In each case, the K_I solutions include those cases where the flaw is in the plate and in the weld material. The K_I solutions for the flaws in the thru-wall weld residual stress whereas the K_I solutions for the plate do not include the thru-wall weld residual stress.

Table 11 provides a summary of the array names before and after the transformation from the FAVLoad mesh to the FAVPFM mesh and the name of the subroutine in which that transformation takes place.

In each case, the transformation from one mesh to another mesh is accomplished by the generation and application of piecewise cubic spline curve fit coefficients. Figure 8 and Figure 9 provide examples of K_I solutions for circumferential flaws of an infinite (360 degrees) and an aspect ratio of 6, respectively.

Note that each of the above 6 subroutines makes a call to the subroutine named SPLINE – which generates the curve fit coefficients that are then applied in the six respective subroutines discussed above and summarized in Table 11.

Following the six above subroutine calls and if VFLAW files are specified, subroutine FLWDIS is called to distribute the flaws among the RPV regions and subregions. An additional call is made subroutine ARATIO to distribute the flaw aspect ratios.

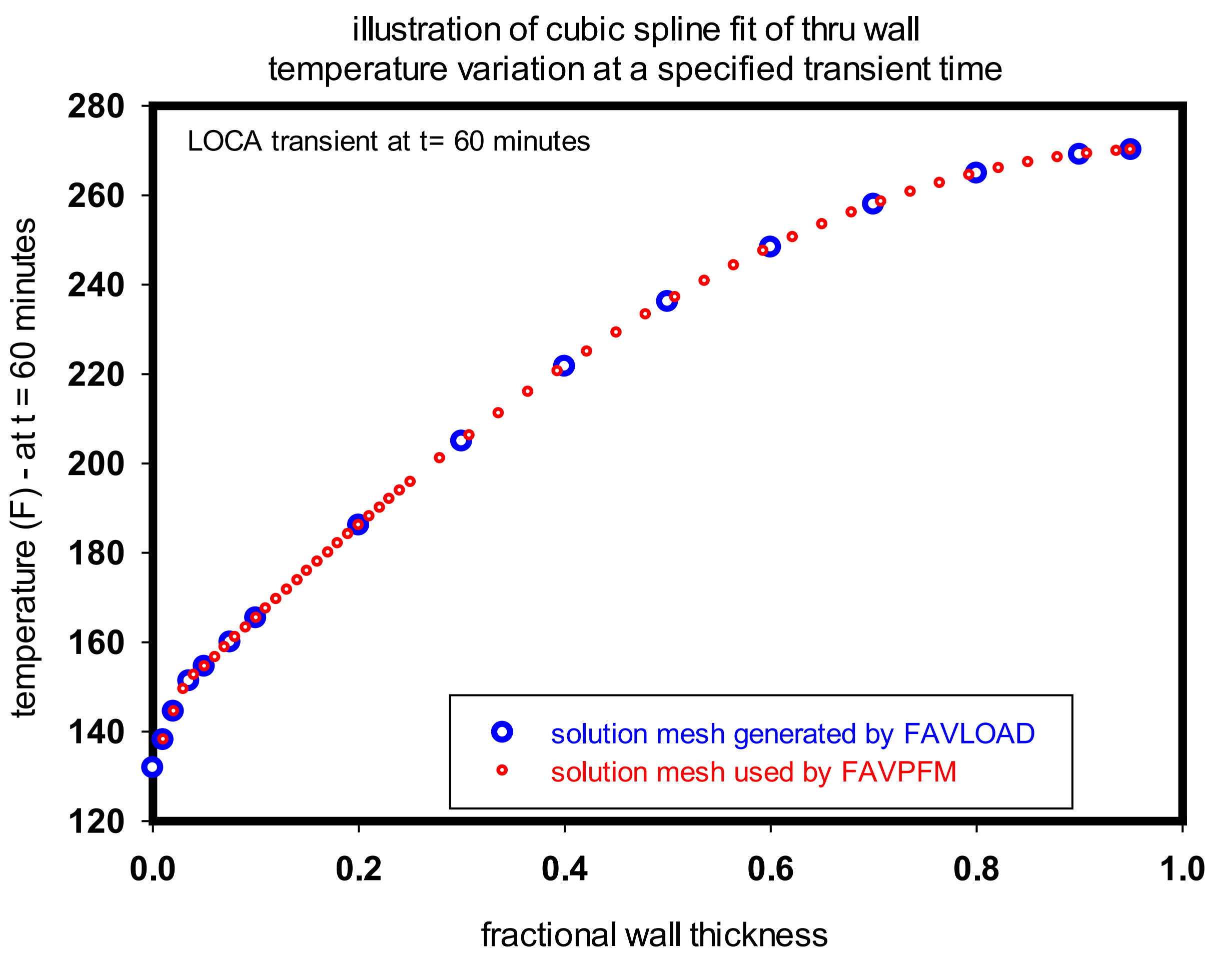


Figure 7: Illustration of Cubic Spline Fit of Thru Wall Temperature Variation at a Specified Transient Time

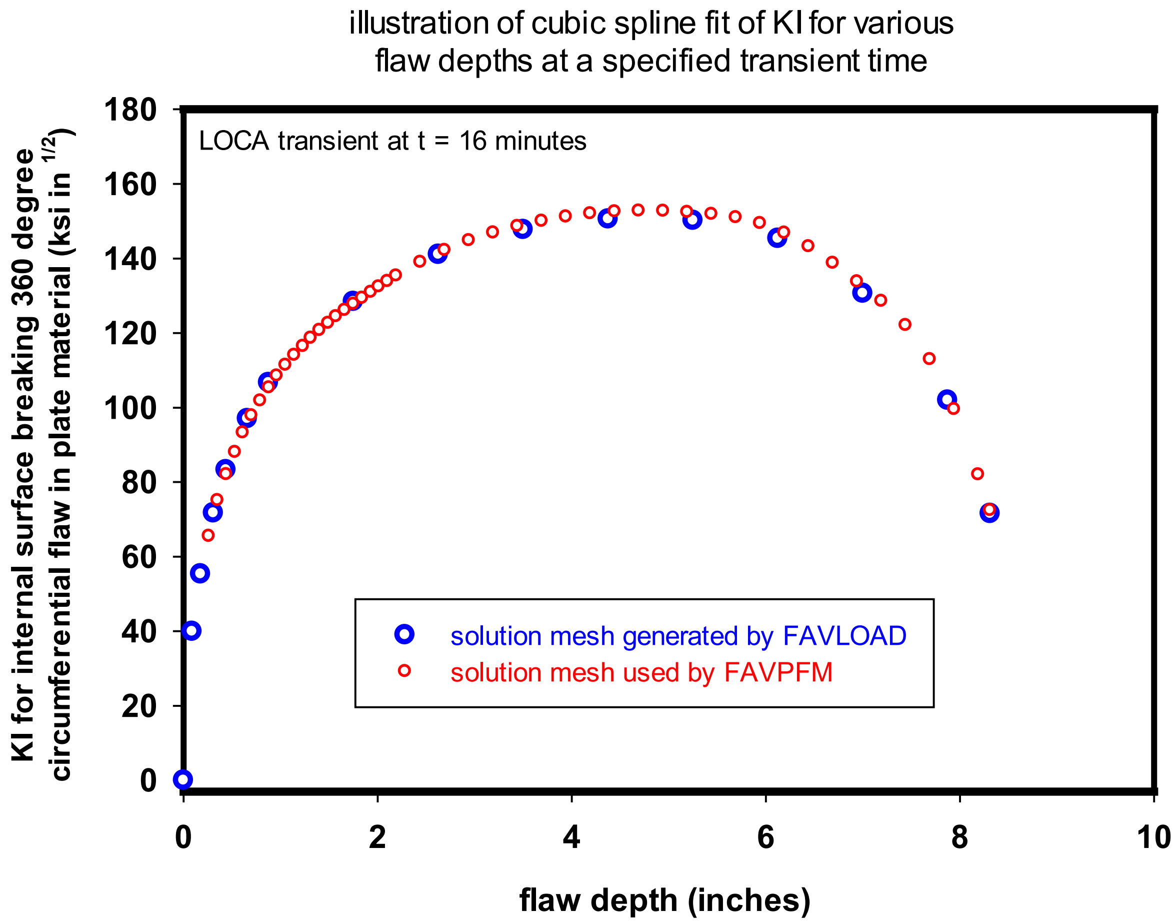


Figure 8: Illustration of Cubic Spline Fit of KI for 360-Degree Circumferential Internal Surface Breaking Flaw in Plate Material.

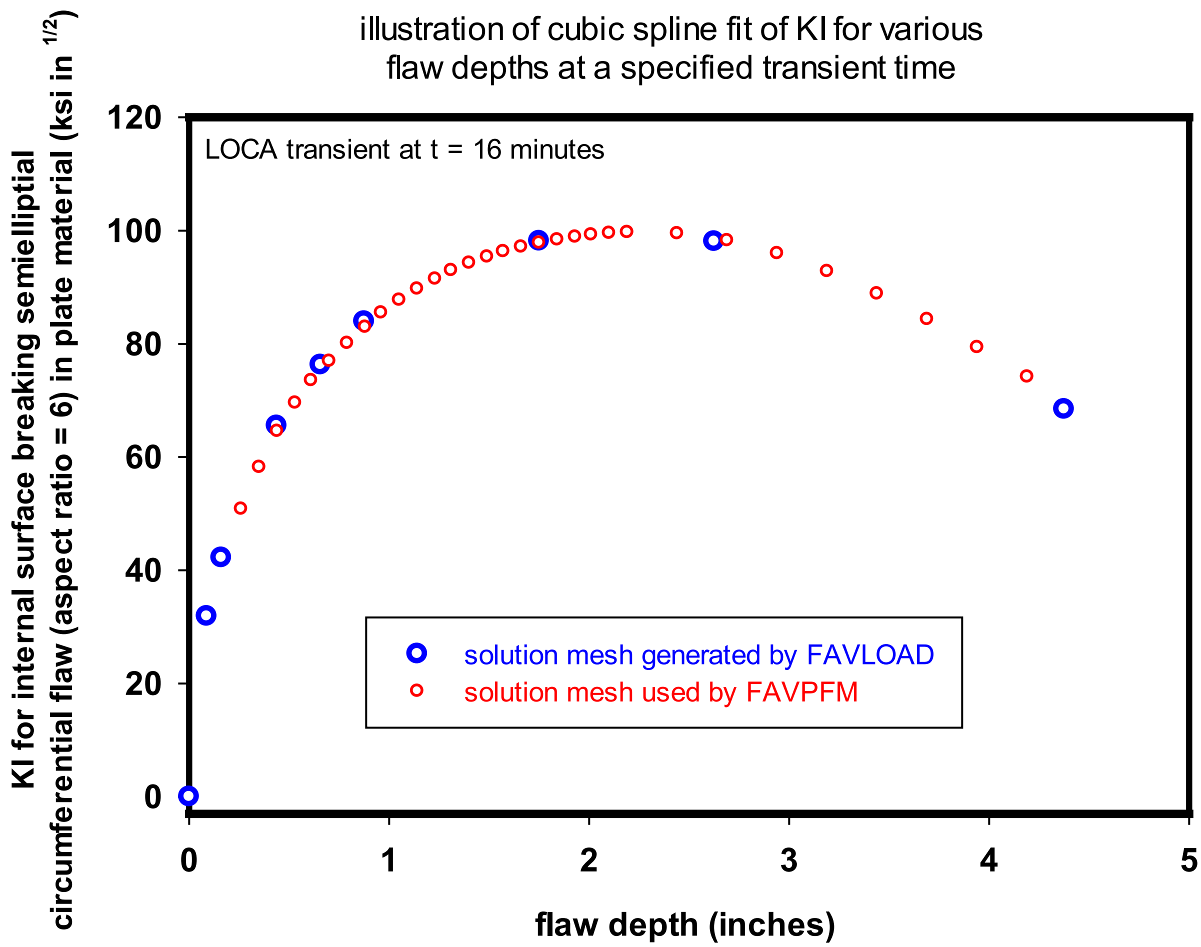


Figure 9: Illustration of Cubic Spline Fit of KI for Finite Length Internal Surface Breaking Semielliptical (Aspect Ratio = 6) Circumferential Flaw in Plate Material.

Table 11: Summary of Array Names and Subroutines Involved with Transformation of Thru Wall Variations of Temperature and KI for Various Flaw Geometries

Array Name as read in from FAVLoad Output	Subroutine where Cubic Spline occurs	Array Name (after Spline Fit Transformation)	Surface	Orientation	Weld Plate	Aspect Ratio
Transform Temperature						
ZSURFT	TMPTIP	TTIP	-	-	-	-
KI for infinite axial internal surface breaking flaws						
ZKAX99	KAX99	AKAX99	internal	axial	plate	infinite
RZKAX99	KAX99	RAKAX99	internal	axial	weld	infinite
KI for infinite circ for internal surface breaking flaws						
ZKCR99	KCR99	AKCR99	internal	circ	plate	infinite
RZKCR99	KCR99	RAKCR99	internal	circ	weld	infinite
KI for infinite axial external surface breaking flaws						
EZKAX99	KAX99ext	EAXIK99	external	axial	plate	infinite
REZKAX99	KAX99ext	REAXIK99	external	axial	weld	infinite
KI for infinite circ external surface breaking flaws						
EZKCR99	KCR99ext	ECIRK99	external	circ	plate	infinite
REZKCR99	KCR99ext	RECIRK99	external	circ	weld	infinite
KI for semielliptical inner surface breaking flaws						
AXK2TOT	SURFK3D	AXK2NEW	internal	axial	plate	2
AXK6TOT	SURFK3D	AXK6NEW	internal	axial	plate	6
AXK10TOT	SURFK3D	AXK10NEW	internal	axial	plate	10
CIRK2TOT	SURFK3D	CIRK2NEW	internal	circ	plate	2
CIRK6TOT	SURFK3D	CIRK6NEW	internal	circ	plate	6
CIRK10TOT	SURFK3D	CIRK10NEW	internal	circ	plate	10
RAXK2TOT	SURFK3D	RAXK2NEW	internal	axial	weld	2
RAXK6TOT	SURFK3D	RAXK6NEW	internal	axial	weld	6
RAXK10TOT	SURFK3D	RAXK10NEW	internal	axial	weld	10
RCIRK2TOT	SURFK3D	RCIRK2NEW	internal	circ	weld	2
RCIRK6TOT	SURFK3D	RCIRK6NEW	internal	circ	weld	6
RCIRK10TOT	SURFK3D	RCIRK10NEW	internal	circ	weld	10
KI for semielliptical external surface breaking flaws						
EAXK2TOT	SURFK3D	EAXK2NEW	external	axial	plate	2
EAXK6TOT	SURFK3D	EAXK6NEW	external	axial	plate	6
EAXK10TOT	SURFK3D	EAXK10NEW	external	axial	plate	10
ECIRK2TOT	SURFK3D	ECIRK2NEW	external	circ	plate	2
ECIRK6TOT	SURFK3D	ECIRK6NEW	external	circ	plate	6
ECIRK10TOT	SURFK3D	ECIRK10NEW	external	circ	plate	10
REAXK2TOT	SURFK3D	REAXK2NEW	external	axial	weld	2
REAXK6TOT	SURFK3D	REAXK6NEW	external	axial	weld	6
REAXK10TOT	SURFK3D	REAXK10NEW	external	axial	weld	10
RECIRK2TOT	SURFK3D	RECIRK2NEW	external	circ	weld	2
RECIRK6TOT	SURFK3D	RECIRK6NEW	external	circ	weld	6
RECIRK10TOT	SURFK3D	RECIRK10NEW	external	circ	weld	10

Design 8 Provide capability to 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 when user selects to perform deterministic fracture analyses.

The design of FAVOR is to perform deterministic and probabilistic fracture mechanics (PFM) analyses of reactor pressure vessels subjected to cool-down or heat-up thermal hydraulic transients imposed on the inner (wetted) surface of the reactor such as those associated with accidental Pressurized Thermal Shock (PTS) conditions and normal transients associated with reactor shutdown or heat-up.

8.1 User Option for Time History or Through-Wall Profiles

When a deterministic analysis is selected in the FAVPFM input, the code was designed to allow the user to select either to generate time history results at a specific location in the RPV wall or generate through-wall profiles of stress and $K_{I,applied}$ at a specific time. An input parameter called IOPT on the LDQA record is used to activate either option: IOPT=1 to activate the time history generation module or IOPT=2 to activate the through-wall profiles. FAVPFM uses the FAVLoad output file containing the Table 9 array information to generate the output from either selected option. The subroutines used to read in the user input, in particular the full LDQA record, are described in the above Design 2 requirement on page 20.

In order to perform the deterministic analysis, FAVPFM requires a flaw orientation (IFLOR), whether residual stresses are included or not (IWELD), type of flaw (inner surface-breaking flaw, embedded flaw, or outer surface-breaking flaw – IKIND), location of inner crack tip from inner surface if a time history analysis is performed or flaw depth if through-wall analysis is performed and embedded flaw is selected (XIN), flaw depth if a time history is performed or time at which the profile is to be produced if through-wall analysis is performed (XVAR), and an aspect ratio (ASPECT). Aspect ratios for surface breaking flaws must be 2, 6, 10, or 99 and for embedded flaws the aspect ratio must be > 0.0.

The FAVLoad output is a load-definition file, which is deterministic in nature, and thereby contains all the necessary information for FAVPFM to output flaw specific time history or through-wall profiles for surface-breaking flaws. Note that embedded flaws are closed form solutions and $K_{I,applied}$ are calculated as needed within FAVPFM, in particular, within subroutine QA_REPORTS, with supporting calls to subroutines QSUB, SUBMM, SUBMB, and STRINT2 to calculate the membrane and bending stresses. The equation used to calculate $K_{I,applied}$ for embedded flaws is described in the previous design description on page 47.

Subroutine STRINT2 is also used for other flaws to performs linear interpolation to determine the stress (Hoop and Axial) at a point in the RPV wall (x) at a specific time step (ntstep) for a specific transient. Subroutine QA_REPORTS is the main routine called by the main FAVPFM routine to print either the time history or through-wall profile based on the user specified flaw characteristics (IFLOR, IWELD, IKIND, XIN, XVAR, and ASPECT) and FAVLoad load definition file.

All the write statements to output the deterministic analysis, either time history or through-wall, are within subroutine QA_REPORTS. The output is written to the FAVPFM output file, Fortran Unit 29. Samples of output for the two deterministic options are shown on the following pages.

8.2 Time History Output

An excerpt of a sample time history report is shown below for a internal surface breaking flaw:

```
******************************************************
TIME HISTORY RESULTS FOR INTERNAL SURFACE BREAKING FLAW
  0.5000 inches IN DEPTH FROM INNER SURFACE
INTERNAL-SURFACE BREAKING FLAW
CIRCUMFERENTIAL FLAW WITH RESIDUAL STRESSES
******************************************************


 TRANSIENT NUMBER   1

                              AXIAL    KX-> X = ASPECT RATIO
NSTEP  TIME    TEMP    PRESS  STRESS    K2      K6      K10     KINF
   1    0.00  544.80    2.30   16.41   14.91   20.59   21.65   23.33
   2    1.00  542.88    0.98   10.71    9.38   12.96   13.61   15.18
    :      :        :        :        :        :        :        :        :
    :      :        :        :        :        :        :        :        :
```

An excerpt of a sample time history report is shown below for an embedded flaw:

```
******************************************************
AXIAL EMBEDDED FLAW WITH RESIDUAL STRESSES
POSITION OF POINT 1 =  8.375 IN.(FROM INNER SURF.)
POSITION OF POINT 2 =  7.875 IN.(FROM INNER SURF.)
FLAW DEPTH (2a)     =  0.500 IN.
ASPECT RATIO        =  6.000
******************************************************


 TRANSIENT NUMBER   1

                               HOOP STRESSES
                             MEMBRANE BENDING                    POINT 1
NSTEP  TIME    TEMP    PRESS   STRM    STRB      Q     SMM     SMB     KI
   1    0.00  532.17    2.10   23.09   -1.64    1.08    1.02    0.96   18.81
   2    1.00  532.17    1.74   19.42   -1.36    1.08    1.02    0.96   15.84
   3    2.00  532.17    1.46   16.55   -1.14    1.08    1.02    0.96   13.51
   4    3.00  532.17    1.21   14.00   -0.95    1.08    1.02    0.96   11.45
   5    4.00  532.17    1.04   12.18   -0.81    1.08    1.02    0.96    9.97
   :      :     :        :       :        :       :       :       :       :
   :      :     :        :       :        :       :       :       :       :
```

8.3 Through-Wall Output

An excerpt of a sample through-wall profile report is shown below:

```
 ******************************************************
 RESULTS FOR  129.000 MIN.  ELAPSED TIME IN TRANSIENT
 INTERNAL-SURFACE BREAKING FLAW
 AXIAL FLAW WITHOUT RESIDUAL STRESSES
 ******************************************************
        FOR FLAW DEPTHS THAT RESIDES IN CLAD REGION
             NO FRACTURE ANALYSES IS PERFORMED
       VALUES OF KI NOT REPORTED FOR SUCH FLAW DEPTHS
 ******************************************************


TRANSIENT NUMBER   1

                                HOOP       KX-> X=ASPECT RATIO
NSTEP  R(IN.)   TEMP    PRESS  STRESS    K2      K6      K10     KINF
 130    0.09  248.98    2.54   34.38
 130    0.18  249.72    2.54   34.13
 130    0.26  250.33    2.54   30.22   22.13   31.90   33.70   38.67
 130    0.35  250.72    2.54   30.10   24.57   35.50   37.58   43.71
 130    0.44  250.97    2.54   29.98   26.72   38.68   41.03   47.62
  :      :       :       :       :       :       :       :       :
 130    1.75  255.49    2.54   28.09   49.61   74.65   82.03  100.87
 130    1.84  255.81    2.54   27.96   50.70   76.62   84.47  104.65
 130    1.93  256.13    2.54   27.83   51.76   78.58   86.91  108.53
 130    2.01  256.44    2.54   27.70   52.78   80.52   89.34  112.50
 130    2.10  256.76    2.54   27.57   53.78   82.44   91.78  116.59
 130    2.19  257.08    2.54   27.45   54.76   84.35   94.22  120.79
 130    2.44  257.98    2.54   27.08   57.39   89.71  101.23  133.49
 130    2.69  258.89    2.54   26.71   59.83   94.96  108.31  147.38
 130    2.94  259.79    2.54   26.35   62.10  100.10  115.50  162.61
  :      :       :       :       :       :       :       :       :
 130    7.19  271.38    2.54   21.57                           809.74
 130    7.44  271.70    2.54   21.42                           870.10
 130    7.69  271.96    2.54   21.28                           923.87
 130    7.94  272.16    2.54   21.14                           967.55
 130    8.19  272.30    2.54   21.04                          1001.07
 130    8.31  272.36    2.54   20.99                           957.62

FOR INTERNAL SURFACE BREAKING-FLAWS; R IS MEASURED FROM THE RPV INNER SURFACE
```

An excerpt of a sample through-wall profile report is shown below for an embedded flaw:

```
 ******************************************************
 AXIAL EMBEDDED FLAW WITHOUT RESIDUAL STRESSES
 RESULTS FOR   14.000 MIN. ELAPSED TIME IN TRANSIENT
 POSITION OF POINT 1 =  1.200 IN.(FROM INNER SURF.)
 ASPECT RATIO        =  6.000
 ******************************************************


TRANSIENT NUMBER   1

                                  HOOP STRESSES
```

				MEMBRANE	BENDING				POINT 1
R	FL DEPTH	TEMP	PRESS	STRM	STRB	Q	SMM	SMB	KI
1.23	0.03	324.00	0.05	-29.39	93.79	1.08	1.00	0.73	7.49
1.31	0.11	329.77	0.05	-29.39	93.79	1.08	1.00	0.73	15.70
1.40	0.20	335.54	0.05	-29.39	93.79	1.08	1.00	0.72	20.68
1.49	0.29	341.31	0.05	-29.39	93.79	1.08	1.00	0.72	24.4
1.58	0.38	347.09	0.05	-29.39	93.79	1.08	1.01	0.71	27.59
1.66	0.46	352.86	0.05	-29.39	93.79	1.08	1.01	0.71	30.22
1.75	0.55	358.63	0.05	-29.39	93.79	1.08	1.01	0.70	32.49
1.84	0.64	363.42	0.05	-27.72	91.48	1.08	1.01	0.70	34.55
1.93	0.73	368.20	0.05	-26.45	89.74	1.08	1.02	0.69	36.40
:	:	:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:	:	:
3.69	2.49	451.23	0.05	-13.79	72.29	1.08	1.11	0.60	54.00
3.94	2.74	459.73	0.05	-12.08	69.94	1.08	1.13	0.59	55.57
4.19	2.99	468.23	0.05	-10.67	67.98	1.08	1.14	0.58	56.98
4.44	0.00	476.17	0.05						
4.69	0.00	482.43	0.05						
4.94	0.00	488.70	0.05						
:	:	:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:	:	:
8.19	0.00	528.53	0.05						
8.31	0.00	528.93	0.05						

Design 9 For probabilistic fracture analyses, implement a Monte Carlo technique, where deterministic fracture analyses are performed on a large number of stochastically generated RPV trials or realizations.

FAVPFM, in particular subroutine PFM, uses a model based on the Monte Carlo technique, where deterministic fracture analyses are performed on many stochastically generated RPV trials or realizations. Each vessel realization can be considered a perturbation of the uncertain condition of the specific RPV under analysis. The condition of the RPV is considered uncertain in the sense that several the vessel’s properties (specifically, material chemistry composition and irradiation fluence) along with the postulated flaw population have uncertainties associated with them. These input uncertainties are described by statistical distributions. The RPV trials propagate the input uncertainties with their interactions through the model, thereby determining the probabilities of crack initiation and through-wall cracking.

The FAVPFM model also provides estimates of the uncertainties in its outputs in terms of discrete statistical distributions. By repeating the RPV trials many times, the output values constitute a random sample from the probability distribution over the output induced by the combined probability distributions over the several input variables.

The assumed fracture mechanism is stress-controlled cleavage initiation (in the transition-temperature region of the vessel material) modeled under the assumptions of linear-elastic fracture mechanics (LEFM). The failure mechanism by through-wall cracking is 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. Flaw growth can be due to either cleavage propagation or stable ductile tearing. In addition, if the conditions for unstable ductile tearing are satisfied, then vessel failure by through-wall cracking is assumed to occur.

The Monte Carlo method involves sampling from appropriate probability distributions to simulate many possible combinations of flaw geometry and RPV material embrittlement subjected to transient loading conditions. The PFM analysis is performed for the beltline of the RPV as defined by the input data and typically assumed to extend from one foot below the reactor core to one foot above the reactor core. The RPV beltline can be divided into major regions such as axial welds, circumferential welds, and plates or forgings that may have their own embrittlement-sensitive chemistries. The major regions may be further discretized into subregions to accommodate detailed neutron fluence maps that can include significant details regarding azimuthal and axial variations in neutron fluence. The general data streams that flow through the FAVPFM module are depicted in Figure 10.

The FAVPFM module requires, as input, load-definition data from FAVLoad and user-supplied data on flaw distributions and embrittlement of the RPV beltline. FAVPFM then generates two matrices: (1) the conditional probability of crack initiation (PFMI) matrix and (2) conditional probability of through-wall cracking (PFMF) matrix. The (i, j)th entry in each array contains the results of the PFM analysis for the jth vessel simulation subjected to the ith transient.

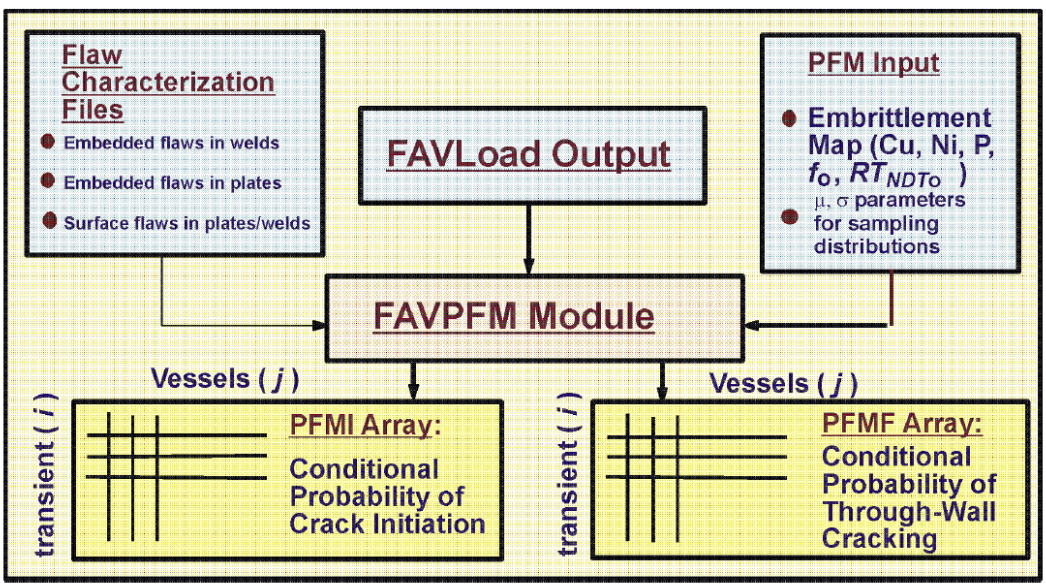


Figure 10: The FAVPFM module takes output from FAVLoad and user-supplied data on flaw distributions and embrittlement of the RPV beltline and generates PFMI and PFMF arrays.

Figure 11 shows a high-level overview of FAVPFM and the subroutines called to perform the functions described in Figure 10.

The descriptive Fortran logic sequence is shown below:

HIGH LEVEL CALLING SEQUENCE for FAVPFM

```
CALL FILE_INIT_PFM
! Queries user for input/output filenames and opens all files.
CALL RDDET
! Reads FAVLoad Output File which contains temperatures, stresses, and KIs.
CALL RDPFM
!  Reads PFM input dataset.
IF (IQA = 0) THEN
! (perform PFM ANALYSES)
       CALL RDSURF, RDWELD and RDPLATE
       ! Reads 3 input flaw files or CALL RDFOUND – Reads As-found flaw file.
       TRANSFORM T and K to new meshes to be used in PFM analyses using SPLINE.
       CALL FLWDIS
       ! Distributes Flaws among subregions.
       CALL PFM
       ! Performs main probabilistic fracture mechanics  calculation.
       10     NTRIAL  = NTRIAL + 1
       ! (RPV Trial Loop)
              5556   NFLAW = NFLAW + 1
              !(Flaw Loop)
                     !Locate sub-region in which this flaw resides.
                     CALL FLUENCE
                     ! Sample neutron fluence.
                     CALL WLDCHEM OR PLCHEM
                     ! Sample chemistry.
                     CALL FLAWCAT
                     ! Determine flaw category.
                     CALL FLAW
                     ! Sample flaw depth.
                     CALL CRTNDT
                     ! Determine RTNDT at crack tip.
                     DO 8888 ITRAN = ITRAN + 1
                     !(Transient Loop)
                            Do 110 NTSTEP = NTSTEP + 1
                            !(Time Loop)
                                   TADJ = T(t)
                                   ! RTNDT
                                   Calculate Weibul a = 19.35 + 8.335 exp (0.02254 *
TADJ)
                                   Calculate cpi  (ITRAN,NFLAW,NTSTEP)
                            110 CONTINUE
                            !  (Close Time Loop)
                            If (CPI > 0)  CALL ACCOUNT
                            ! Performs accounting procedures to acquire data to
generate
                            ! output reports.  Also serves as the driver for calling
                            ! subroutine PROP which performs a thru-wall analysis to
                            ! determine the conditional probability of failure.
                     8888 CONTINUE
                     !  (Close Transient Loop)
              5556  CONTINUE
              !  (Close Flaw Loop)
       CALL OUTCPI
       ! Writes CPI to screen and to INITIATE.DAT for current RPV trial.
       CALL OUTCPF
       ! Writes CPF to screen and to FAILURE.DAT for current RPV trial.
       10 CONTINUE
       !  (Close RPV Trial Loop)
       CALL REPORT
```

```
       !  Creates PFM Output file.
ELSE   (IQA = 1)
       PERFORM Deterministic Analysis
END IF
```

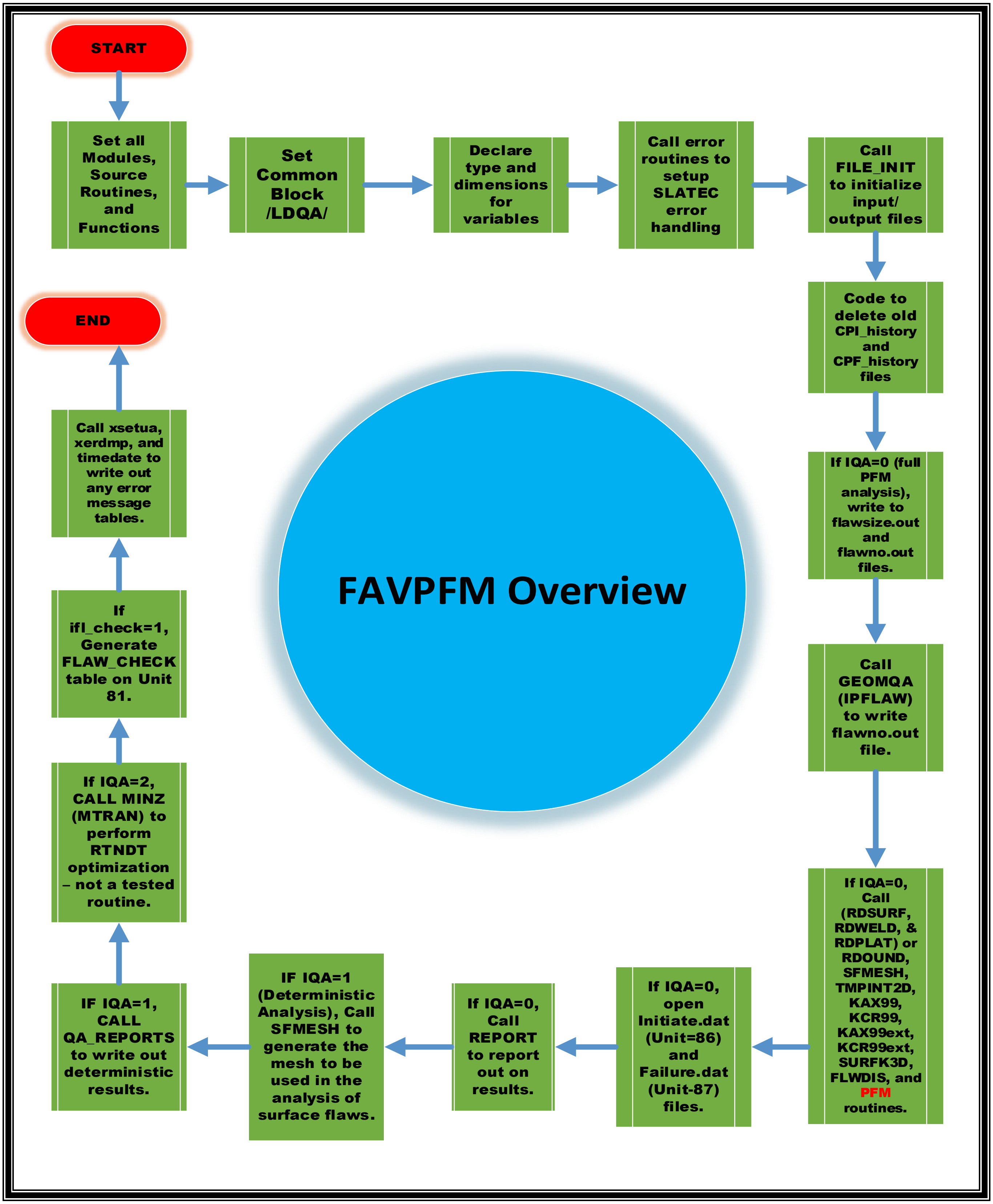

START
Set all Modules, Source Routines, and Functions
Set Common Block /LDQA/
Declare type and dimensions for variables
Call error routines to setup SLATEC error handling
Call FILE_INIT to initialize input/ output files
Code to delete old CPI_history and CPF_history files
If IQA=0 (full PFM analysis), write to flawsize.out and flawno.out files.
Call GEOMQA (IPFLAW) to write flawno.out file.
If IQA=0, Call (RDSURF, RDWELD, & RDPLAT) or RDOUND, SFMESH, TMPINT2D, KAX99, KCR99, KAX99ext, KCR99ext, SURFK3D, FLWDIS, and PFM routines.
If IQA=0, open Initiate.dat (Unit=86) and Failure.dat (Unit-87) files.
If IQA=0, Call REPORT to report out on results.
IF IQA=1 (Deterministic Analysis), Call SFMESH to generate the mesh to be used in the analysis of surface flaws.
IF IQA=1, CALL QA_REPORTS to write out deterministic results.
If IQA=2, CALL MINZ (MTRAN) to perform RTNDT optimization – not a tested routine.
If ifl_check=1, Generate FLAW_CHECK table on Unit 81.
Call xsetua, xerdmp, and timedate to write out any error message tables.
END
FAVPFM Overview

Figure 11: High Level Overview of FAVPFM Module

To further describe the Fortran routines and processing within FAVPFM, content is broken into several parts as follows:

- Part 9.1 details the listing of FAVPFM file allocations used to perform the many internal computations.
- Parts 9.2 and 9.3 describe the package of random number generators that are used throughout FAVPFM; initially sets seeds for random number generator.
- Parts 9.4 through 9.8 provide the Probabilistic Fracture Mechanics (PFM) analysis logic through the use of flowcharts and references to subroutines. A detailed description of subroutines and variables are provided.

9.1 FAVPFM File Allocations

Due to the detailed characterization of flaws within FAVPFM and the desire to follow crack propagation through arrest or failure, a number of files are used to account for the many variables used to process FAVPFM internal computations. These files are captured in Table 12.

Table 12: FAVPFM File Allocations

Unit #	File Name	Input/Output/Internal
5,*	Not applicable	Screen and Command prompt
15	User defined FAVPFM input file (FNAME1)	Input
16	F16	Internal
17	F17	Internal
29	User defined FAVPFM output file (FNAME6)	Output
30	*.echo	Output file
39	User defined Flaw file for embedded flaws in plate (FNAME5)	Input
41	User defined FAVLOAD output file (FNAME2)	Input
42	F42 (equivalent to Unit 41 except no comments)	Internal
48	User defined Flaw file for surface breaking flaws (FNAME3)	Input
49	User defined Flaw file for embedded flaws in weld (FNAME4)	Input
50	User defined As-Found flaw file (FNAME8)	Input
71	CPI_history.out	Output
72	CPF_history.out	Output
81	TRACE.OUT	Output
82	FLAWSIZE.OUT	Output
83	FLAWNO.OUT	Output
84	ARREST.OUT	Output

Unit #	File Name	Input/Output/Internal
85	RTNDT.OUT	Output
86	INITIATE.DAT	Output
87	FAILURE.DAT	Output
88	Not used anymore	Debug CPI Output for Mark Kirk
89	Not used anymore	Debug CPF Output for Mark Kirk
91	restart.bin	Binary Input/Output
92	PFMI.BIN	Binary Output
93	PFMF.BIN	Binary Output
94	TRACE_embedded.OUT	Output (Debug file – No longer used.)

9.2 Seeds for Random Number Generator

FAVPFM requires the ability to set seeds for random numbers. A portable random number generator, written in Fortran, has been implemented and tested in FAVOR. This portable generator, based on a composite of two multiplicative linear congruential generators using 32-bit integer arithmetic, has a reported theoretical minimum period of 2.3×10^{18}. This implementation was successfully tested by the HSST Program at ORNL for statistical randomness using the NIST *Statistical Test Suite for Random and Pseudorandom Number Generators*.

Random sampling is required in multiple places within FAVPFM. In fact, *two sampling blocks* exist in FAVOR, 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 crack *Initiation-Growth-Arrest* sub-model6 draws from sets of random number sequences created in the second sampling block. These set-aside random number sequences remain fixed for the current flaw and 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*. The above approach involves an implementation of a variance reduction technique called *common random numbers* (CRN) which, in the terminology of classical experimental design, is a form of *blocking*. CRN has also been called *correlated sampling* or *matched streams* in some statistical simulation contexts.

9.3 Subroutine Calls Related to Random Numbers and Error Handling

The following shows the sequence of FAVPFM subroutine calls to initialize random number generators and to set up the error handling variables.

Module random_num_generator_m – Initializes random number generator (This is a translation from Pascal to Fortran of routine Get_State from [15].

Within this module a module **subroutine random_seed** is used - which sets all the random number generators. Sets the initial seed of generator 1 to ISEED1 and ISEED2. The initial seeds of the other generators are set accordingly, and all generators' states are set to these seeds. This is a translation from Pascal to Fortran of routine Set_Initial_Seed from the paper.

Also within this module another **module subroutine random_number_(harvest)** is used, which emulates the behavior of the similarly named intrinsic subroutine.

Submodule(random_num_generator_m) random_num_generator_s – Used with the above module to set initial values for the seeds. This submodule also contains a **module procedure random_seed** and **procedure random_number_** with an **integer function random_integer()**

Note that FAVPFM confines 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 is drawn from sets of random number sequences created in the second sampling block (e.g., get_grab_bag function and the use of the grab_bag array (dimensioned to 5000) of saved random numbers used in snorm2a). These set-aside random number sequences (i.e., grab_bag array) 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. This approach allows the transients to be ordered in any fashion without changing the results.

```
CALL XERMAX – Sets up SLATEC error handling variables.
CALL XSETUA                      "
CALL XSETF                 "
```

9.4 Probabilistic Fracture Mechanics Analysis

A high-level flowchart for the Probabilistic Fracture Mechanics (PFM) analysis is shown in Figure 12. An additional flowchart showing how subroutine PFM calls other subroutines is shown in Figure 13. Figure 13 presents a flowchart illustrating the essential elements of the nested-loop structure of the PFM Monte Carlo model – (1) RPV Trial Loop, (2) Flaw Loop, (3) Transient Loop, and (4) Time integration Loop. The outermost RPV Trial Loop is indexed for each RPV trial included in the analysis, where the number of RPV trials is specified by the user in the FAVPFM input stream. Since each RPV trial can be postulated to contain multiple flaws, the next innermost loop (the Flaw Loop) is indexed for the number of flaws for this trial. Each postulated flaw is positioned (through sampling) in an RPV beltline subregion having its own distinguishing embrittlement-related parameters. Next, the flaw geometry (depth, length, aspect ratio, and location within the RPV wall) is determined by sampling from appropriate distributions derived from expert judgment and nondestructive and destructive examinations of RPV steels. Each of the embrittlement-related parameters [nickel and manganese (alloying elements), copper and phosphorus (contaminants), neutron fluence, and an estimate of the epistemic and aleatory uncertainties in the unirradiated RTNDT(0)] are sampled from distributions, as described in the various sub-sections in section 5.2 of Reference [1]. The neutron fluence is attenuated to the crack tip location, and a value for the irradiated reference index, RT_{NDT} (serving as a quantitative estimate of radiation damage), is calculated.

A deterministic fracture analysis is then performed on the current flaw for each of the postulated transients; thus, the deterministic component of the analysis involves two inner nested loops – a Transient Loop and a Time-integration Loop. The temporal relationship between the applied Mode I stress intensity factor (KI) and the static cleavage fracture initiation toughness (K_{Ic}) at the crack tip is calculated at discrete transient time steps. The fracture-toughness, K_{Ic} , statistical model is a function of the normalized temperature, $T(\tau) - RT_{NDT}$, where $T(\tau)$ is the time-dependent temperature at the crack tip. Analysis results are used to calculate the conditional probability of crack initiation (CPI), i.e., the probability that pre-existing fabrication flaws will initiate in cleavage fracture. Also, the PFM model calculates the conditional probability of failure (CPF) by through-wall cracking, i.e., the probability that an initiated flaw will propagate through the RPV wall. These probabilities are conditional in the sense that the thermal-hydraulic transients are assumed to occur. The values of CPI and CPF calculated for individual flaws become the statistically independent marginal probabilities used in the construction of the joint conditional probabilities of initiation and failure.

9.5 PFM Analysis Flowchart and Subroutines

The Probabilistic Fracture Mechanics (PFM) analysis is triggered by the user specification of IQA being set to zero. Software logic proceeds to a call to subroutine PFM which is the driver routine for the PFM analysis. Four major flowcharts describe the inner workings of the FAVPFM iterative structure. These are described in the FAVOR Theory Manual (i.e., Figure 16, Figure 17a, Figure 17b, and Figure 17c) and reproduced herein. Figure 16 of the theory manual is reproduced as Figure 12 and is discussed above. A further breakdown of that flowchart shows that many subroutine calls are made to calculate CPI and CPF. These are shown in Figure 13 alongside the flowchart from Figure 12. The seventeen subroutines shown have a description of their intended purpose and a listing of the passed parameters from the calling routines. Below Figure 13, Table 13 provides a listing of definitions for key variables used in the call statements.

Similarly, Figure 15 describes the subroutine ACCOUNT which is called from subroutine PFM (as shown in Figure 13) and shows the *Initiation-Growth-Arrest (IGA)* sub-model logic. Each step, G1 through G10, is explained in detail and shows the relevant program steps associated with implementing the flowchart logic. The IGA logic is primarily controlled by subroutine ACCOUNT. Additional information is provided in Figure 16, which shows the calls from ACCOUNT to subroutine PROP and the continued calls to other routines from subroutine PROP. At the bottom of Figure 15, Table 14 provides a listing of definitions for key variables used in the ACCOUNT routine.

Continuing with the inner loops with FAVPFM, the *IGA "propagation"* sub-model is described in Figure 17. The programming logic that implements the IGA propagation sub-model resides in subroutine PROP. Each step, P1 through P10, is explained in detail and shows the relevant program steps in subroutine PROP associated with implementing the flowchart logic. The primary objective within this sub-model is to determine if vessel failure occurs and whether the failure was caused by plastic collapse, by exceeding the limit on flaw depth, or by unstable ductile tearing. There are calls to other routines to determine if a new weld layer has been entered and if so, resampling of weld chemistry parameters is performed. Additional calls to calculate RT_{Arrest}, K_{Ia}, and K_{Ic} (with warm pre-stress on or off) are performed to determine if the $K_{I,Applied}$ results in a stable arrest or if flaw growth is re-initiated. At the bottom of Figure 17, Table 15 provides a listing of definitions for key variables used in the PROP routine.

Lastly, the FAVPFM inner-most loop is the *Ductile-Tearing* sub-model, which is described in Figure 18. This model is called if the option is turned on and uses the current position and orientation of the crack tip along with the time within the selected transient. Other data coming from the IGA propagation sub-model includes the temperature, driving force (K_I), sampled flow stress (σ_f), elastic modulus, Poisson's ratio, irradiated upper shelf energy, and current value for J_R^*. Each step, D1 through D5, is explained in detail and shows the relevant program steps in subroutine ductile_tearing associated with implementing the flowchart logic. The primary objectives within this sub-model are to:

1. Determine If ductile tearing is unstable or stable (i.e., Logical variables "FAIL_UDT" and "STABLE_DT" set to ".TRUE." or ".FALSE.").

2. Determine $J_{applied}$ and compare it to JIC and JR* to determine the above status of "FAIL_UDT" and "STABLE_DT". Two ductile tearing models are available. One based on $\widehat{J_{Ic}}$ and the other based on the JR-curve parameters, $\widehat{J_{Ic}}$, $\widehat{C}$, and $\widehat{m}$.

3. If ductile tearing is predicted, the sub-model advances the position of the flaw by the amount of ductile crack extension produced by the known value of $J_{applied}$. Figure 19 illustrates how the flaw position and local material tearing modulus are calculated based on second-order finite-difference ratio.

Following the calls to the *Ductile-Tearing* sub-model, execution is returned to the IGA sub-model.

In summary, the main FAVPFM logic is illustratively presented in four flowcharts, Figures 8 through 13. The main Fortran subroutines are provided alongside the relevant flowchart logic. In addition, key variables and their definitions supporting the FAVPFM logic are provided in Tables 11 through 13. A detailed narrative of the logic is also provided at the end of the above figures. These flowcharts provide the design description for Design 9, which consists of implementing a Monte Carlo technique in which deterministic fracture analyses are performed on a large number of stochastically generated RPV trials or realizations.

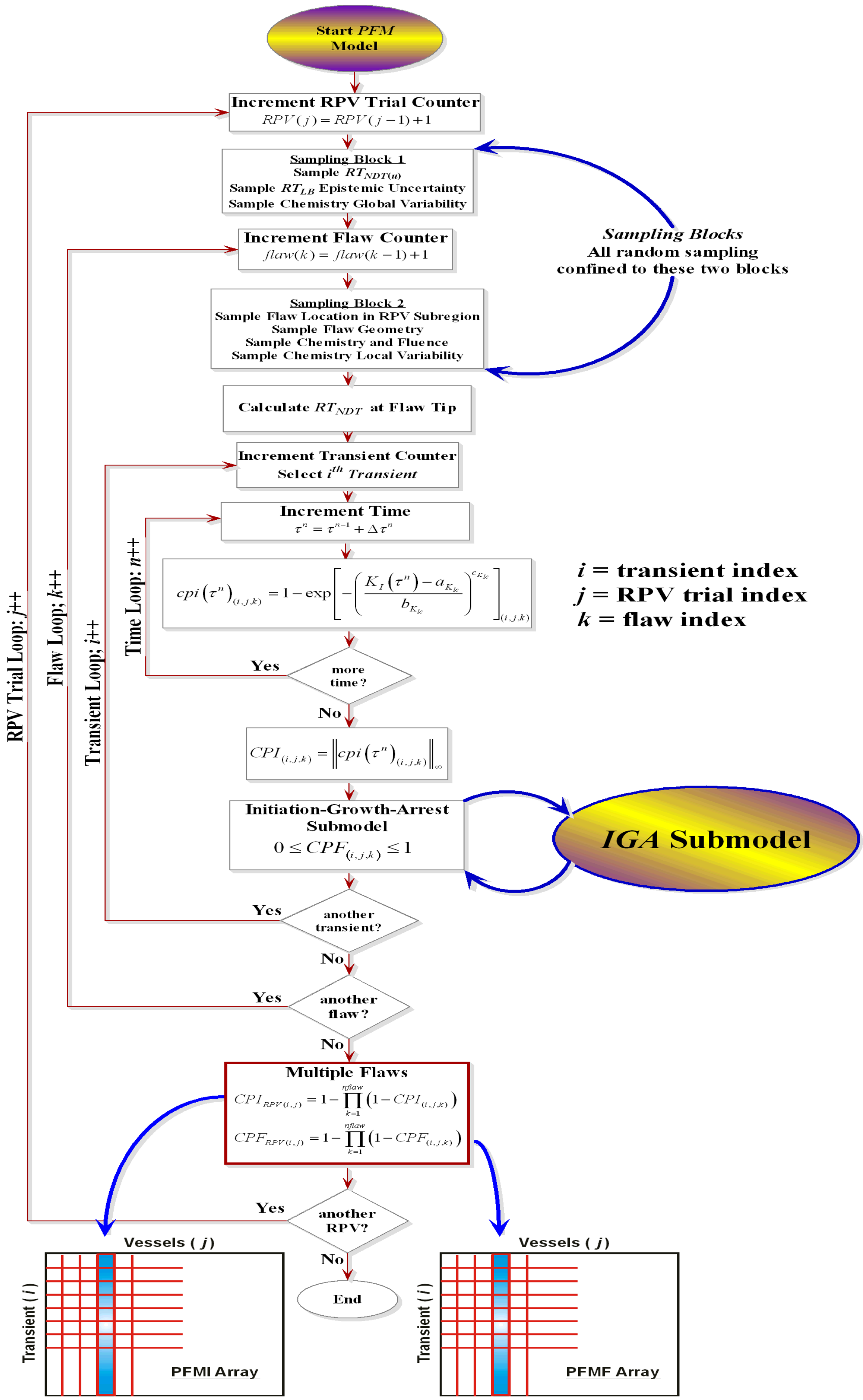
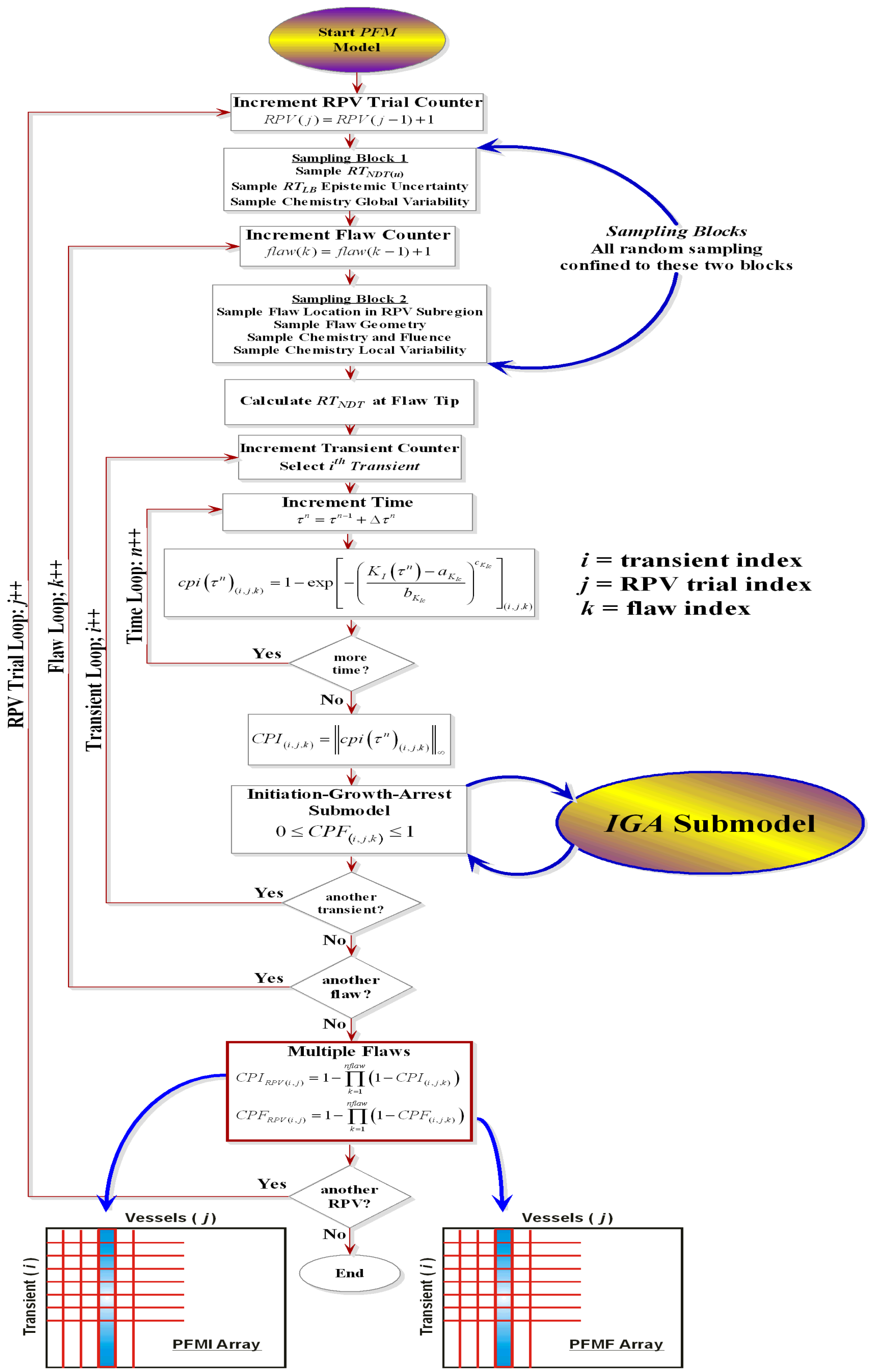


Figure 12: High Level FAVPFM Flowchart showing the four primary nested loops – (1) RPV Trial Loop, (2) Flaw Loop, (3) Transient Loop, and (4) Time Loop. Note: ++ notation indicates increment index by 1, e.g., i++ means i=i+1.



- **PFM** — Subroutine PFM (MTRAN, TC, KHALF, xinmesh). Called by Main Program FAVPFM16-1.
  Calls random_seed_(), RTCALC1, MARK, WCFCT199, PCFCT199, read_restart_file(), setup_Long_output, write_restart_file(), random_number_(), and the below routines. Uses various Functions which are contained in varoius modules specified below.
- **RTCALC1** — Module Procedure RTCALC1 (RTCALC,USE_CALC, ZSURF,CFDIFF,CU,ANI,PHOS,AMN,FO,SIGDEL, SIGRTO,TC,NTSUB,iheat,iheat_embedded) - Calculates RTNDTs for each subregion. Contained within submodule(rtndt_calculation_m) rtndt_calculation_s.
- **sample major region variables** — For each major region, sample values for standard deviations of chemistry: Ni, P, Cu, and Mn. Also sample major region values for unirradiated RTNDT. Calls rtlb and G05DDF, get_Weibull_Q, get_Johnson_SB_Q, and random_number_(rndu). GO5DDF, get_Weibull_Q, and get_Johnson_SB_Q are functions defined in module distributions_m and submodule(distributions_m) distributions_s.
- **FLUENCE** — FLUENCE (SIGFGL,SIGFLC,FO, NSBR,NTSUB,GLBSIG,SFID) - Generates value of surface fluence from normal distribution and sets lower bound on surface fluence to prevent numerical problems.
- **WLDCHEM** — WLDCHEM (IPASS,CHMPAS, CHMPAS_DT) - Implements the rules for stochastically simulating chemistry in weld. Routine in module chemistry_m and submodule(chemistry_m) chemistry_s.
- **PLCHEM** — PLCHEM (IPASS,CHMPAS_PL) - Implements the rules for stochastically simulating chemistry in plate material. Routine in module chemistry_m and submodule(chemistry_m) chemistry_s.
- **FLAWCAT** — FLAWCAT (ITYPE,IFILE,RXINNER) - Determines the flaw category (1-3) based on the flaw category cumulative distribution function that is in array WELDCAT. CAT 1 (IFLCAT=1) - ISB flaw, CAT 2 (IFLCAT=2) - embedded flaw (0 < R < t/8), and CAT 3 (IFLCAT=3) - embedded flaw (t/8 < R < 3t/8). R = location of inner crack tip and t = RPV wall thickness. Array WELDCAT(3,I) contains CDF for all flaw categories. Routine in moudule flaw_m and submodule(flaw_m) flaw_s.
- **FLAW** — FLAW (KHALF,ZSURF,NCDP,CLTH,THICK,NSBR,ICORR,ITYPE,LOAD,IFILE,IPFLAW,iheat, iheat_embedded,IWDEP1,IPDEP1,RXINNER,LFIRST,NTSUB,nflaw,iorient,xinmesh) - Determines flaw depths for embedded flaws and XINNER (L is pointer for surface breaking flaw), simulates the flaw aspect ratio, and determines time-independent parameters that will be used in Subroutine PFM to calculate KI. Routine in moudule flaw_m and submodule(flaw_m) flaw_s.
- **CRTNDT** — Module Procedure CRTNDT(IFLAG,SIGDEL,SIGRTO,ZSURF,TC,STOR2,NSBR1,iheat, iheat_embedded) - Calculates RTNDT. Contained within submodule(rtndt_calculation_m) rtndt_calculation_s.
- **QSUB** — QSUB (SUBASPECT,Q) - Calculates Q factor using formulation in EPRI Report NP-1181 as required for computing KI for embedded flaw.
- **SUBMM** — SUBMM (AT2,ECC,ESUM,A,SMM) - Calculates free surface correction factor for membrane stress using formulation in EPRI Report NP-1181 as required for computing KI for embedded flaw. Contained in module correction_factor_m and submodule(correction_factor_m) correction_factor_s.
- **SUBMB** — SUBMB (AT2,ECC,ESUM,THICK, SMB) - Calculates free surface correction factor for bending stress using formulation in EPRI Report NP-1181 as required for computation of KI for embedded flaw. Contained in module correction_factor_m and submodule(correction_factor_m) correction_factor_s.
- **TMPINT** — TMPINT(NTSTEP,X,ITRAN, TINNER) - Performs linear interpolation of temperatures when calculating KIc at the inner tip (X) of an embedded flaw. Contained in module linear_interpolation_m and submodule(linear_interpolation_m) linear_interpolation_s.
- **STRINT** — STRINT (THICK,ITYPE,NTSTEP, X,ITRAN, ICLAD,NSBR1,SIGZ) - Performs linear interpolation to determine what the stress (SIGZ) is at a point in the RPV wall (X) at a specific time step (NSTEP) for a specific transient (ITRAN). Calls INTCLD. STRINT is contained in module linear_interpolation_m and submodule(linear_interpolation_m) linear_interpolation_s.
- **ACCOUNT** — ACCOUNT (NTRIAL,NFLAW, ITRAN,ITYPE, ITYPE_C,NTIMES, NSBR1,THICK, PFTHWL,TC, LFIRST,STORE, STOR2,TIME, IHEAT,KI_Check,MTRAN, NTIME_FIRST, NTIME_LAST, IORIENT,iheat_embedded, IPFLAW) - Performs accounting of the acquired data to generate output reports. Calls Subroutine PROP to determine CPF. Largest value of instantaneous probability of crack initiation for ITRAN transient, NTSTEP timestep, and NFLAW flaw of the current vessel is stored and used later to combine with the largest value of CPI for other flaws that reside in this vessel.
- **OUTCPI** — OUTCPI (mline,irmd,mtran,ntrial, pfmi,create_binary) - Writes out cpi to the screen and to appropriate output file.
- **OUTCPF** — OUTCPF (MLINE,IRMD,MTRAN, NTRIAL,PFMF,cpism,cpfsm,create_binary) - Writes out cpf to the screen and to output file.

Figure 13: Flowchart for PFM Model and CALL TO IGA Sub-model – based on Figure 16 in FAVOR Theory Manual (page 75)

Notes:

- The driver for the PFM Model resides in subroutine PFM.
- Flowchart for PFM model – the Initiation-Growth-Arrest (*IGA*) sub-model can be viewed as a Monte Carlo model nested within the larger PFM Monte Carlo model. For a given flaw, the *IGA* sub-model is called after the *CPI* for the current transient has been calculated. Note: ++ notation indicates increment index by 1; e.g., *i*++ means *i*=*i*+1.

Table 13: Definition of Key Variables used in Call Statements

AT2	Equal to the length of the minor axis of an elliptical flaw (XDEPTH) divided by vessel wall thickness, THICK.
CFDIFF	Difference between chemistry factor for the weld and the user specified chemistry-factor override (field 19 on embrittlement map record).
CHMPAS, CHMPAS_DT, and CHMPAS_PL	Sampled chemistry parameter array for Copper, Nickel, Phosphorus, and Manganese for weld, weld (ductile tearing), and plate, respectively.
CLTH	Clad thickness in inches.
cpfsm	Conditional probability of failure for a trial.
cpism	Conditional probability of crack initiation for a trial.
create_binary	A logical parameter that is set to .true. if restart is being performed, which will generate both cpi and cpf binary files (PFMI.BIN and PFMF.BIN, respectively).
CU, ANI,PHOS,AMN	User input best estimates of copper, nickel, phosphorus, and manganese content in wt% (entered on embrittlement map record).
ECC	Absolute difference of one-half the vessel wall thickness (WHALF=1/2*THICK) and location of the midpoint of the crack (XC). XC is a function of flaw population (inner, outer, thru-wall). For inner flaw population option 1, XC = (XOUTER + XINNER) / 2 where XINNER is inner crack tip and XOUTER is depth of crack. For flaw population option 2, XC = THICK - (XOUTER+XINNER)/2), where XOUTER is outer distance of crack and XINNER is inner crack tip location in inches. For flaw population option 3, if XINNER is less than WHALF, then XC is equivalent to option 1 XC calculation. If XINNER is greater or equal to WHALF, then XC is equivalent to option w XC calculation.
ESUM	The sum of 2*ECC/THICK and XDEPTH/THICK, where ECC and THICK are described within the table, and XDEPTH is the flaw depth of embedded flaws.
FO	User input best estimate neutron fluence at RPV inside surface in 10^{13} neurons/cm^2 (entered on embrittlement map record).
GLBSIG	The global uncertainty (i.e., number of standard deviations associated with all flaws in the current simulated RPV). Also, the number of standard deviations which the user-input (best estimate) neutron fluence is perturbed for all flaws in the current RPV, prior to simulating the local uncertainty for each flaw. GLBSIG is sampled from a standard normal distribution once for each simulated RPV. It is applied for all flaws in the current RPB. The function G05DDF is used to determine the random sampled value for GLBSIG.
ICLAD	Largest Index value where the clad resides within the 16 indexed mesh points generated by FAVLoad.
ICORR	User input product-form flag for chemistry-factor (CF) override, where 11=weld with no CF override, 12=weld with CF override, 21=plate with no CF override, 22=plate with CF override, and 31=forging.
IFILE	Index that varies from 1 to 1000 to cover the entire range specified in the VFLAW based flaw files.

iheat and iheat_embedded	iheat is set equal to 1 for inner surface flaws and is set to 2 for outer surface flaws. iheat_embedded is similar to iheat except it is used for embedded flaws, where iheat_embedded = 1 for embedded flaws within the inner 3/8 of base metal wall thickness and iheat_embedded=2 for embedded flaws within the outer 3/8 of the wall thickness.
IORIENT	IORIENT is set to 1 for axial oriented flaws and is set to 2 for circumferential oriented flaws.
IPASS	An integer array that tracks the number of flaws in each subregion, NSBR. IPASS is initialized to zero for each new vessel (NTRIAL) analyzed.
IPFLAW	User specified integer value for flaw population model on Record 1 of FAVPFM input file. IPFLAW flag sets the distributions of surface-breaking and embedded flaws within the RPV wall. IPFLAW=1 is for internal surface-breaking flaws and embedded flaws uniformly distributed within the inner $3/8^{th}$ of the RPV base metal. IPFLAW=2 is for external surface-breaking flaws and embedded flaws uniformly distributed in the outer $3/8^{th}$ of the RPV base metal. Lastly, IPFLAW=3 is for surface-breaking flaws that are 50% internal surface-breaking flaws and 50% external surface-breaking flaws, where embedded flaws are distributed uniformly throughout the entire RPV base metal thickness.
IRMD	Index counter to assist in writing out cpi and cpf results per vessel and number of input transients to the screen, Files 86, and 87.
ITRAN	User specified transient number input on Record 7 – TRAC. This is the transient number in the transient stack supplied in the FAVLoad output file. Transient sequence number (1, 2, 3….)
ITYPE	Integer value which is set to 0 for welds and 1 for plates and forgings.
ITYPE_C	Integer value which is set to 0 for welds when they are controlling ductile tear and 1 for plates and forgings if they are controlling ductile tear.
IWDEP1,IPDEP1	Arrays specifying the number of simulated Category 1, 2, and 3 flaws. IWDEP1 is for welds and IPDEP1 is for plates.
LFIRST	Integer index indicating the location in ZSURF(i) of the flaw depth location prior to propagation.
KHALF	Integer index indicating the location in ZSURF(i) of the midpoint of the vessel wall thickness.
KI_CHECK	Real type array that stores the $K_{Applied}$ for all NTSTEPs. NTSTEP is defined below.
MLINE	Integer index indicating the number of output lines for each vessel used in printing cpi and cpf results. Used with variable IRMD described above.
MTRAN	Integer number of Transients evaluated.
NCDP	Integer index used in ZSURF(j) to indicate 95% of vessel wall thickness.
NFLAW	Integer flaw number, which ranges from 1 to NUMFLW (maximum number of flaws).
NSBR,NSBR1	Internal integer index used for vessel subregion number, which corresponds to the subregion on the user specified embrittlement map. NSBR1 is the same as NSBR.

NTIME_FIRST	Integer start time step for FAVPFM analysis for transient, ITRAN. Typically, 0.0 from the FAVLoad output file, unless specified on Record DTRF in FAVPFM file where the FAVLoad entered transient timeframe is contracted to a smaller one.
NTIME_LAST	Integer end time step for FAVPFM analysis for transient, ITRAN. Typically, the last time specified in the FAVLoad output file, unless specified on Record DTRF in FAVPFM file where the FAVLoad entered transient timeframe is contracted to a smaller one.
NTIMES	Integer number of time steps specified in the FAVLoad output file. This value is based on the FAVLoad input values of "TIME" and "DT" specified on Record 7, TIME. Calculated in FAVLoad as NTIMES = [TIME/DT + 1].
NTSTEP	Integer time step index that ranges from NTIME_FIRST to NTIME_LAST.
NTRIAL	Integer counter for number of simulated RPV trials.
NTSUB	Integer number of total weld and plate subregions.
PFMI	Probability of crack initiation as a function of RPV trial. Written to INITIATE.DAT.
PFMF	Probability of vessel failure as a function of RPV trial. Written to FAILURE.DAT.
PFTHWL	An array dimensioned by (1000,4,4) which captures various random probabilities (based on function rndu()) used in the PFM analysis. That is, PF,
Q	Shape parameter based on the EPRI methodology using the infinite-series approximation of the elliptical integral (see equation 88 of Theory manual).
RTCALC	One dimensional array that contains calculated RT_{NDT} for each subregion.
RXINNER	Random number sampled from a uniform distribution in subroutine FLAWCAT.
SFID	Sampled fast-neutron fluence at the crack tip depth.
SIGDEL	Not currently used. Is echoed in the echo file, but not defined. Might have been used in initial testing.
SIGFGL	The user-input definition of one standard deviation of global uncertainty, defined in terms of fractional part of the user-input value. One standard deviation of the global variability of neutron fluence is SIFFGL*FO(NSBR) where FO(NSBR) is the user-input best-estimate neutron fluence for the neutron fluence of the current flaw located in subregion NSBR.
SIGFLC	The user-input definition of one standard deviation of local uncertainty, defined in terms of fractional part of the best-estimate neutron fluence of the current flaw, including the global uncertainty, GLBSIG (described above), such that the local variability of neutron fluence is SIGFLC*FLMEAN where FLMEAN = FO + GLBSIG*SIGFGL*FO, where FLMEAN is the mean varied fluence.
SIGRTO	The user-input standard deviation for RT_{NDT0} (°F) specified on the embrittlement record field 13.
SIGZ	Linearly interpolated stress at location x within RPV wall.
SMB	Free-surface correction factor for bending stresses (M_b). See Equation 90 in the FAVOR Theory Manual.
STORE	Storage array for $KI_{applied}$ and Temperature at crack tip for each time step.

STOR2	**One dimensional Storage array for 17 elements. These elements include the important sampled (simulated) chemistry concentrations for copper, nickel, phosphorus, manganese, fluence, etc. The following list is pulled from subroutine CRTNDT which calculates RT_{NDT}.** **STOR2(1) = RTNDTO ≡ $RT_{NDT(0)}$** **STOR2(2) = DRTEPI ≡ Epistemic uncertainty in the unirradiated value of $RT_{NDT(0)}$** **STOR2(3) = SDRTNDT ≡ Irradiation-shift in RT_{NDT}, ΔRT_{NDT}** **STOR2(4) = RTNDT ≡ RT_{NDT}** **STOR2(5) = DT30 ≡ 30 ft-lbf CVN transition temperature (ΔT_{30})** **STOR2(6) = SCU ≡ Sampled (simulated) Copper concentration** **STOR2(7) = SNI ≡ Sampled (simulated) Nickel concentration** **STOR2(8) = SPHOS ≡ Sampled (simulated) Phosphorus concentration** **STOR2(9) = SMN ≡ Sampled (simulated) Manganese concentration** **STOR2(10) = SFID ≡ Sampled (simulated) fast-neutron fluence at the crack tip depth.** **STOR2(11) = USE0 ≡ Initial upper-shelf energy.** **STOR2(12) = USEi ≡ Irradiated upper-shelf energy.** **STOR2(13) = SCU_DT ≡ Sampled Copper concentration under ductile-tearing.** **STOR2(14) = SNI_DT ≡ Sampled Nickel concentration under ductile-tearing.** **STOR2(15) = SPHOS_DT ≡ Sampled Phosphorus concentration under ductile-tearing.** **STOR2(16) = SMN_DT ≡ Sampled Manganese concentration under ductile-tearing.** **STOR2(17) = p_rtepi ≡ Sampled percentile (0 to 1) to be used in sampling T_O.**
SUBASPECT	**Equal to 2**a* / *L* of the elliptical subsurface flaw used in calculating the flaw shape parameter, Q.**
TC	**User entered value for initial RPV coolant temperature (^oF).**
THICK, A	**Reactor vessel wall thickness including clad.**
TIME	**Elapsed time in transient in minutes.**
TINNER	**Interpolated temperature at the inner crack tip.**
USE_CALC	**Upper Shelf Energy one dimensional array dependent on NSUBR (vessel subregion number), where NSUBR(NSBR,1) = Subregion number (NSBR), NSUBR(NSBR,2) = Subregion of 1st adjacent plate material, and NSUBR(NSBR,3) = Subregion of 2nd adjacent plate material.**
X	**Location of the inner crack tip. Used in interpolation subroutines STRINT and TMPINT as described above. Also used in subroutines INTCLD and INTCLD2.**
xinmesh	**A 32 by 5 dimensioned array which is no longer used. Originally developed for investigative purposes.**
ZSURF	**Position of crack tip relative to inner surface in inches.**

Additional Notes to subroutine PFM and called subroutines presented in Figure 13.

- Each stochastically generated RPV is based on perturbations in its chemistry and fluence properties along with uncertainties in postulated flaw population.
- When using VFLAW based input, each postulated flaw is 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) is also performed.
- When using the as-found flaw input option, each specified flaw has its own distinguishing location (i.e. embrittlement) and geometry parameters, specified by the user.
- Global and Local Uncertainties in fast-neutron fluence attenuation is considered in determining the sampled fast-neutron fluence at the crack tip.
- The attenuation is taken as follows and is evaluated in subroutine FLUENCE:

  $$\widehat{f_0(a)} = \widehat{f}_0\,(0) \times exp(-0.24a)$$

  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:

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

  $$\widehat{f}_{mean} \leftarrow N(fluence_{subregion}, \sigma_{global})$$
  $$\widehat{\sigma_{local}} = SIGFLC \times \widehat{f}_{mean}$$
  $$\widehat{f_0}\,(0) \leftarrow N\left(\widehat{f}_{mean}, \widehat{\sigma_{local}}\right)$$

  where the best estimate fluence, $fluence_{subregion}$, and the global standard deviation, σ_{global}, are input by the user at the subregion level. The global *SIGFGL* and local *SIGFLC* multipliers are also supplied as input by the user.
- Plane-Strain Static Cleavage Initiation Toughness (K_{Ic})and Plane-Strain Crack Arrest Toughness (K_{Ia}) correlations are based on measured data using (T - RT_{NDT}) as an index and industry standard statistical models. (Design Description 10). The data used to establish these correlations meets the validity requirements given in ASTM Standard E-399 to maintain consistency with the LEFM driving forces applied in the fracture model. Furthermore, the unirradiated RT_{NDT0}, determined according to the ASME Boiler and Pressure Vessel Code, Section III, NB-2331 must be available for the K_{IC} and K_{Ia} data used in establishing the correlations. Plane-Strain Static Cleavage Initiation Toughness, K_{Ic}, as a function of (T-RT_{NDT}) is based on a Weibull statistical distribution and the use of a lower-bounding reference temperature using fracture toughness data. Plane-Strain Crack Arrest Toughness, K_{Ia}, as a function of (T-RT_{NDT}) is based on a Lognormal statistical

distribution and the use of a normalized arrest reference temperature using fracture toughness data.

- Both epistemic and aleatory uncertainties are considered in the evaluation of RT_{NDT}. Reference [16] recommends that the uncertainty in the sampled CVN transition shift values be treated as *epistemic*. Having used information concerning composition and irradiation conditions to estimate the CVN transition temperature shift, it is necessary to transform these $\widehat{\Delta T_{30}}$ values into shifts in the fracture-toughness transition temperature. Figure 14 provides an empirical basis for the following least-squares fits for of $\widehat{\Delta RT_{NDT}}$ using data extracted from the literature as discussed in [16]. The module procedure get_dt30 in the radiation_shift_s module performs this correction.

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

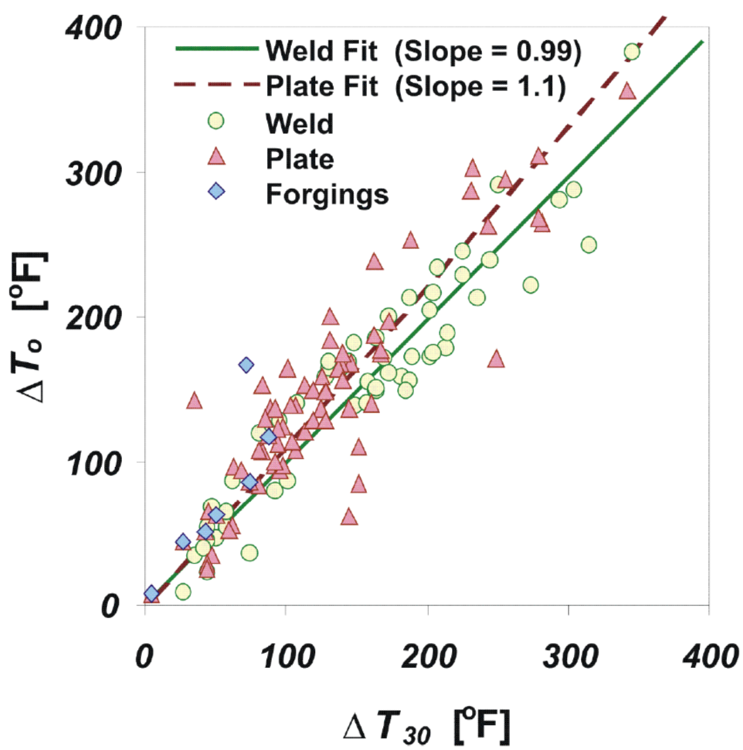


Figure 14: Relationship between the change in the fracture-toughness index temperature (ΔT0 ≈ ΔRTNDT) change in the 30 ft-lbf CVN transition temperature (ΔT30) for welds and plates/forgings produced by irradiation. The difference in the best-fit slopes is statistically significant (from [16]).

- RT_{Arrest} is 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 curve.

- Stochastically sampled methods are applied on material chemistry (i.e., Cu, Mn, Ni, and P) for plates, forgings, and welds used in the reactor vessel beltline model. The material chemistry sampling protocols 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 are perturbations of the first sampled flaw chemistry for this subregion. This variation in chemistry shall simulate local variability in the subregion chemistry. Initial sampling uses a normal distribution, and any uncertainties are based on well recognized and credible published data for plates, welds, and forgings. When sampling either for the first flaw or subsequent flaws, negative chemistry values are prevented by truncating to a prescribed value of 0.0. When sampling a subregion for subsequent flaws, local variability is sampled using a logistic distribution for Cu, Ni, and P, and a Johnson SB distribution for Mn. Chemistry resampling in plates and forgings is not performed as a flaw is propagated through the wall. In contrast, chemistry resampling in welds is performed once the flaw propagates from one 1/4t of the vessel wall thickness to an adjoining 1/4t region. 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. Resampled chemistry values that exceed the bounds of an embrittlement correlation are truncated back to the appropriate upper bound or saturation limit (e.g., Cu).

- FAVPFM makes the following stochastic tools available to apply:

  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.

- Each RPV trial propagates 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.

- 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 is evaluated at each discrete transient time step for determining probability of crack initiation.

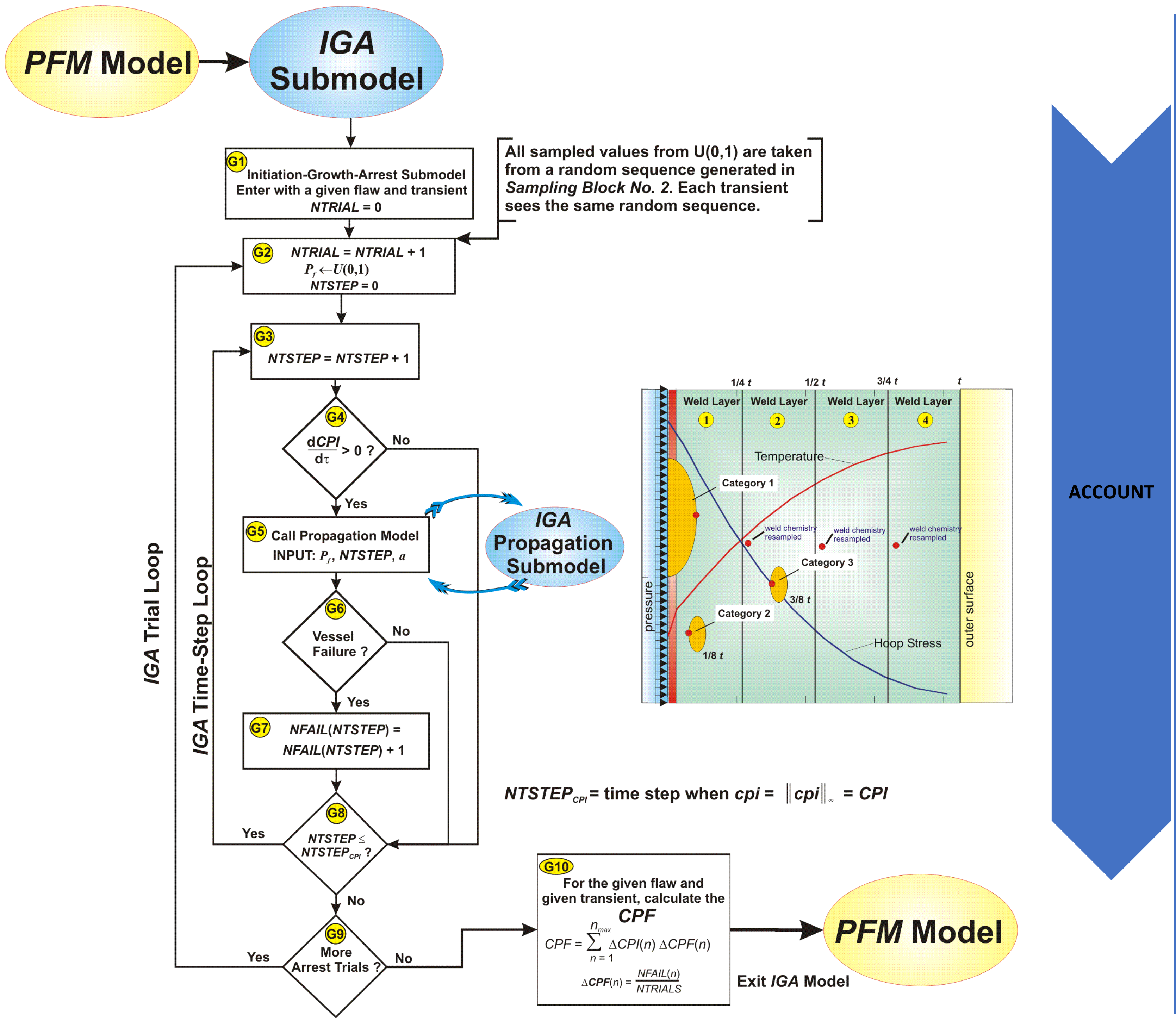
- An optional warm prestress (WPS) model exists to ascertain whether crack initiation occurs. The model assumes a flaw is in a state of WPS when the time-rate-of-change of the applied-K_I is negative. See Section 4.3.4 of Reference [1] for further background and basis for WPS.

1 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.

2 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.

- Flaws that are postulated to be in a weld are assumed to reside on the fusion line between the weld and adjacent plate or forging.
- The higher value of RTNDT between the plate (or forging) and weld subregion is used before entering the PFM Monte Carlo loop.
- PFM output provides 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 ($\mathbf{0 \leq \mathit{CPI} \leq 1}$) and conditional probability of failure ($\mathbf{0 \leq \mathit{CPF} \leq 1}$) 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.



- **Subroutine ACCOUNT** (NTRIAL,NFLAW, ITRAN,ITYPE, ITYPE_C,NTIMES, NSBR1,THICK,PFTHWL, TC, LFIRST,STORE, STOR2,TIME, IHEAT,KI_Check,MTRAN, NTIME_FIRST, NTIME_LAST, IORIENT, iheat_embedded, IPFLAW) performs accounting of the acquired incremental data to generate output reports. Calls Subroutine PROP to determine CPF. Largest value of instantaneous probability of crack initiation for ITRAN transient, NTSTEP timestep, and NFLAW flaw of the current vessel is stored and used later to combine with the largest value of CPI for other flaws that reside in this vessel.
- ***G2***: Step 10 in Program PFM increments NTRIAL counter. NTRIAL is the counter for number of vessel simulations (Maximum is defined by NSIM). NTRIAL counter, as displayed in flowchart, refers to the number of Initiation-Growth-Arrest (IGA) trials per flaw (specified by input parameter IGATR). DO LOOP 2015 controls iterations on IGA trials (using J counter) where NTEST is set to IGATR. Note that transient and flaw type are not varied within Subroutine ACCOUNT.
- ***G3***: Step 110 in Program PFM increments NTSTEP and DO LOOP 2020 in Subroutine ACCOUNT performs a nested NTSTEP loop. Subroutine ACCOUNT is called by Subroutine PFM. When ACCOUNT is called from Subroutine PROP, the maximum CPI (i.e., variable BIG) and corresponding timestep (i.e., variable IBIG) is first determined. Note that two time loops are being used; one in PFM and one in ACCOUNT.
- ***G4***: DO LOOP 2010 in Subroutine ACCOUNT determines CPI distribution over discrete time steps. First, the change in CPI that occurs between two transient time steps is calculated and stored in ARRAY DCPI. A positive value of DCPI is an increase (i.e., dCPI/dt > 0).
- ***G5***: First, vessel failure counters are initialized to zero before calling Subroutine PROP. Then the code determines quantile for weld-layer and set Copper, Nickle, Phosphorus, Manganese, and fluence and associated uncertainties using the STOR2 array. DO LOOP 2020 goes through NTSTEP = NTIME_FIRST(ITRAN), IBIG where delta CPI is always increasing. Within the DO LOOP, IPFLAW is tested before going to Subroutine PROP. When IPFLAW=2 (i.e., external surface-breaking flaw) or IPFLAW=3 (i.e., both internal and surface breaking flaws) through-wall propagation of external surface flaws to the inner surface is conservatively assumed to occur upon crack initiation. Finally for embedded flaws that reside in the outer half (i.e., IFLCAT.NE.1 and iheat_embedded=2), propagation to failure is also assumed upon crack growth initiation.
- ***G6. G7, and G8***: End of DO LOOP 2020, where fail counters are updated based on IMODE = 0 (No Failure), 1 (Fail by Cleavage Fracture), and 2 (Fail by Ductile Tearing). NTSTEP is then incremented for DO LOOP 2020 until it reaches IBIG (time step corresponding to largest cpi for that transient and flaw).
- ***G9***: End of DO LOOP 2015, where Number of IGA Trials counter (i.e., J) is checked against the input number of IGA trials (i.e., IGATR).
- ***G10***: CPF is calculated along with parent and child subregions by performing another DO LOOP 2021. The calculated CPF is for a given flaw and transient. Both CPI and CPF are stored in array CPI(ITRAN,NTIMES+1(2),NFLAW), respectively. See notes below.

Figure 15: Flowchart for IGA Model and CALL TO IGA Sub-model Figure 17a in FAVOR Theory Manual (page 76). The driver for IGA Model resides in subroutine ACCOUNT which calls subroutine PROP

Table 14: Definition of Key Variables Passed into Subroutine ACCOUNT

ITYPE	**ITYPE = 0 for weld; ITYPE = 1 for plate**
ITYPE_C	**Integer value which is set to 0 for welds when they are controlling ductile tear and 1 for plates and forgings if they are controlling ductile tear.**
TC	**User entered value for initial RPV coolant temperature (^oF).**
LFIRST	**Integer index indicating the location in ZSURF(i) of the flaw depth location prior to propagation.**
iheat and iheat_embedded	**iheat is set equal to 1 for inner surface flaws and is set to 2 for outer surface flaws.** **iheat_embedded is similar to iheat except it is used for embedded flaws, where iheat_embedded = 1 for embedded flaws within the inner 3/8 of base metal wall thickness and iheat_embedded=2 for embedded flaws within the outer 3/8 of the wall thickness.**
IPFLAW	**User specified integer value for flaw population model on Record 1 of FAVPFM input file. IPFLAW flag sets the distributions of surface-breaking and embedded flaws within the RPV wall. IPFLAW=1 is for internal surface-breaking flaws and embedded flaws uniformly distributed within the inner $3/8^{th}$ of the RPV base metal. IPFLAW=2 is for external surface-breaking flaws and embedded flaws uniformly distributed in the outer $3/8^{th}$ of the RPV base metal. Lastly, IPFLAW=3 is for surface-breaking flaws that are 50% internal surface-breaking flaws and 50% external surface-breaking flaws, where embedded flaws are distributed uniformly throughout the entire RPV base metal thickness.**
IORIENT	**IORIENT is set to 1 for axial oriented flaws and is set to 2 for circumferential oriented flaws.**
ITRAN	**Transient sequence number (1, 2, 3….).**
KI_CHECK	**Real type array that stores the $K_{Applied}$ for all NTSTEPs (integer time step). NTSTEP goes from NTIME_FIRST to NTIME_LAST.**
MTRAN	**Integer number of Transients evaluated.**
NFLAW	**Integer flaw number, which ranges from 1 to NUMFLW (maximum number of flaws).**
NSBR1	**Internal integer index used for vessel subregion number, which corresponds to the subregion on the user specified embrittlement map.**
NTIME_FIRST	**Integer start time step for FAVPFM analysis for transient, ITRAN. Typically, 0.0 from the FAVLoad output file, unless specified on Record DTRF in FAVPFM file where the FAVLoad entered transient timeframe is contracted to a smaller one.**
NTIME_LAST	**Integer end time step for FAVPFM analysis for transient, ITRAN. Typically, the last time specified in the FAVLoad output file, unless specified on Record DTRF in FAVPFM file where the FAVLoad entered transient timeframe is contracted to a smaller one.**
NTRIAL	**Integer counter for number of simulated RPV trials.**
PFTHWL	**Array of probabilities used in sampling various parameters.**
STORE	**Storage array for AKICHEK (i.e., $K_I(t)$ used in Weibull distribution to determine cpi) and TMP (i.e., temperature at inner crack tip location) variables for all timesteps (NTSTEP).**
STOR2	**One dimensional Storage array for 17 elements. These elements include the important sampled (simulated) chemistry concentrations for copper, nickel,**

	phosphorus, manganese, fluence, etc. The following list is pulled from subroutine CRTNDT which calculates RT_{NDT}. **STOR2(1) = RTNDTO ≡ $RT_{NDT(0)}$** **STOR2(2) = DRTEPI ≡ Epistemic uncertainty in the unirradiated value of $RT_{NDT(0)}$** **STOR2(3) = SDRTNDT ≡ Irradiation-shift in RT_{NDT}, ΔRT_{NDT}** **STOR2(4) = RTNDT ≡ RT_{NDT}** **STOR2(5) = DT30 ≡ 30 ft-lbf CVN transition temperature (ΔT_{30})** **STOR2(6) = SCU ≡ Sampled (simulated) Copper concentration** **STOR2(7) = SNI ≡ Sampled (simulated) Nickel concentration** **STOR2(8) = SPHOS ≡ Sampled (simulated) Phosphorus concentration** **STOR2(9) = SMN ≡ Sampled (simulated) Manganese concentration** **STOR2(10) = SFID ≡ Sampled (simulated) fast-neutron fluence at the crack tip depth.** **STOR2(11) = USE0 ≡ Initial upper-shelf energy.** **STOR2(12) = USEi ≡ Irradiated upper-shelf energy.** **STOR2(13) = SCU_DT ≡ Sampled Copper concentration under ductile-tearing.** **STOR2(14) = SNI_DT ≡ Sampled Nickel concentration under ductile-tearing.** **STOR2(15) = SPHOS_DT ≡ Sampled Phosphorus concentration under ductile-tearing.** **STOR2(16) = SMN_DT ≡ Sampled Manganese concentration under ductile-tearing.** **STOR2(17) = p_rtepi ≡ Sampled percentile (0 to 1) to be used in sampling T_O.**
TC	**User entered value for initial RPV coolant temperature (°F).**
THICK	**RPV thickness.**
TIME	**Elapsed time in transient in minutes.**

9.6 ACCOUNT Procedure

As shown in Figure 12, after the value of *CPI* has been calculated for the current flaw and transient, the conditional probability of vessel failure, *CPF*, by through-wall cracking is determined by the flaw Initiation-Growth-Arrest (*IGA*) sub-model. The *IGA* sub-model may be viewed as a small Monte Carlo model nested within the larger PFM Monte Carlo model. The following steps in the *IGA* sub-model are shown in Figure 15:

Step G1. The *IGA* sub-model is entered from the *PFM* model with a given flaw and transient. The *IGA* trial counter, *NTRIAL*, is initialized to zero. The pointer to the vector holding the random number sequence containing the values of P_f [5] is reset to 1. Each transient for this flaw will start with the same random number sequence for internal sampling; however, each flaw has a different vector of random numbers. Go to Step G2.

Step G2. The *NTRIAL* counter is incremented; the time-step counter *NTSTEP* is initialized to zero; and a random number P_f is drawn from a uniform distribution on the open interval (0,1). Go to Step G3.

Step G3. The time-step counter is incremented up to the time step corresponding to when CPI occurred; time advances to the next time step. Go to Step G4.

Step G4. For the given flaw, subjected to the current transient, the change in *cpi* with respect to time is checked. If $dcpi/dt > 0^{th}$, then the flaw becomes a candidate for propagation through the wall. (This sub-model will be described in detail in the following.) If $dcpi/dt \leq 0$, then control branches to Step G8.

Step G5. The *IGA Propagation* sub-model is entered for this flaw, providing the sub-model with the current time step, flaw depth, and value of P_f. Go to Step G6.

Step G6. Control returns from the *IGA Propagation* sub-model with the fate of the flaw, either a vessel failure or a stable arrest (no failure). If a vessel failure occurred, control is transferred to Step G7. If a stable arrest occurred, control is transferred to Step G8.

Step G7. The vessel failure counter, *NFAIL*(*NTSTEP*), for this time step is incremented. Go to Step G8.

Step G8. If the transient has completed, i.e., $NTSTEP > NTSTEP_{CPI}$, branch to Step G9. If the transient is not finished, cycle to Step G3. Note that $NTSTEP_{CPI} = NTSTEP$ at which $cpi(t) = \|cpi(t)\|_\infty = CPI$.

Step G9. A check is made to see if the required number of trials has been completed. If there are more *NTRIALS* to be run, control is transferred to Step G2. If the *IGA* sub-model has completed its sample trials for the current transient, then control is transferred to Step G10.

Step G10. The $CPF_{(i,j,k)}$ for the *i*th transient, and *j*th RPV trial, and *k*th flaw is calculated by the following:

---

[5] The value of P_f represents the percentile used in sampling $\widehat{\Delta RT}_{ARREST}$ (see Step 11 in Sect. 5.5 of FAVOR Theory Manual) and $\widehat{K_{Ia}}$ (see Step 15 in Sect. 5.5 of FAVOR Theory Manual) in Step P6 and in sampling $\widehat{K_{Ic}}$ in Step P8 of the *IGA Propagation Sub-model*, and is used to ensure that the calculated initiation and failure probabilities are not affected by the order in which transients are analyzed. The *IGA Propagation Sub-model* is an embedded Monte Carlo model that is repeated a user-set number of times using a different value of P_f each time.

$$CPF_{(i,j,k)} = \sum_{m=1}^{NTSTEP_{CPI}} \Delta cpi(t^m)_{(i,j,k)} P(F \mid I)^m$$

$$P(F \mid I)^m = \frac{NFAIL(m)}{NTRIALS}$$

where $NTSTEP_{CPI}$ is the time step at which the value of $CPI_{(i,j,k)}$ was calculated for this *i*th transient, *j*th RPV trial, and *k*th flaw. CPF is calculated along with parent and child subregions by performing another loop. The calculated CPF is for a given flaw and transient. Both CPI and CPF are stored in the same array CPI(ITRAN,NTIMES+1(2),NFLAW), respectively. That is, CPI is stored in CPI(ITRAN, NTIMES+1,NFLAW), an CPF is stored in CPI(ITRAN,NTIMES+2,NFLAW).

Steps G2 through G9 are repeated NTRIAL cycles through the IGA sub-model.

ACCOUNT

- ACCOUNT (NTRIAL,NFLAW, ITRAN,ITYPE, ITYPE_C,NTIMES, NSBR1,THICK,PFTHWL, TC, LFIRST,STORE, STOR2,TIME, IHEAT,KI_Check,MTRAN, NTIME_FIRST, NTIME_LAST, IORIENT,iheat_embedded, IPFLAW) - Performs accounting of the acquired incremental data to generate output reports. Calls Subroutine PROP to determine CPF. Largest value of instantaneous probability of crack initiation for ITRAN transient, NTSTEP timestep, and NFLAW flaw of the current vessel is stored and used later to combine with the largest value of CPI for other flaws that reside in this vessel.

PROP

- PROP (ITYPE,TC,LFIRST, NTSTEP, ITRAN,XDEPTH,PF, P_T0,P_JIc,P_m,NTRIAL, NFLAW,MNTEST,PFTHWL, THICK,STORE,NSBR2,IPROP,IMODE) - Following flaw crack intiation, first propagates the flaw and then determines whether the initiatied flaw propagates to failure or results in a stable arrest. Both failure by cleavage or ductile tearing is checked.

- Cleavage Propagation: KI > KIA
- Cleavage Arrest: KI < KIA
- Cleavage Reinitiatio n: KI > KIc and KIc < KJIc
- Stable Ductile Tearing: JI > JIc
- Tearing Reinitiation: JI > JIc and KI < KIA
- Unstable Ductile Tearing: JI > JIc and dJ/da_app > dJ/da_JR

- Ductile tearing is only checked when Temp > 200 F (T_DT). This value has been hard-wired in the code based on the results of the initial sensitivity study which showed that for T_DT < 300 F, the value of T_DT had no effect on the final CPF.

- Initiation is by cleavage only. Pre-cleavage ductile tearing for the initial event not modeled. With exception to the above, the following accomodates mixed-mode such as experimentally observed in PTSE-2b. No ductile tearing is allowed until the first cleavage arrest event. Cleavage propagation can be interrupted (overtaken) by ductile tearing prior to cleavage arrest or failure. A flaw that is propagating by ductile tearing (by one or more stable ductile tears) can stop tearing and resume propagation by cleavage if KI > KIa, but still not arrest. If no arrest, then further propagation will be by cleavage propagation.

- Calls to FKIA, ARRHEAD, ductile_tearing, flaw_track, FAILWR, RECHEM, DRTARREST, STABLE, PROPA, ARRT, FKIC, REINI, REINI2, NREINI, and functions get_dt30 and get_Kapplied.

FKIA

- FKIA (PF,AKINIT,TADJ,TADJINI, SMKIA,ILAYER,KIa_Model) - Calculates and returns the value of KIa corresponding to the input probability of crack extension. KIa distrubution is a lognormal distribution. Inputs are PF = cumulative probability of crack extension, AKINIT = current value of KIC, TADJ = T(r,t) - RTArrest (F), TADJINI = T(r,T) - RTArrest (F) at initiation, ILAYER = WELD LAYER COUNTER, and KIa_Model = KIa model 1 or 2 Output is SMKIA = sampled crack arrest at this percentile and relative temperature (ksi-in^1/2). Calls functions KIACDF and dnrminv.

ARRHEAD

- ARRHEAD (NFLAW,MTSTEP,L, ITRAN,DT30,RTNDTO,RTNDTII,AKICHEK) - Writes out output header for either ductile tear or no ductile tear.

ductile_tearing

- ductile_tearing (ITYPE,IFLCAT,L, MTSTEP,ITRAN,IORIENT,KJIc, KJRstar,T_DT,da0,SFLOW,P_T0, P_JIc,P_m,Emod,Nu,C_DT,m_DT,STABLE_DT,FAIL_UDT) - Tests for unstable ductile tearing. Calls functions get_Kapplied.

fkaw_track

- flaw_track(ktype,itype,itran,ntrial,nflaw,iorient,nsbr2,nsbr1)- Creates a log file of flaw types for QA purposes. Contained in module flaw_m and submodule(flaw_m).

FAILWR

- FAILWR (NFLAW,L,P,DT30, RTNDTO,DRTEPA,DRTARR, DRTNDX,RTNDTA,RTNDTII,ITRAN,MTSTEP,TADJII,AKICHEK, SMKIC,SMKIA,KJIc,KJRstar,USEi,C_DT, m_DT,da0,P_T0,P_JIc,P_m,sflow,KWRITE) - Writes out flaw failure headers and failure data.

RECHEM

- RECHEM (NTRIAL,ITRAN, NFLAW) - Resimulates the chemistry at each t/4 location as the flaw propagates thru the RPV wall. Calls COPPER2, NICKEL2, PHOSPH2, MANGANESE2 and functions G05DDF2 and get_Weibull_Q. Contained in module chemistry_m and submodule(chemistry_m).

DRTARREST

- DRTArrest(PF,DRTEPI,RTNDTO) - Calculates and returns the value of DRTArrest for the input cumulative probability as quantified by the variable PF. DRTArrest distribution is a lognormal distribution. Inputs are PF = cumulative probability of crack extension, DRTepis = episitemic uncertainty term [F], RTNDTO - sampled unirradiated value for RTNDT [F]. Output is DRTArr = sampled DRTArrest at this percentile and RTNDTO temperature [F]. Calls functions dnrminv and get_Diff.

STABLE

- STABLE (NFLAW,MTSTEP,L, ITRAN,P,DT30,RTNDTO,DRTEPA, DRTARR,DRTNDX,RTNDTA, RTNDTII,TADJII,AKICHEK, SMKIC,SMKIA,KJIc, KJRstar,USEi,C_DT,m_DT,da0,P_T0,P_JIc, P_m,sflow) - Writes out stable ductile tear-related data to ARREST.OUT.

PROPA

- PROPA (NFLAW,MTSTEP,L, ITRAN,P,DT30,RTNDTO,DRTEPA,DRTARR,DRTNDX,RTNDTA,RTNDTII,TADJ,TADJII,AKICHEK, SMKIA) - Writes out flaw propagation-related data to ARREST.OUT.

ARRT

- ARRT (NFLAW,MTSTEP,L,ITRAN, P,DT30,RTNDTO,DRTEPA,DRTARR,DRTNDX,RTNDTA,RTNDTII, TADJII,AKICHEK,SMKIA) - Writes out crack-arrest-related data to ARREST.OUT.

FKIC

- FKIC (PF,TADJ,SMKIC) - Calculates the value of KIC corresponding to PF.

REINI

- REINI (NFLAW,MTSTEP,L,ITRAN, P,DT30,RTNDTO,DRTEPA,DRTARR,DRTNDX,RTNDTA,RTNDTII,TADJII,AKICHEK,SMKIC,KJIc,KJRstar, USEi,C_DT, m_DT,da0,P_T0, P_JIc,P_m,sflow) - Writes out flaw re-initiation data to ARREST.OUT when the trace option is selected and ductile tearing was predicted. Contained in module write_arrest_data_m and submodule(write_arrest_data_m).

REINI2

- REINI2 (NFLAW,MTSTEP,L, ITRAN,P,DT30,RTNDTO,DRTEPA,DRTARR,DRTNDX,RTNDTA, RTNDTII,TADJII,AKICHEK, SMKIC) - Writes out flaw re-initiation data to ARREST.OUT when the trace option is selected and ductile tearing was not predicted. Contained in module write_arrest_data_m and submodule(write_arrest_data_m).

NREINI

- NREINI (NFLAW,MTSTEP,L, ITRAN,P,DT30,RTNDTO,DRTEPA,DRTARR,DRTNDX,RTNDTA,RTNDTII,TADJ,AKICHEK,SMKIC,KJIc,KJRstar,USEi,da0, P_T0,P_JIc,P_m,sflow) - Writes out flaw related data for a stable-arrest to ARREST.OUT. Contained in module write_arrest_data_m and submodule(write_arrest_data_m).

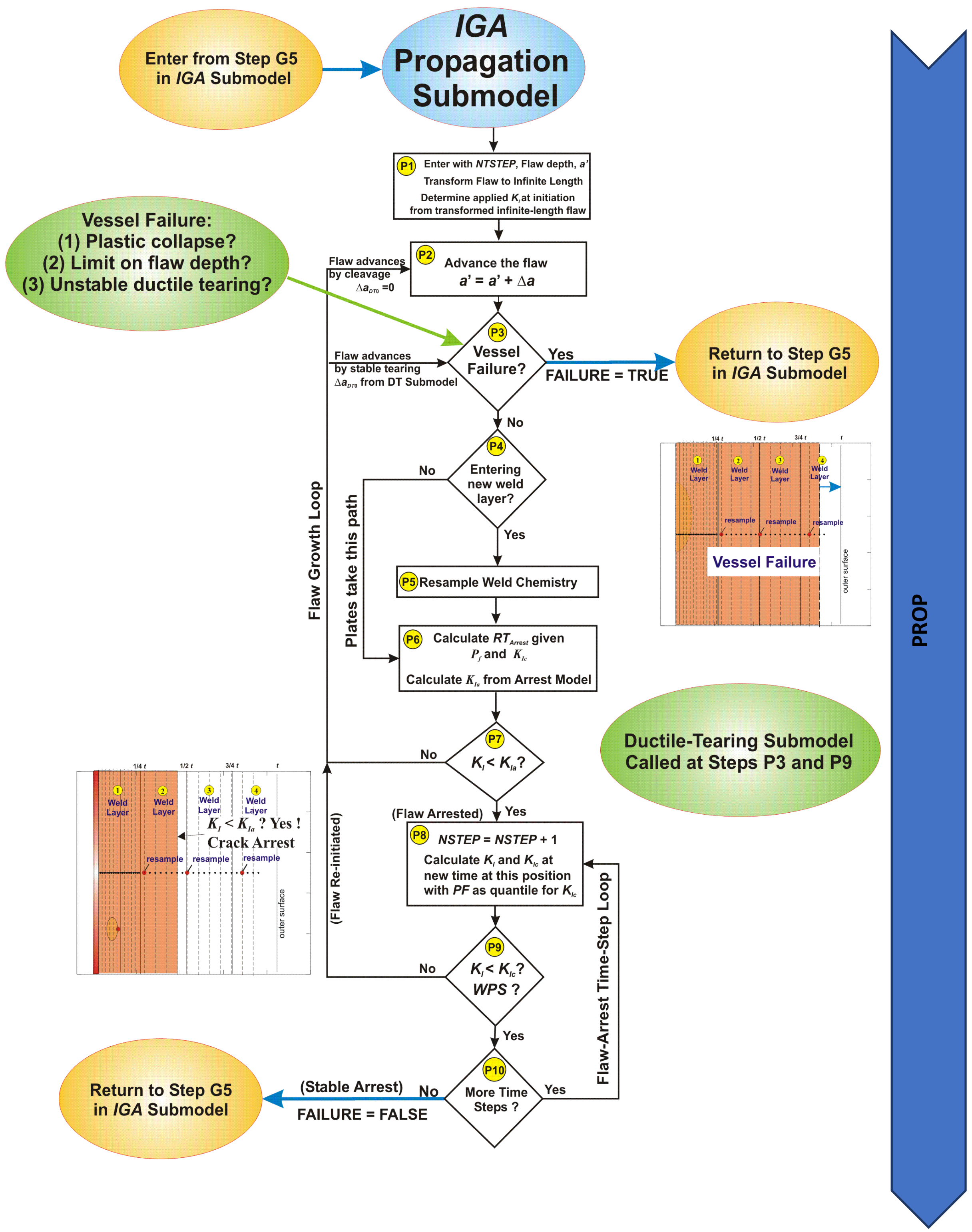
get_dt30

- get_dt30(IFLAG,TC,IHEAT, iheat_embedded) RESULT (DT30_current) - Calculates the radiation embrittlement shift, DT30 (DT30). Calls EWO1998, RG199W, WCFCT199, RG199B, PCFCT199, E2000, E2006, TCURVE2, TCURVE3, TCURVE4, and EWO1998. Contained in module write_arrest_data_radiation_shift_m and submodule(radiation_shift_m).

get_Kapplied

- get_Kapplied(IFLCAT,ITYPE,L,ITRAN,MTSTEP,IORIENT) RESULT (Kapplied) - Calculates K applied, KI.

Figure 16: Subroutine Calls from ACCOUNT to PROP and all of PROP called Subroutines and Functions



- **P1**: Call to subroutine PROP (see step G5 in Figure 17A) (ITYPE,TC,LFIRST, NTSTEP, ITRAN,XDEPTH, PF, P_T0,P_JIc,P_m,NTRIAL, NFLAW,MNTEST,PFTHWL,THICK,STORE,NSBR2,IPROP,IMODE) - Following flaw crack intiation, first propagates the flaw and then determines whether the initiatied flaw propagates to failure or results in a stable arrest. Both failure by cleavage or ductile tearing is checked. (1) Cleavage Propagation: KI > KIA; (2) Cleavage Arrest: KI < KIA; (3) Cleavage Reinitiation: KI > KIc and KIc < KJIc; (4) Stable Ductile Tearing: JI > JIc; (5) Tearing Reinitiation: JI > JIc and KI < KIA; and (6) Unstable Ductile Tearing: JI > JIc and dJ/da_app > dJ/da_JR.
  - Ductile tearing is only checked when Temp > 200 F (T_DT). This value has been hard-wired in the code based on the results of the initial sensitivity study which showed that for T_DT < 300 F, the value of T_DT had no effect on the final CPF.
  - Initiation is by cleavage only. Pre-cleavage ductile tearing for the initial event not modeled.With exception to the above, the following accomodates mixed-mode such as experimentally observed in PTSE-2b. No ductile tearing is allowed until the first cleavage arrest event.
  - Cleavage propagation can be interrupted (overtaken) by ductile tearing prior to cleavage arrest or failure. A flaw that is propagating by ductile tearing (by one or more stable ductile tears) can stop tearing and resume propagation by cleavage if KI > KIa, but still not arrest. If no arrest, then further propagation will be by cleavage propagation.
  - Subroutine PROP calls FKIA, ARRHEAD, ductile_tearing, flaw_track, FAILWR, RECHEM, DRTARREST, STABLE, PROPA, ARRT, FKIC, REINI, REINI2, NREINI, and functions get_dt30 and get_Kapplied. See Figure 11 for description of called subroutines.
  - Subroutine PROP returns IPROP and IMODE values based on the the following possilbe failure information back to subroutine ACCOUNT:
    IPROP=0===>NON-FAILURE===>STABLE ARREST
    IPROP=1===>FAILURE
    MODE=0===>NON-FAILURE===>STABLE ARREST
    IMODE=1===>Failure by cleavage
    IMODE=2===>Failure by ductile tearing
- **P2**: Before advancing the flaw, initial values for DT30, AKICHEK, and SMKIA are calculated. This is done by calling functions get_DT30 and get_Kapplied. Then a call to subroutine FKIA is made to calculate and return the value of KIa corresponding to the input probability of crack extension. KIa distribution is a lognormal distribution. At step 7932 in subroutine PROP increments L by 2 indexes which advances the flaw. L is the pointer index for array ZSURF(L). ZSURF is the one-dimensional array of crack tip positions relative to inner surface in inches. First 25 positions is set equal to ASIZE (25% of RPV thickness) with each increment being 0.01 x (t). Positions 26 to 60 are sequentially incremented by 0.25 inches. Subroutine FLAW is used to determine flaw depth where variable XDEPTH is used for embedded flaws and L is used for surface breaking flaws. For embedded flaws, variable XINNER is also determined. Subroutine SFMESH generates the mesh to be used for surface breaking flaws. It also determines the pointer for array ZSURF that corresponds to the user-specified failure criteria. Subroutine PROP uses the following vessel failure tests: (1) ZSURF(L) > FAILCR*THICK > ZSURF(IFAIL); (2) NOMINAL STRESS > INSTABILITY STRESS (FLOW STRESS), where flow stress increases with radiation damage and is linearly proportional to EASON's DT30 correlation; and (3) UNSTABLE DUCTILE TEARING if option is turned on.
- **P3**: As mentioned in P2 above, ZSURF array holds a mesh showing crack tip position and Subroutine SFMESH determines the pointer for array ZSURF corresponding to the user-specified failure criteria. Subroutine PROP uses the following vessel failure tests: (1) ZSURF(L) > FAILCR*THICK > ZSURF(IFAIL); (2) NOMINAL STRESS > INSTABILITY STRESS (FLOW STRESS), where flow stress increases with radiation damage and is linearly proportional to EASON's DT30 correlation; and (3) UNSTABLE DUCTILE TEARING if option is turned on. For failure test (2), Nominal Stress (SIGNOM) is compared to the instability flow stress (SIGINS) to test for vessel failure. SIGNOM = PRESS(MTSTEP,ITRAN)* ((ZSURF(L)+RI)/(RO-RI)). SIGNOM is multiplied by 0.5 if circumferential flaw. The variable, SIGINS is defined for welds and for plates. SIGINS = (FLWSTR + 0.112d0*DT30) *(ONE-(ZSURF(L)/(RO-RI))) for welds, and SIGINS = (FLWSTR + 0.131d0*DT30)*(ONE-(ZSURF(L)/(RO-RI))) for plates. "PRESS" is the time dependent pressure. "ZSURF" is the current flaw depth. "RI" and "RO" are the inner and external vessel radii, respectively. "FLWSTR" is an input parameter on Control Record CNT3, the unirradiated flow stress used in predicting failure by remaining ligament instability. "ONE" is double precision 1.000, and "DT30" is the irradiation shift on flow stress.
- **P4**: Subroutine PROP tests if crack tip exceeds 1/4 thickness threshold in the weld layer. This step is bypassed if in plate or forging
  T4=1 ====> CRACK TIP JUST ENTERED t/4 < zsurf(l) < t/2
  IT2=1 ====> CRACK TIP JUST ENTERED t/2 < zsurf(l) < 3t/4
  IT34=1====> CRACK TIP JUST ENTERED 3t/4 < zsurf(l) < thick
- **P5**: Paramater ILAYER is set to 1, 2, 3, or 4 based on P4 above. PF, P_T0, P_JIc, and P_m are acquired for the new weld layer using array PFTHWL. A Call to subroutine RECHEM is made to resample chemistry content for the new weld layer.
- **P6**: A call is made to DTRARREST which uses the lognormal KIa distribution and returns the value of DRTArr (i.e., Arrest Reference Temperature) via Common Block TRACE. Inputs are PF = cumulative probability of crack extension, DRTepis = episitemic uncertainty term [F], RTNDTO - sampled unirradiated value for RTNDT [F]. See Step P6 notes below for detail calculations performed.
- **P7**: Variable AKICHEK.LT.SMKIA (i.e., KI < KIa) is checked to determine if flaw is arrested. If arrested, enter time loop to check for reinitiation of the arrest flaw by stepping thru transient timesteps (program step 794). MTSTEP is variable name for transient time step. If the transient is over, set IPROP=0 (no failure) and return to subroutine PFM.
- **P8**: Once MTSTEP is incremented, KI and KIC are recalculated by call function get_Kapplied and subroutine FKIC, respectively. In addition, if WPS option is selected, the maximum KI(t) for arrested flaw needs to be checked and updated, if required. AREMAX is the variable name for maximum KI(t).
- **P9**: Multiple conditional if/then statements are used to handle WPS and ductile-tearing options. Depending on the options, different calls to subroutines ductile_tearing, FKIA, REINI, REINI2, NREINI, FAILWR, and flaw_track and functions get_Kapplied and get_dt30 are used to ultimately determine if the (1) vessel failed by unstable ductile tearing, (2) flaw has re-initiated by ductile-tearing event, (3) flaw has re-initiated by cleavage, or (4) flaw was arrested.
- **P10**: If more timesteps are required, the status of the flaw (see P9 above) is used to determine rentry step: program step 794 (flaw arrested), 7932 (flaw advanced due to cleavage), or 7933 (flaw advanced due to ductile tearing). If no time steps left, returns to subroutine ACCOUNT (G5 in flowchart).

Figure 17: Flowchart for IGA Propagation Sub-model Figure 17b in FAVOR Theory Manual (page 77). The driver for the Propagation Sub-model resides in Subroutine PROP

Table 15: Variables Called in Subroutine PROP

ITYPE	**ITYPE = 0 for weld; ITYPE = 1 for plate.**
TC	**User entered value for initial RPV coolant temperature (°F).**
LFIRST	**L = LFIRST – index into zsurf mesh for initial flaw depth – prior to any propagation.**
NTSTEP	**Time step at which initiation occurs.**
ITRAN	**Transient sequence number (1, 2, 3….).**
XDEPTH	**Depth of flaw.**
PF	**PF = PFTHWL (J, 1, 1) - set in ACCOUNT for each NTRIAL – Cumulative probability of crack extension.**
P_T0	**P_T0 = PFTHWL (J, 1, 2) - Uniform random number used in sampling T0.**
P_JIc	**P_JIc = PFTHWL (J, 1, 3) - Uniform random number used in sampling JIc – updated for each flaw in PFM.**
P_m	**P_m = PFTHWL (J, 1, 4) - Uniform random number used in sampling C2 (JR Curve exponent) – updated for each flaw in PFM.**
NTRIAL	**Current RPV trial in PFM looping structure.**
NFLAW	**Current FLAW in PFM looping structure.**
J	**Replacement Variable for MNTEST, which is set to IGATRL = Input number of IGA trials per flaw.**
PFTHWL	**Array of probabilities used in sampling various parameters.**
THICK	**RPV thickness.**
STORE	**Storage array for AKICHEK (i.e., $K_I(t)$ used in Weibull distribution to determine cpi) and TMP (i.e., temperature at inner crack tip location) variables for all timesteps (NTSTEP).**
NSBR2	**NSBR2 = NPARENT(NSBR) which is the applicable parent subregion.**
IPROP	**Return to ACCOUNT: IPROP = 0 for nonfailure; IPROP = 1 for failure**
IMODE	**3 possible outcomes from subroutine PROP that are returned to subroutine ACCOUNT: IMODE = 0 for non-failure; stable arrest no failure, IMODE = 1 for failure by cleavage, or IMODE = 2 for failure by ductile tearing.**

9.7 IGA Propagation Sub-model (PROP Procedure)

Step P1. Enter the sub-model with the initiating time step, *NTSTEP*, and the flaw depth. Set the *IGA Propagation Sub-model* time-step counter *NSTEP* = *NTSTEP*. Transform the Category 1, 2, or 3 flaw into its corresponding infinite-length flaw, and calculate the applied stress-intensity factor, K_I, for the transformed flaw at this time and designate it $K_{I\text{-}initiation}$. This value of K_I will be higher than the K_I for the finite-flaw at initiation. Go to Step P2.

Step P2. Advance the infinite-length flaw to its next position in the *IGA* mesh (see Fig. 18). Proceed to Step P3.

Step P3. Check for vessel failure by through-wall cracking. At this new flaw depth and current time, calculate the current sampled estimate for the flow stress of the material. The current sampled value of $\widehat{\Delta T_{30}}$ (to be discussed in Chapter 5) is also used to estimate the effects of irradiation on the unirradiated flow stress, $\sigma_{flow(u)}$. After each resampling of $\widehat{\Delta T_{30}}$, the flow stress will have been adjusted by the following relation:

$$\widehat{\sigma_{flow}} = \sigma_{flow(u)} + \gamma\,\widehat{\Delta T_{30}} \text{ where } \gamma = \begin{cases} 0.112 \text{ ksi/°F for welds} \\ 0.131 \text{ ksi/°F for plates} \end{cases}$$

This sampled value of $\widehat{\sigma_{flow}}$ is then used in the vessel-failure test against the pressure-induced membrane stress in the remaining ligament, checking for net-section plastic collapse. The membrane stress is equal to

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

where $p_i(\tau)$ is the time-dependent internal pressure, R_i and R_o are the inner and external vessel radii, respectively, and a is the current flaw depth.

For the initial entry into the *IGA Propagation* sub-model, the flaw is growing due to a cleavage initiation; therefore, the ductile-tearing model will not be applied until the flaw has experienced its first arrest event. After the flaw has arrested, the ductile-tearing model is called at this point to check for unstable ductile tearing. This check for unstable tearing is made only if the flaw has re-initiated in ductile tearing. If the flaw has re-initiated as a cleavage event, the ductile-tearing sub-model is not called. If the conditions for unstable ductile tearing are encountered, the logical variable FAIL_UDT is set to TRUE in the ductile-tearing sub-model and returned to the IGA Propagation Sub-model.

The vessel failure criterion is

if REINITIATED_BY_DUCTILE_TEARING is TRUE then

$$\text{if } \left\{ \begin{matrix} \sigma_m > \widehat{\sigma_{flow}} \\ \text{or} \\ FAIL\_UDT \text{ is TRUE} \\ \text{or} \\ \left(\dfrac{a}{R_o - R_i}\right) > FAILCR \end{matrix} \right\} \text{ then}$$

vessel failure = TRUE during ductile tearing
return to Step G5 in IGA Model

$$\text{elseif } \left\{ \begin{matrix} \sigma_m > \widehat{\sigma_{flow}} \\ or \\ \left(\dfrac{a}{R_o - R_i}\right) > FAILCR \end{matrix} \right\} \text{ then}$$

vessel failure = TRUE during flaw growth by cleavage
return to Step G5 in IGA Model

else

vessel failure = FALSE
proceed to Step P4

where $0.25 \leq FAILCR \leq 0.95$ is a user-supplied failure criterion.

Step P4. If the material is a plate or forging product form, proceed directly to Step P6. If the material is a weld, check to see if the flaw has advanced into a new weld layer. Weld subregions are sectioned into through-wall quadrants to simulate, in an approximate manner, multiple weld layers. As the flaw advances from one weld-layer quadrant into the next, the weld chemistry will be resampled with the attenuated fluence. If the flaw has just advanced into a new weld layer, go to Step P5. If not, then proceed to Step P6.

Step P5. Resample the weld chemistry $\left(\widehat{Cu}, \widehat{Ni}, \widehat{Mn}, \widehat{P}\right)$ using the sampling distributions given in Chapter 5. Update the irradiation shift, $\widehat{\Delta RT_{NDT}}$, and the irradiated value of the upper shelf energy, $\widehat{USE_{(i)}}$, using the resampled weld chemistry. If the weld-layer-resampling option is turned on and the flaw has just entered layer 2, 3, or 4, then resample for a new value of P_f to replace the value of P_f sampled in Step G2 of the *IGA* sub-model. The random iterate P_f is drawn from a uniform distribution on the open interval *U*(0,1).

Step P6. Using the current chemistry content and current value of P_f, recalculate the arrest reference temperature. Calculate the epistemic uncertainty in the arrest reference temperature by Eqs. (103) and (107) given in Sect. 5.5 of the Theory Manual.

Retrieve the previously sampled unirradiated value of $\overline{RT}_{NDT(0)}$ for this subregion and the sampled value of the irradiation shift for this flaw, $\widehat{\Delta RT_{NDT}}(r, \ldots)$, determined from the embrittlement model applied for this flaw at its current position in the RPV wall or from weld-chemistry resampling if Step P5 was executed. Calculate the shift in the arrest reference temperature, relative to the initiation reference temperature using Eqs in Step 11 of Sect. 5.5 of the Theory manual.

$$\widehat{\Delta RT}_{ARREST} \leftarrow \Lambda(\overline{\mu}_{ln(\Delta RT_{ARREST})}, \overline{\sigma}_{ln(\Delta RT_{ARREST})}) \ \ [°F]$$

where (see Appendix F of the FAVOR Theory Manual (Reference [1]) for the development of this protocol)

$$\overline{\mu}_{ln(\Delta RT_{ARREST})} = ln\left[\overline{\Delta RT}_{ARREST(mean)}\right] - \frac{\overline{\sigma}^2_{ln(\Delta RT_{ARREST})}}{2}$$

$$\overline{\Delta RT}_{ARREST(mean)} = 44.122\, exp\left[-0.005971 \times \overline{T}_0\right] \ \ [°C]$$

$$\overline{T}_0 = \left(\overline{RT}_{NDT_0} - \overline{\Delta RT}_{epist-arrest} - 32\right)/1.8 \ \ [°C]$$

$$\overline{\sigma}_{ln(\Delta RT_{ARREST})}$$

$$= \sqrt{ln\left\{exp\left[0.38998^2 + 2\, ln\left(\overline{\Delta RT}_{ARREST(mean)}\right)\right] - var\left(\overline{T}_0\right)\right\} - 2\, ln\left[\overline{\Delta RT}_{ARREST(mean)}\right]}$$

$$var(\overline{T_0}) = \begin{cases} (12.778)^2 & \text{for } \overline{T_0} < -35.7\,°C \\ 99.905972 - 1.7748073\,\overline{T_0} & \text{for } -35.7\,°C \le \overline{T_0} \le 56\,°C \\ 0 & \text{for } \overline{T_0} > 56\,°C \end{cases}$$

Calculate the estimated arrest temperature[6] by Eq. (109) in Step 12 of Sect. 5.5

$$\widehat{RT}_{ARREST}\,(r,\dots) = \overline{RT}_{NDT_0} - \overline{\Delta RT}_{epist-arrest} + \widehat{\Delta RT}_{ARREST} + \Delta\overline{RT_{NDT}}\,(r,\dots)$$

Calculate the normalized (relative to $\widehat{RT}_{ARREST}$) temperature of the vessel at the current location, *r*, in the RPV wall by Eq. (140) in Step 13 of Sect. 5.5

$$\widehat{\Delta T}_{RELATIVE}\,(r,\dots) = T(r,t) - \widehat{RT}_{ARREST}\,(r,\dots)$$

If this is the first pass through the sub-model for this flaw, calculate (by Eqs. (118) or (119) and (141) in Steps 14 and 15 in Sect. 5.5) the fractile, $\Phi_{K_{I-initiation}}$, associated with this value of $K_{I\text{-}initiation}$ from the arrest model, given the current value of the applied $K_{I\text{-}initiation}$ from the infinite-length flaw in the *IGA* sub-model

$$\Phi_{K_{I-initiation}} = \frac{1}{2}\left[erf\left(\frac{ln(K_{I-initiation}) - \mu_{ln(K_{Ia})}(\widehat{\Delta T}_{RELATIVE})}{\sigma_{ln(K_{Ia})}\sqrt{2}}\right) + 1\right]$$

where

$$erf(x) = \text{ error function } = \frac{2}{\sqrt{\pi}}\int_0^x exp(-\xi^2)\,d\xi\,;\; erf(-x) = -erf(x)$$

if K_{Ia}_Model is equal to 1

$$K_{Ia(\text{mean})}(\widehat{\Delta T}_{RELATIVE})$$

$$= 27.302 + 69.962\,exp\left[0.006057(\widehat{\Delta T}_{RELATIVE})\right] \quad [\text{ksi}\sqrt{\text{in.}}]$$

$$\sigma_{ln(K_{Ia})} = 0.18$$

else if K_{Ia}_Model is equal to 2

$$K_{Ia(\text{mean})}(\widehat{\Delta T}_{RELATIVE})$$

$$= 27.302 + 70.6998\,exp\left[0.008991(\widehat{\Delta T}_{RELATIVE})\right] \quad [\text{ksi}\sqrt{\text{in.}}]$$

$$\sigma_{ln(K_{Ia})} = 0.34$$

[6] The major region variate $\overline{RT_{NDTo}}$ is not re-sampled in this step.

$$\mu_{ln(K_{Ia})}(\widehat{\Delta T}_{RELATIVE}) = ln\left[K_{Ia(\text{mean})}(\widehat{\Delta T}_{RELATIVE})\right] - \frac{\sigma^2_{ln(K_{Ia})}}{2}$$

In the above relation for $\Phi_{K_{I-initiation}}$, $\mu_{ln(K_{Ia})}$ is calculated at the location of the initiation of the flaw. For this flaw, the value of $\Phi_{K_{I-initiation}}$ remains fixed in the *IGA Propagation* sub-model until P_f is resampled in Step G2 of the *IGA* sub-model. Using the current value of P_f, scale by $\Phi_{K_{I-initiation}}$ (if this is the weld layer in which the crack initiation originally occurred) such that (from Eq. (142) in Step 15 of Sect. 5.5)

$$\Phi_{K_{Ia}} = (P_f)(\Phi_{K_{I-initiation}})$$

For subsequent weld layers do not perform the above scaling. When the flaw advances into a new weld layer, any linkage between the flaw's initiation and its continued propagation is assumed to be broken.

With this $\Phi_{K_{Ia}}$ fractile, draw a value of K_{Ia} from its lognormal distribution as given by Eq. (143) of Step 15 in Sect. 5.5

$$K_{Ia}\left(\Phi_{K_{Ia}}, \widehat{\Delta T}_{RELATIVE}\right) = \exp\left[\sigma_{\ln\,(K_{Ia})} Z_{\Phi_{K_{Ia}}} + \mu_{ln(K_{Ia})}(\widehat{\Delta T}_{RELATIVE})\right]$$

$$Z_{\Phi_{K_{Ia}}} = \text{standard normal deviate corresponding to the } \Phi_{K_{Ia}} \text{ fractile.}$$

In the above relation for K_{Ia}, $\mu_{ln(K_{Ia})}$ is calculated at the current location of the flaw. The scaling procedure in Step P6 ensures that the initial value of K_{Ia}, calculated immediately after initiation, does not exceed the initiating value of $K_{I\text{-}initiation}$, thus producing an initial extension. Once the value of $Z_{\Phi_{K_{Ia}}}$ has been determined for this *IGA* trial, the arrest toughness during flaw advancement through the wall changes due to changes in $\widehat{\Delta T}_{RELATIVE}$ only. These changes are caused by variations in $T(r,t)$ and RT_{Arrest} (due to the resampling of the weld chemistry when passing into new weld layers).

For Ductile-Tearing Model No. 2, update the current value of the irradiated upper-shelf energy by

$$\widehat{USE}_{(i)} = A + 0.0570 \cdot \widehat{USE}_{(u)}^{1.456} - \left[17.5 \cdot f\left(\widehat{Cu}\right) \cdot \left(1 + 1.17\,\widehat{Ni}^{0.8894}\right) + 305\,\widehat{P}\right]\left(\frac{\hat{f}_0\,(r)}{10^{19}}\right)^{0.2223} \quad \text{[ft-lbf]}$$

Go to Step P7.

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

if $K_I < K_{Ia}$ then
 the flaw has arrested
 proceed to Step P8
else
 the flaw has not arrested

Proceed to Step P2

Step P8. Hold the flaw at this position and advance the time to check for re-initiation or new ductile tearing.

$$NSTEP = NSTEP + 1$$

For this new time station, bring up the wall temperature, $T(r,\tau)$, at this position along with the current irradiated and attenuated value of RT_{NDT} to calculate

$$\widehat{\Delta T}_{RELATIVE}\,(r,\dots) = T(r,\tau) - \widehat{RT}_{RTNDT}\,(r,\dots)$$

Now calculate the parameters of the K_{Ic} model

$$a_{K_{Ic}}(\widehat{\Delta T}_{RELATIVE}) = 19.35 + 8.335\,exp\left[0.02254(\widehat{\Delta T}_{RELATIVE})\right] \quad [\text{ksi}\sqrt{\text{in.}}]$$

$$b_{K_{Ic}}(\widehat{\Delta T}_{RELATIVE}) = 15.61 + 50.132\,exp\left[0.008(\widehat{\Delta T}_{RELATIVE})\right] \quad [\text{ksi}\sqrt{\text{in.}}]$$

$$c_{K_{Ic}} = 4$$

with K_{Ic} in ksi√in and $\Delta T = (T\text{-}RT_{NDT})$ in °F.

The static initiation toughness, K_{Ic}, is calculated from its Weibull distribution by

$$K_{Ic}(\widehat{\Delta T}_{RELATIVE}) = \widehat{a_{K_{Ic}}}\,(\widehat{\Delta T}_{RELATIVE}) + \widehat{b_{K_{Ic}}}\,(\widehat{\Delta T}_{RELATIVE})\left[-\,ln(\,1 - P_f)\right]^{1/c_{K_{Ic}}} \quad \text{for} \quad a_{K_{Ic}}(\widehat{\Delta T}_{RELATIVE}) \le K_{Ic} \le K_{Ic(max)}$$

Proceed to Step P9.

Step P9. If the warm prestressing (WPS) analysis option has been turned on by the user, check to see if the flaw is in a state of WPS. If the ductile-tearing option is turned on, then call the ductile-tearing model to determine if there is stable or unstable ductile tearing. If the WPS option is on and WPS = TRUE, go to Step P10. If the WPS option is off or WPS = FALSE, check the current applied K_I for re-initiation by the test

if $K_I < K_{Ic}$ and $STABLE_DT$ and $FAIL_UDT$ are both FALSE then

No re-initiation.

Proceed to Step P10.

else if WPS_OPTION is on and WPS is TRUE then

No re-initiation

Proceed to Step P10.

else if $FAIL_UDT$ is TRUE then

the vessel has failed by unstable ductile tearing

set vessel failure to TRUE

return to Step G5 of IGA model.

else if $STABLE_DT$ is TRUE and $K_{J_{Ic}}$ is less than K_{Ic} then

the flaw has re-initiated by a ductile-tearing event

REINITIATED_BY_DUCTILE_TEARING = TRUE

the current level of tearing Δa_0 is set by the ductile-tearing model

Proceed to Step P3.

else

The flaw has re-initiated by a cleavage event.

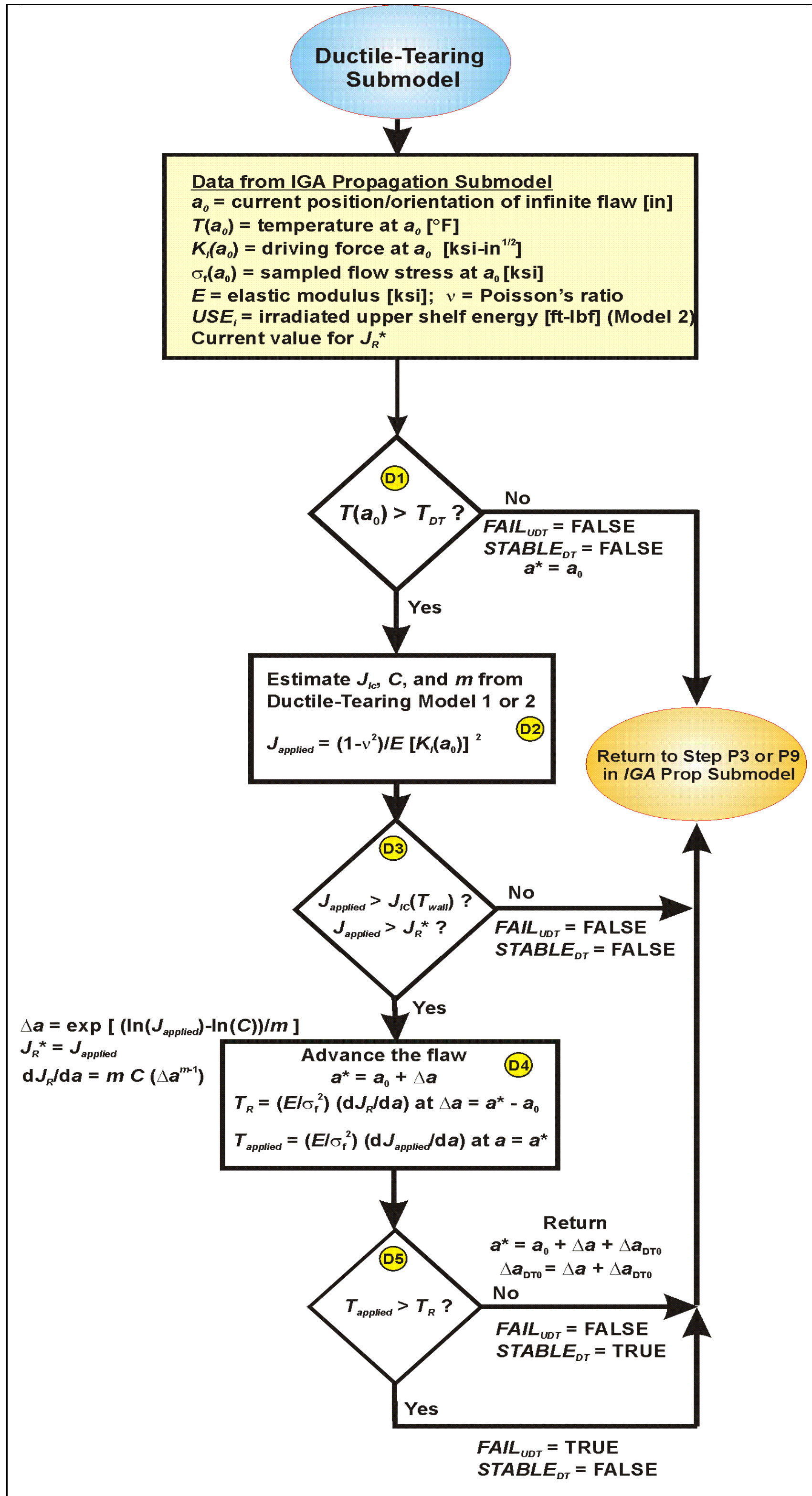
REINITIATED_BY_DUCTILE_TEARING = FALSE

Reset the current level of tearing $\Delta a_0 = 0$

Proceed to Step P2 and advance the flaw.

Step P10. If there are time steps remaining in the transient, proceed to Step P8 and advance the time. If the transient is complete, set vessel failure = FALSE, and return to Step 5 of the *IGA* sub-model.

Note that in the *IGA Propagation* sub-model, the flaw is assumed to advance instantaneously; i.e., the time station remains fixed during flaw growth. Time will advance only if the flaw is in a state of arrest. If the flaw remains in arrest until the end of the transient, then the flaw is said to have experienced a *Stable Arrest*.



ductile-tearing

•**Call to Subroutine ductile_tearing (see steps P3 and P9 in Figure 12)** to test for ductile tearing instability. Inputs include:

ITYPE = 0 ==> Weld
ITYPE = 1 ==> Plate or Forging
IFLCAT = Flaw Category
L = Crack Position Index in wall ==> ZSURF(L)
MTSTEP = Time Step in Transient
ITRAN = Transient
IORIENT = 1 ==> Axial
IORIENT = 2 ==> Circumferential
KJIc = Ductile Fracture Toughness [ksi$\sqrt{\text{in}}$]
KJRstar = KJapplied corresponding to previous time step at which stable ductile tear occurred.
T_DT = Ductile-Tearing Transition Temperature [degF] = 200 °F
da0 = initial tearing (in.)
SFLOW = Current sampled flow stress [ksi]
P_T0 = p_rtepi = Random percentile (0 to 1) to be used in sampling T_O [-]
P_JIc = PFTHWL (1, 1, 3) = Random percentile (0 to 1) to be used in sampling JIc [-]
P_m = PFTHWL (1, 1, 4) = Random percentile (0 to 1) to be used in sampling JR curve exponent [-]
Emod = Elastic Modulus [ksi]
Nu = Poisson's Ratio [-]

Outputs include:

FAIL_UDT = TRUE or FALSE (failure by unstable ductile tearing)
STABLE_DT = TRUE or FALSE (flaw experienced stable ductile tearing)
L = New Crack Position Index in wall ==> ZSURF(L)
da0 = new level of stable tearing (in.)

•Subroutine ductile_tearing calls functions get_Kapplied and get_JIc. Function get_JIc incorporates the ductile-tearing models described in section 4.3.11.1 and 4.3.11.2 of FAVOR's theory manual.

•*D1:* The program enters the sub-model with the current position and orientation of the crack tip and the time within the selected transient. The sub-model first checks the current wall temperature (TEMP(L,ITRAN,MTSTEP) at the crack tip with the ductile-tearing transition temperature, T-DT = T_{DT}. The value of T_{DT} is hardwired to 200 °F. If this is not the first entry into the model, a current value of J_R^* will be known, where J_R^* is a measure of the current deformation state due to tearing. Japplied = J_a is tested against JIc = J_{IC} and JRstar = J_R^* initially to see if flaw advances. A call to Function get_JIc calculates J_{IC}.

•*D2*: The call to Function get_JIc also provides the initial estimates for the J_R-curve parameters C and m. The program uses variables C_DT_ini and m_DT_ini for C and m, respectively. Function get_JIc captures the two ductile-tearing models (1 - newer upper-shelf model and 2 - older upper-shelf model based on USE_i).

•*D3*: If Japplied = J_a is greater than JIc = J_{IC} and/or JRstar = J_R^*, the flaw is advanced. If not the logical varialbes FAIL_UDT are STABLE_DT are set to ".FALSE.".

•*D4*: If the flaw is advanced, da_DT ("Δa" in flowchart description) is calculated using the equation in STEP D4 to calculate the ductile crack extension. Also the new flaw depth is calculated: astar = ZSURF(L) + da_DT ($a^* = a_0 + \Delta a$ in flowchart). The flaw then is advanced to a depth a^{**}, which is the first nodal position deeper than a^*. It is at this nodal position, called "ai" in the subroutine that the local material tearing modulus, TR (i.e., T_R) and applied tearing modulus, Tapplied (i.e., $T_{applied}$), are calculated.

•*D5*: If Tapplied > TR, the logical variable FAIL_UDT is set to ".TRUE." and STABLE_DT is set ".FALSE." to capture that vessel failed due to unstable ductile tearing. If Tapplied < TR, the logicals are set opposite and updated L and da0 variables are returned to Subroutine PROP (i.e., either Step *P3* or P9 in the IGA Propagation Sub-model flowchart.)

Figure 18: Ductile Tearing Sub-Model – Figure 17c in Theory Manual Subroutine Ductile_Tearing. Called from two locations within Subroutine PROP

9.8 Ductile Tearing Model

Step D1. The program enters the sub-model with the current position and orientation of the crack tip and the time within the selected transient. The sub-model first checks the current wall temperature at the crack tip with the ductile-tearing transition temperature, T_{DT}. Based on a previous study, the value of T_{DT} is set to 200 $°F$. If this is not the first entry into the model, a current value of J_R^* will be known, where J_R^* is a measure of the current deformation state due to tearing.

if $T_{wall} < T_{DT}$ then
  $FAIL_{UDT}$ = FALSE
  $STABLE_{DT}$ = FALSE
  Return to Step P3 or P9 of IGA Sub-model
else

Proceed to Step D2

Step D2. Given the location and orientation of the flaw tip, the sub-model converts the known value of $K_{I\text{-}applied}$ to $J_{applied}$ using a plane-strain conversion. The sub-model then proceeds to calculate/sample estimates for the J_R-curve parameters, J_{Ic}, C, and m.

$$J_{applied} = \frac{(1-\nu^2)}{E} K_{I-applied}^2 \text{ [in-kips/in}^2\text{]}$$

get $\widehat{J_{Ic}}$ from either Ductile-Tearing Model No. 1 or 2
get $\widehat{C}$, and $\widehat{m}$ from either Ductile-Tearing Model No. 1 or 2

Proceed to Step D3

Step D3. The sub-model then compares the $J_{applied}$ to the estimated value of J_{Ic} obtained in Step D2 and the known value of J_R^*. If this is the first entry into the model or if a cleavage reinitiation has occurred since the last entry into the model, then $J_R^* = 0$. J_R^* is the value of $J_{applied}$ corresponding to a previous time step at which a stable ductile tear ocurred. For a ductile tear to occur at the current time, it is necessary for $J_{applied}$ to be equal to or greater than the current value of J_R^*.

if $(J_{applied} < J_{Ic})$ or $(J_{applied} \leq J_R^*)$ then
  $FAIL\_UDT$ = FALSE
  $STABLE\_DT$ = FALSE
  Return to Step P3 or P9 of IGA Sub-model
else

Proceed to Step D4

Step D4. The sub-model then advances the position of the flaw, a_0, by the amount of ductile crack extension, Δa, produced by the known value of $J_{applied}$, and the new flaw depth is $a^* = a_0 + \Delta a$. The flaw then is advanced to a depth a^{**}, which is the first nodal position deeper than a^*. It is at this nodal position, $a^{**} = x_n$, that the local material tearing modulus, T_R, and applied tearing modulus, $T_{applied}$, are calculated. The local tearing modulus, T_R, characterizes the tearing resistance of the material.

$$J_R^* = J_{applied}$$
$$\Delta a = exp\left[\frac{ln(J_R^*) - ln(C)}{m}\right] \text{, [in]}$$
$$a* = a_0 + \Delta a$$

The *IGA Propagation* sub-model mesh is searched to find the closest node point, node *n*, that is deeper into the wall than the current flaw position at a^*. The flaw is then repositioned to this node point such that $a^{**} = x_n$ (see Fig. 19). Based on the new position of the flaw, the local material tearing modulus is calculated at a^{**} and the applied tearing modulus is estimated from a second-order finite-difference ratio.

$$\Delta a^{**} = a^{**} - a_0$$
$$T_R = \left(\frac{E}{\sigma_{flow}^2}\right)\frac{dJ_R^*}{da}\bigg|_{\Delta a^{**}} = \left(\frac{E}{\sigma_{flow}^2}\right)\times m \times C \times \left(\Delta a^{**}\right)^{m-1}$$

and

$$\frac{dJ_{applied}}{da} \approx \frac{J_{n+1} + (\alpha - 1)J_n - \alpha^2 J_{n-1}}{\alpha(\alpha+1)\Delta x} \quad , \quad \mathrm{O}\left(\Delta x^2\right)$$

where

$$\Delta x = x_n - x_{n-1}$$
$$\alpha = \frac{x_{n+1} - x_n}{x_n - x_{n-1}}$$
$$T_{applied} = \left(\frac{E}{\sigma_{flow}^2}\right)\frac{dJ_{applied}}{da}\bigg|_{a=a^{**}}$$

Step D5. A check is now made for unstable ductile tearing. If the applied tearing modulus is greater than T_R , then a state of unstable ductile tearing is declared.

if $T_{applied} > T_R$ then

$FAIL\_UDT$ = TRUE
$STABLE\_DT$ = FALSE
Return to Step P3 or Step P9 in the $IGA\ Propagation$ Sub-model
else
$FAIL\_UDT$ = FALSE
$STABLE\_DT$ = TRUE
$\Delta a_0 = \Delta a$
$a_0 = a*$

Return to Step P3 or Step P9 in the $IGA\ Propagation$ Sub-model

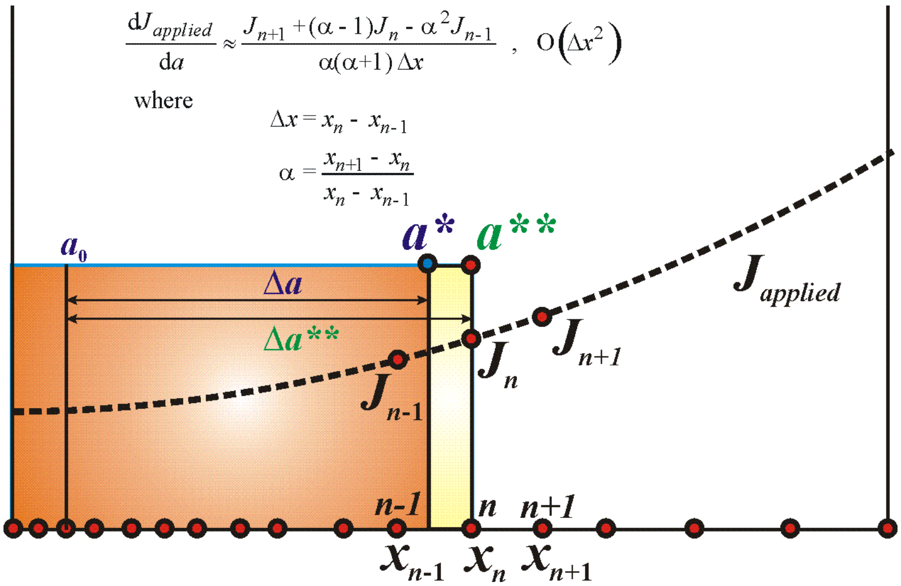


Figure 19: IGA Propagation sub-model mesh used to estimate $dJ_{applied}$ / da using a second-order central finite-difference ratio.

Design 10 Initial fracture mechanism is based on stress-controlled cleavage initiation (in the transition-temperature region of the vessel material) modeled under the assumptions of linear-elastic fracture mechanics (LEFM)

FAVLoad and FAVPFM have been designed using LEFM. The methods used to calculate hoop, axial stresses, and applied stress intensity factors are based on the LEFM model, as described in the previous Design Descriptions. For crack initiation, the FAVPFM model assumes a fracture mechanism based on stress-controlled cleavage initiation (in the transition-temperature region of the vessel material) modeled under the assumptions of LEFM. The failure mechanism by through-wall cracking is 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. In FAVOR, flaw growth can be due to either cleavage propagation or stable ductile tearing. In addition, if the conditions for unstable ductile tearing are satisfied, then vessel failure by through-wall cracking is assumed to occur.

Design 9 provides the details of the software logic flow used to calculate the probability of crack initiation. The temporal relationship between the applied Mode I stress intensity factor (K_I), as previously described, and the static cleavage fracture initiation toughness (K_{IC}) at the crack tip is calculated at discrete transient time steps. This design description will focus on the fracture-toughness, K_{Ic}. K_{Ic} is based on a statistical model which is a function of the normalized temperature, $T(\tau) - RT_{NDT}$, where $T(\tau)$ is the time-dependent temperature at the crack tip. Analysis results are used to calculate the conditional probability of crack initiation (*CPI*), i.e., the probability that pre-existing fabrication flaws will initiate in cleavage fracture. Also, the PFM model calculates the conditional probability of failure (*CPF*) by through-wall cracking, i.e., the probability that an initiated flaw will propagate through the RPV wall. These probabilities are conditional in the sense that the thermal-hydraulic transients are assumed to occur.

The computational model for quantification of fracture-toughness uncertainty has been improved (relative to the models used in the 1980s that supported the PFM calculations that informed 10 CFR 50.61) in three ways: (1) the K_{Ic} and K_{Ia} databases were extended by 84 and 62 data values, respectively, relative to the databases in the EPRI NP-719-SR[7] report [17]; (2) the statistical representations for K_{Ic} and K_{Ia} were derived through the application of rigorous mathematical procedures; and (3) a method for estimating the *epistemic* uncertainty in the transition-reference temperature was developed. Bowman and Williams [18] provide details regarding the extended database and mathematical procedures employed in the derivation of a Weibull distribution for fracture-toughness data. Listings of the extended ORNL 99/27 K_{Ic} and K_{Ia} database are given in Appendix C of the FAVOR Theory Manual (Reference [1]). A Weibull statistical distribution, in which the parameters were calculated by the *Method of Moments* point-estimation technique, forms the basis for the K_{Ic} model. For the Weibull distribution, there are three parameters to estimate: the location parameter, *a*, of the random variate; the scale parameter, *b*, of the random variate; and the shape parameter, *c*. The Weibull probability density, f_W, is given by:

$$f_W(x|a,b,c) = \begin{cases} 0 \quad ; & x \le a \\ \frac{c}{b} y^{c-1} \, exp(-y^c) \, ; & (y = (x-a)/b, x > a, b, c > 0) \end{cases}$$

where the parameters of the K_{Ic} distribution are a function of $\widehat{\Delta T}_{RELATIVE}$:

$$a_{K_{Ic}}\left(\widehat{\Delta T}_{RELATIVE}\right) = 19.35 + 8.335 \, exp\left[0.02254\left(\widehat{\Delta T}_{RELATIVE}\right)\right] \quad \left[ksi\sqrt{in.}\right]$$
$$b_{K_{Ic}}\left(\widehat{\Delta T}_{RELATIVE}\right) = 15.61 + 50.132 \, exp\left[0.008\left(\widehat{\Delta T}_{RELATIVE}\right)\right] \quad \left[ksi\sqrt{in.}\right]$$
$$c_{K_{Ic}} = 4$$

where $\widehat{\Delta T}_{RELATIVE} = \left(T(t) - \widehat{RT}_{NDT}\right)$ in $°F$. The curve, "$\widehat{X}$", above a variable indicates that it is a randomly sampled value.

For each postulated flaw, a deterministic fracture analysis is performed by stepping through the transient time history for each transient. At each time step, τ^n, for the i^{th} transient and j^{th} RPV trial, an

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[7] The fracture-toughness database given in EPRI NP-719-SR (1978) [17] served as the technical basis for the statistical K_{Ic} / K_{Ia} distributions used in the IPTS studies of the 1980s.

instantaneous *cpi*(τ^n)$_{(i,j,k)}$ is calculated for the k^{th} flaw from the Weibull K_{Ic} cumulative distribution function at time, τ, to determine the fractional part (or fractile) of the distribution that corresponds to the applied $K_I(\tau^n)_{(i,j,k)}$:

$$\Pr\left(K_{Ic} \le K_I(\tau^n)_{(i,j,k)}\right) = cpi(\tau)_{(i,j,k)} = \begin{cases} 0 \quad ; & K_I(\tau^n)_{(i,j,k)} \le a_{K_{Ic}} \\ 1 - \exp\left\{ -\left[\dfrac{K_I(\tau^n)_{(i,j,k)} - a_{K_{Ic}}}{b_{K_{Ic}}} \right]^{c_{K_{Ic}}} \right\} ; & K_I(\tau^n)_{(i,j,k)} > a_{K_{Ic}} \end{cases}$$

Here, *cpi*(τ^n)$_{(i,j,k)}$ is the instantaneous conditional probability of initiation at the crack tip at time τ^n. Figure 20 illustrates the interaction of the applied K_I time history and the Weibull K_{Ic} distribution for an example case, in which an embedded flaw 0.67-in. in depth, 4.0-in. in length, with the inner crack tip located 0.5-in. from the inner surface, is subjected to a severe PTS transient. The RT_{NDT} of the RPV material is 270 °F. A Weibull distribution, as a lower-bounded continuous statistical distribution, has a lower limit (referred to as the *location parameter,* $a_{K_{Ic}}$) such that any value of K_I below the location parameter has a zero probability of initiation. As described in Figure 20, the applied K_I must be greater than the local value of $a_{K_{Ic}}$ before *cpi* > 0. The region designated as *cpi* > 0 in the figure represents the finite probability K_{Ic} initiation space, and outside of this region *cpi* = 0.

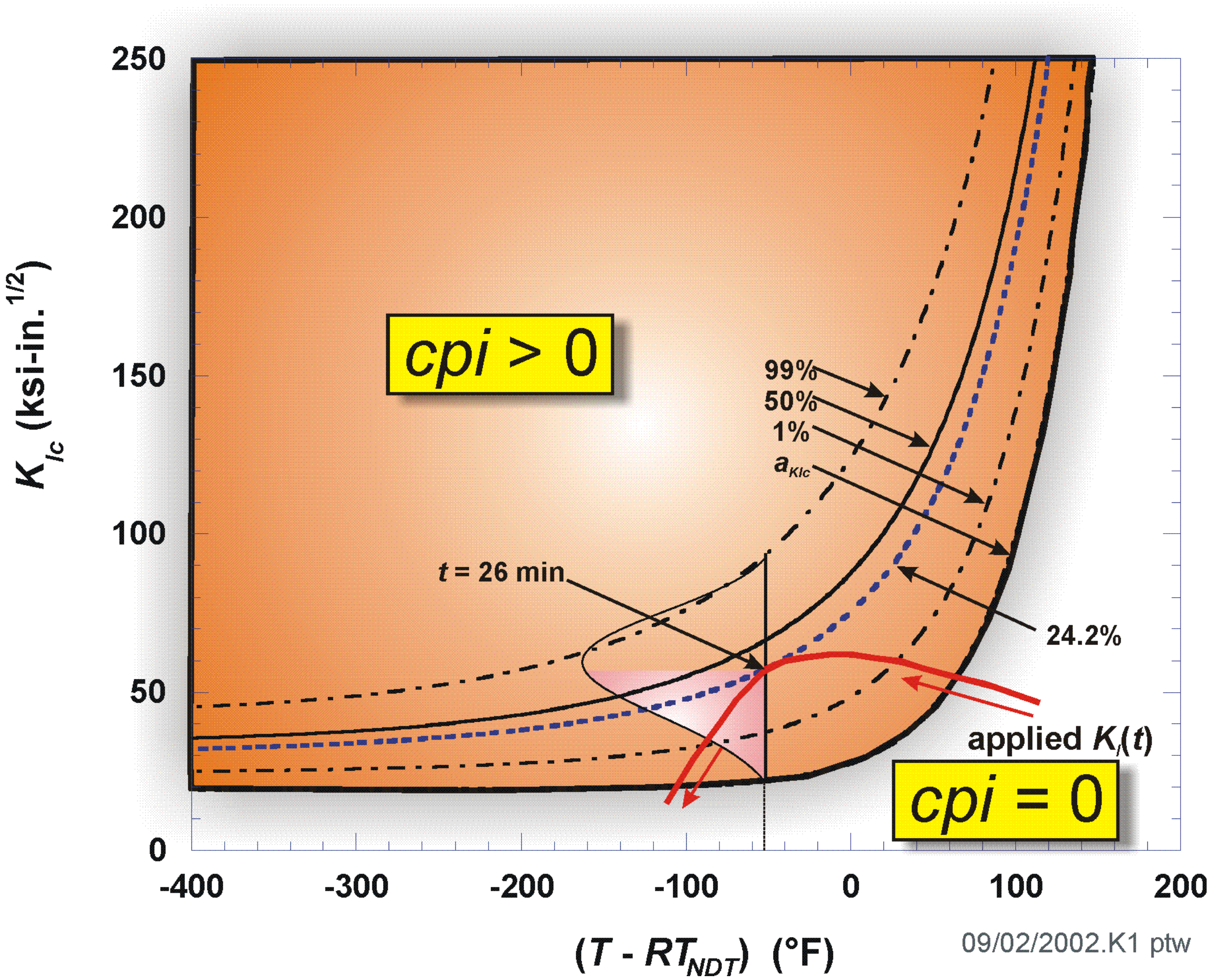

Figure 20: Interaction of the Applied K_I Time History and Weibull K_{Ic} Statistical Model for a Postulated Flaw

Subroutine PFM calculates the conditional probability of crack initiation (*CPI*) using the above Weibull K_{Ic} model.

Design 11 Radiation embrittlement is considered when determining the Plane-Strain Static Cleavage Initiation Toughness, KIc, and that the correlation is based on an industry acceptable standard or one that has been benchmarked to a valid standard.

Irradiation damage of RPV steels in U.S. reactor vessels occurs as a consequence of two hardening mechanisms: *matrix hardening* and *age hardening*. Details of these mechanisms are taken from [1]:

Matrix Hardening – Matrix damage develops continuously during irradiation, producing hardening that has a square root dependence on fluence. Matrix damage can be divided into two components: unstable matrix defects (UMD), and stable matrix defects (SMD). Unstable matrix defects are formed at relatively low fluence and are small vacancy or interstitial clusters, complexed with solutes such as phosphorous. UMDs are produced in displacement cascades. Increasing flux causes increasing hardening due to these defects, but they occur relatively independently of alloy composition. In low copper alloys, at low fluence and high flux, UMD is the dominant source of hardening; however, in high copper steels, these defects delay the copper-rich precipitate contribution to hardening by reducing the efficiency of radiation-enhanced diffusion. Stable matrix features form at high fluence and include nanovoids and more highly complexed clusters. These defects cause hardening that increases with the square root of exposure and is especially important at high fluence levels.

Age Hardening – Radiation accelerates the precipitation of copper held in solid solution, forming copper-rich precipitates (CRPs) that inhibit dislocation motion and, thereby, harden the material. This hardening rises to a peak value and is then unaffected by subsequent irradiation because no copper remains in solid solution to precipitate out and cause damage. The magnitude of this peak depends on the amount of copper initially in solution, which is available for subsequent precipitation. Post-weld heat treatment (PWHT) performed before the RPV is placed into service can also precipitate copper, removing its ability to cause further damage during irradiation. Thus, different materials are expected to have different peak hardening values due to differing pre-service thermal treatments. Additionally, the presence of nickel in the alloy further enhances its age-hardening capacity. Nickel precipitates together with copper, forming larger second-phase particles that present greater impediments to dislocation motion and, thereby, produce a greater hardening effect.

These physical insights helped to establish the functional form of a 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. A quantitative relationship was developed from the database of Charpy shift values, ΔT_{30}, generated in US commercial reactor surveillance programs. Currently, five correlations are available within FAVPFM based on these data.

11.1 Eason 2000 Correlation Implemented in FAVOR, v05.1, and Earlier Versions

$$\widehat{\Delta T}_{30}\left(\widehat{Ni},\widehat{Cu},\widehat{P},\widehat{f}_0(r),\tau_{exposure},T_c,productform\right)[°F] =$$
$$A\,exp\left(\frac{19310}{T_c+460}\right)\left(1+110\,\widehat{P}\right)\left(\widehat{f}_0(r)\right)^{0.4601}+B\left(1+2.40\,\widehat{Ni}^{1.250}\right)f\left(\widehat{Cu}\right)g\left(\widehat{f}_0(r)\right)+Bias$$

$$A=\begin{Bmatrix} 8.86\times 10^{-17}\ for\ welds \\ 9.30\times 10^{-17}\ for\ forgings \\ 12.7\times 10^{-17}\ for\ plates \end{Bmatrix};\ B=\begin{Bmatrix} 230\ for\ welds \\ 132\ for\ forgings \\ 206\ for\ plates\ in\ CE\ vessels \\ 156\ for\ other\ plates \end{Bmatrix}\begin{bmatrix} CE\ \rightarrow\ manufactured\ by \\ Combustion\ Engineering \end{bmatrix}$$

$$g\left(\widehat{f}_0(r)\right)=\frac{1}{2}+\frac{1}{2}tanh\left[\frac{log_{10}\left(\widehat{f}_0(r)+4.579\times 10^{12}\tau_{exposure}\right)-18.265}{0.713}\right]$$

$$f\left(\widehat{Cu}\right)=\begin{cases} 0 & for\ \widehat{Cu}\le 0.072\ wt\ \% \\ \left(\widehat{Cu}-0.072\right)^{0.659} & for\ \widehat{Cu}>0.072\ wt\ \% \end{cases};\ \begin{bmatrix} subject\ to\ copper\text{-}saturation\ limit \\ \widehat{Cu}=min\left(\widehat{Cu},Cu_{max}\right) \end{bmatrix} \qquad (1)$$

$$Cu\begin{Bmatrix} 0.25\ for\ Linde\ 80\ or\ Linde\ 0091\ weld\ fluxes \\ 0.305\ for\ all\ other\ weld\ fluxes \end{Bmatrix}_{max}$$

and

$$Bias = \begin{Bmatrix} 0\ for\, \tau_{exposure} < 97000\ h \\ 9.4\ for\, \tau_{exposure} \geq 97000\ h \end{Bmatrix}$$

11.2 Eason 2006 Correlation Implemented in FAVOR, v06.1

$$\widehat{\Delta T}_{30}(\widehat{Ni}, \widehat{Cu}, \widehat{P}, \widehat{Mn}, \widehat{f}_0(r), \tau_{\text{exposure}}, T_c, \text{product form})\left[{}^\circ\text{F}\right] =$$

$$A(1-0.001718\,T_c)\left(1+6.13\,\widehat{P}\,\widehat{Mn}^{2.471}\right)\sqrt{\widehat{f}_0(r)_{eff}} +$$

$$B\left(1+3.769\,\widehat{Ni}^{1.191}\right)\left(\frac{T_c}{543.1}\right)^{1.100} f\left(\widehat{Cu}, \widehat{P}\right)\, g\left(\widehat{Cu}, \widehat{Ni}, \widehat{f}_0(r)\right)$$

$$A=\begin{cases}1.140\text{x}10^{-7} & \text{for forgings}\\ 1.561\text{x}10^{-7} & \text{for plates}\\ 1.417\text{x}10^{-7} & \text{for welds}\end{cases};\quad B=\begin{cases}102.3 & \text{for forgings}\\ 102.5 & \text{for plates in non-CE vessels}\\ 135.2 & \text{for plates in CE vessels}\\ 155.0 & \text{for welds}\end{cases};$$

$$\left[\begin{matrix}\text{CE} \rightarrow \text{ manufactured by}\\ \text{Combustion Engineering}\end{matrix}\right];\quad \widehat{f_0}(r)=\left\{\begin{matrix}\text{sampled and attenuated}\\ \text{neutron fluence}\end{matrix}\left[\frac{\text{neutrons}}{\text{cm}^2}\right]\right\};$$

$$\text{neutron flux: } \phi=\frac{\widehat{f_0}(r)}{3600\ \tau_{\text{exposure}}}\left[\frac{\text{neutrons}}{\text{cm}^2\text{-sec}}\right];$$

$$\widehat{f_0}(r)_{eff}=\begin{cases}\widehat{f_0}(r) & \text{for } \phi\geq 4.3925\times10^{10}\left[\frac{\text{neutrons}}{\text{cm}^2\text{-sec}}\right]\\ \widehat{f_0}(r)\left(\frac{4.3925\times10^{10}}{\phi}\right)^{0.2595} & \text{for } \phi< 4.3925\times10^{10}\left[\frac{\text{neutrons}}{\text{cm}^2\text{-sec}}\right]\end{cases}$$

$\widehat{f_0}(r)_{eff}$ is bounded from above by $3\widehat{f_0}(r)\rightarrow\ \widehat{f_0}(r)_{eff}=\min\left[\widehat{f_0}(r)_{eff},\left(3\widehat{f_0}(r)\right)\right]$.

$$g\left(\widehat{Cu},\widehat{Ni},\widehat{f_0}(r)\right)=\frac{1}{2}+\frac{1}{2}\tanh\left[\frac{\log_{10}\left(\widehat{f_0}(r)_{eff}\right)+1.139\widehat{Cu}_{eff}-0.4483\widehat{Ni}-18.12025}{0.6287}\right]$$

$$f\left(\widehat{Cu},\widehat{P}\right)=\begin{cases}0 & \widehat{Cu}\leq 0.072\\ \left[\widehat{Cu}_{eff}-0.072\right]^{0.6679} & \text{for } \widehat{Cu}>0.072 \text{ and } \widehat{P}\leq 0.008\\ \left[\widehat{Cu}_{eff}-0.072+1.359(\widehat{P}\text{-}0.008)\right]^{0.6679} & \text{for } \widehat{Cu}>0.072 \text{ and } \widehat{P}>0.008\end{cases}$$

$$\text{where } \widehat{Cu}_{eff}=\begin{cases}0 & \text{for } \widehat{Cu}\leq 0.072 \text{ wt\%}\\ \widehat{Cu} & \text{for } \widehat{Cu}>0.072 \text{ wt\%}\end{cases};\quad\left\{\left[\begin{matrix}\text{subject to copper-saturation upper bound}\\ \widehat{Cu}_{eff}=\min\left(\widehat{Cu}_{eff},Cu_{\max}\right)\end{matrix}\right]\right\}$$

$$\text{with copper saturation defined by } Cu_{\max}\equiv\begin{cases}0.3700 \text{ wt\%} & \text{for } \widehat{\text{Ni}}<0.5 \text{ wt\%}\\ 0.2435 \text{ wt\%} & \text{for } 0.5\leq\widehat{\text{Ni}}\leq 0.75 \text{ wt\%}\\ 0.3010 \text{ wt\%} & \text{for } \widehat{\text{Ni}}>0.75 \text{ wt\%}\\ 0.3010 \text{ wt\%} & \text{all welds with L1092 flux}\end{cases}$$

11.3 Kirk 2007 Correlation Implemented in FAVOR, v07.1

$$\widehat{\Delta T}_{30}(\widehat{Ni},\widehat{Cu},\widehat{P},\widehat{f}_0(r),\tau_{\text{exposure}},T_c,\text{product form})[°\text{F}]=\widehat{\Delta T}_{30(MD)}+\widehat{\Delta T}_{30(CRP)}$$

where:

Matrix Damage

$$\widehat{\Delta T}_{30(MD)}=PF_{MD}\times\widehat{CF}_{MD}\times TF_{MD}\times\widehat{\phi F}_{MD}\times\widehat{f_0F}_{MD}$$

$$PF_{MD}=\begin{Bmatrix}6.70\ ; & \text{for welds}\\ 8.10\ ; & \text{for plates}\\ 4.75\ ; & \text{for forgings}\end{Bmatrix}\times 10^{-9}$$

$$\widehat{CF}_{MD}=\left[1+35\widehat{P}\right]$$

$$TF_{MD}=\left(\frac{T_c}{550}\right)^{-14.64}$$

$$\widehat{\phi F}_{MD}=\left(\frac{\log_{10}\left(\widehat{\phi}\right)}{10.7}\right)^{-3.44}$$

$$\widehat{f_0F}_{MD}=\sqrt{\widehat{f}_0(r)}$$

$$\text{neutron flux: }\phi=\frac{\widehat{f}_0(r)}{3600\ \tau_{\text{exposure}}}\left[\frac{\text{neutrons}}{\text{cm}^2\text{-sec}}\right]$$

Copper Rich Precipitation

$$\widehat{\Delta T}_{30(CRP)}=PF_{CRP}\times\widehat{CF}_{CRP}\times TF_{CRP}\times\widehat{f_0F}_{CRP}$$

$$PF_{CRP}=\begin{Bmatrix}0.301\ ; & \text{for welds}\\ 0.233\ ; & \text{for plates}\\ 0.233\ ; & \text{for forgings}\end{Bmatrix}$$

$$CF_{CRP}=f\left(\widehat{Cu}\right)_{eff}+2500.3\times\text{MIN}\left[0.32,\text{MAX}\left(0,\widehat{Cu}-0.048\right)\right]\times\widehat{Ni}$$

$$f\left(\widehat{Cu}\right)_{eff}=\begin{Bmatrix}0\ ; & \text{for } f\left(\widehat{Cu}\right)<0\\ f\left(\widehat{Cu}\right)\ ; & \text{for } 0\le f\left(\widehat{Cu}\right)\le 185\\ 118.5\ ; & \text{for } f\left(\widehat{Cu}\right)>185\end{Bmatrix}$$

$$\text{where } f\left(\widehat{Cu}\right)=-116.3+530.8\sqrt{\widehat{Cu}}$$

$$TF_{CRP} = \left(\frac{T_c}{550}\right)^{-1.74}$$

$$\widehat{f_0 F}_{CRP} = \left\{1 - \exp\left(\frac{-\widehat{f_0(r)}}{2.38\times 10^{18}}\right)\right\}$$

11.4 RADAMO Correlation [Implemented in FAVOR, v07.1

$$\widehat{\Delta T}_{30}(\widehat{Ni}, \widehat{Cu}, \widehat{P}, \widehat{f}_0(r), \tau_{\text{exposure}}, T_c, \text{product form})[°\text{F}] = \begin{Bmatrix} 1.39\ ; & \text{for welds} \\ 1.18\ ; & \text{for plates} \\ 0.84\ ; & \text{for forgings} \end{Bmatrix} \times \Delta\widehat{YS}$$

where;

$$\Delta\widehat{YS}\ [\text{MPa}] = \Delta\widehat{YS}_{(MD)} + \sqrt{\Delta\widehat{YS}^2_{(CRP)} + \Delta\widehat{YS}^2_{(PRP)}}$$

Matrix Damage

$$\Delta\widehat{YS}_{(MD)} = \begin{Bmatrix} 0\ ; & \text{for } f_0(r) \le 10^{19}\ \text{n/cm}^2 \\ \left\{ \begin{matrix} 585\exp\left[-1250\exp\left(\frac{-0.345}{kT_{c(K)}}\right)\right] + \\ \left(3880 - 6.3T_{c(K)}\right)\widehat{Ni} \end{matrix} \right\} \times \sqrt{1 - \exp\left[-0.01\left(\frac{\widehat{f}_0(r)}{10^{19}} - 1\right)\right]}; & \text{for } f_0(r) > 10^{19}\ \text{n/cm}^2 \end{Bmatrix}$$

$$T_{c(K)} = \frac{(T_c - 32)}{1.8} + 273\ \ [\text{K}]$$

Copper Rich Precipitation

$$\Delta\widehat{YS}_{(CRP)} = \widehat{\Delta}_{CRP(PEAK)} \times f\left(\widehat{\phi}, \tau_{\text{exposure}}, T_c, \widehat{Cu}\right)$$

$$\widehat{\Delta}_{CRP(PEAK)} = \begin{Bmatrix} 0\ ; & \text{for } \widehat{Cu} \le Cu_{\min} \\ 215\left\{1 - \exp\left[-2.7\left(\widehat{Cu} - Cu_{\min}\right)\right]\right\}\ ; & \text{for } \widehat{Cu} > Cu_{\min} \end{Bmatrix}$$

$$f\left(\widehat{\phi},\tau_{\text{exposure}},T_c,\widehat{Cu}\right)=\begin{Bmatrix} 0\ ; & \text{for } \tau_{\text{exposure(EFPY)}}<\left(\tau_{peak}/20\right) \\ \dfrac{\ln\left(20\times\tau_{\text{exposure(EFPY)}}/\tau_{peak}\right)}{\ln(20)}\ ; & \text{for } \left(\tau_{peak}/20\right)\le\tau_{\text{exposure(EFPY)}}<\tau_{peak} \\ 1\ ; & \text{for } \tau_{\text{exposure(EFPY)}}\ge\tau_{peak} \end{Bmatrix}$$

$$\widehat{\tau}_{peak}=\frac{10^{\left[\frac{10684}{T_{c(K)}}-\left(15.3-\frac{0.3}{\widehat{Cu}}\right)\right]}}{1+\dfrac{\widehat{\phi}\times10^{-32}}{\exp\left(-\dfrac{\widehat{E}}{kT_{c(K)}}\right)}}$$

$$\widehat{E}=\begin{Bmatrix} \widehat{E_0}\ ; & \text{for } \widehat{\phi}<\phi_{LIM} \\ \widehat{E_0}-0.03\ln\left(\dfrac{\widehat{\phi}}{\phi_{LIM}}\right); & \text{for } \widehat{\phi}\ge\phi_{LIM} \end{Bmatrix}$$

$$\widehat{E_0}=-kT_{c(K)}\ln\left\{\frac{\phi_{LIM}\times10^{-32}}{\dfrac{10^{\left[\frac{10684}{T_{c(K)}}-\left(15.3-\frac{0.3}{\widehat{Cu}}\right)\right]}}{\tau_{peak}^{Cu_{\max}}}-1}\right\}$$

$$\tau_{peak}^{Cu_{\max}}=\frac{10^{\left[\frac{10684}{T_{c(K)}}-\left(15.3-\frac{0.3}{Cu_{\max}}\right)\right]}}{1+\dfrac{\phi_{LIM}\times10^{-32}}{\exp\left(\dfrac{-2.8}{kT_{c(K)}}\right)}}$$

$$Cu_{\min}=0.03\text{ wt\%};\ \ Cu_{\max}=0.425\text{ wt\%};\ \ \phi_{LIM}=6\times10^{12}\ \left[\text{n/cm}^2/\text{sec}\right];\ k=8.617\times10^{-5}\ [\text{eV/K}]$$

$$\text{neutron flux: }\phi=\frac{\widehat{f_0}(r)}{3600\tau_{\text{exposure}}}\left[\frac{\text{neutrons}}{\text{cm}^2-\text{sec}}\right];\ \ T_{c(K)}=\frac{T_c-32}{1.8}+273\ \ [\text{K}]$$

Phosphorous Rich Precipitation

$$\Delta\widehat{YS}_{(PRP)} = \left\{ \begin{array}{lr} 0\ ; & \text{for } \widehat{P} \le 0.012 \\ \min\left[\max\left(\dfrac{\log_{10}\left(\widehat{f}_0(r)\right)-16}{3},0\right),1\right]\left(44470.5-70T_{c(K)}\right)\left(\widehat{P}-0.012\right)\ ; & \text{for } \widehat{P} > 0.012 \end{array} \right\}$$

11.5 Kirk 2007 + RADAMO Correlation Implemented in FAVOR, v07.1

$$\widehat{\Delta T}_{30}(\widehat{Ni}, \widehat{Cu}, \widehat{P}, \widehat{f}_0(r), \tau_{\text{exposure}}, T_c, \text{product form})[°\text{F}] = \left(1 - \widehat{W}\right)\widehat{\Delta T}_{30}^{LOW} + \widehat{W}\,\widehat{\Delta T}_{30}^{HIGH}$$

where:

$$\widehat{W} = \begin{cases} 0\ ; & \text{for } \widehat{f}_0(r) \le 2\times10^{19}\ \text{n/cm}^2 \\ \dfrac{1}{2}\left(\dfrac{\widehat{f}_0(r)}{10^{19}} - 2\right)\ ; & \text{for } 2\times10^{19} < \widehat{f}_0(r) \le 4\times10^{19}\ \text{n/cm}^2 \\ 1\ ; & \text{for } \widehat{f}_0(r) > 4\times10^{19}\ \text{n/cm}^2 \end{cases}$$

for low fluences

$$\widehat{\Delta T}_{30}^{LOW} = \widehat{\Delta T}_{30(MD)} + \widehat{\Delta T}_{30(CRP)}$$

Matrix Damage

$$\widehat{\Delta T}_{30(MD)} = PF_{MD} \times \widehat{CF}_{MD} \times TF_{MD} \times \widehat{\phi F}_{MD} \times \widehat{f_0 F}_{MD}$$

$$PF_{MD} = \begin{cases} 6.70\ ; & \text{for welds} \\ 8.10\ ; & \text{for plates} \\ 4.75\ ; & \text{for forgings} \end{cases} \times 10^{-9}$$

$$\widehat{CF}_{MD} = \left[1 + 35 \cdot \widehat{P}\right]$$

$$TF_{MD} = \left(\frac{T_c}{550}\right)^{-14.64}$$

$$\widehat{\phi F}_{MD} = \left(\frac{\log_{10}\left(\widehat{\phi}\right)}{10.7}\right)^{-3.44}$$

$$\widehat{f_0 F}_{MD} = \sqrt{\widehat{f}_0(r)}$$

$$\text{neutron flux: } \phi = \frac{\widehat{f}_0(r)}{3600\ \tau_{\text{exposure}}}\left[\frac{\text{neutrons}}{\text{cm}^2\text{-sec}}\right]$$

Copper Rich Precipitation

$$\widehat{\Delta T}_{30(CRP)} = PF_{CRP} \times \widehat{CF}_{CRP} \times TF_{CRP} \times \widehat{f_0 F}_{CRP}$$

$$PF_{CRP} = \begin{Bmatrix} 0.301\ ; & \text{for welds} \\ 0.233\ ; & \text{for plates} \\ 0.233\ ; & \text{for forgings} \end{Bmatrix}$$

$$CF_{CRP} = f\left(\widehat{Cu}\right)_{eff} + 2500.3 \times \text{MIN}\left[0.32, \text{MAX}\left(0, \widehat{Cu} - 0.048\right)\right] \times \widehat{Ni}$$

$$f\left(\widehat{Cu}\right)_{eff} = \begin{Bmatrix} 0\ ; & \text{for } f\left(\widehat{Cu}\right) < 0 \\ f\left(\widehat{Cu}\right)\ ; & \text{for } 0 \le f\left(\widehat{Cu}\right) \le 185 \\ 118.5\ ; & \text{for } f\left(\widehat{Cu}\right) > 185 \end{Bmatrix}$$

$$\text{where } f\left(\widehat{Cu}\right) = -116.3 + 530.8\sqrt{\widehat{Cu}}$$

$$TF_{CRP} = \left(\frac{T_c}{550}\right)^{-1.74}$$

$$\widehat{f_0 F}_{CRP} = \left\{1 - \exp\left(\frac{-\widehat{f_0(r)}}{2.38 \times 10^{18}}\right)\right\}$$

for high fluences

$$\widehat{\Delta T}_{30}^{HIGH} = \begin{Bmatrix} 1.39\ ; & \text{for welds} \\ 1.18\ ; & \text{for plates} \\ 0.84\ ; & \text{for forgings} \end{Bmatrix} \times \Delta\widehat{YS}$$

where

$$\Delta\widehat{YS}\ [\text{MPa}] = \Delta\widehat{YS}_{(MD)} + \sqrt{\Delta\widehat{YS}^2_{(CRP)} + \Delta\widehat{YS}^2_{(PRP)}}$$

Matrix Damage

$$\Delta\widehat{YS}_{(MD)} = \left\{ \begin{array}{ll} 0\ ; & \text{for } f_0(r) \le 10^{19}\ \text{n/cm}^2 \\ \left\{ \begin{array}{c} 585\exp\left[-1250\exp\left(\dfrac{-0.345}{kT_{c(K)}}\right)\right] + \\ \left(3880 - 6.3T_{c(K)}\right)\widehat{Ni} \end{array} \right\} \times \sqrt{1 - \exp\left[-0.01\left(\dfrac{\widehat{f_0}(r)}{10^{19}} - 1\right)\right]}; & \text{for } f_0(r) > 10^{19}\ \text{n/cm}^2 \end{array} \right\}$$

$$T_{c(K)} = \frac{(T_c - 32)}{1.8} + 273 \ \ [\mathrm{K}]$$

Copper Rich Precipitation

$$\Delta \widehat{YS}_{(CRP)} = \widehat{\Delta}_{CRP(PEAK)} \times f\left(\widehat{\phi}, \tau_{\text{exposure}}, T_c, \widehat{Cu}\right)$$

$$\widehat{\Delta}_{CRP(PEAK)} = \begin{Bmatrix} 0\ ; & \text{for } \widehat{Cu} \le Cu_{\min} \\ 215\left\{1 - \exp\left[-2.7\left(\widehat{Cu} - Cu_{\min}\right)\right]\right\}\ ; & \text{for } \widehat{Cu} > Cu_{\min} \end{Bmatrix}$$

$$f\left(\widehat{\phi}, \tau_{\text{exposure}}, T_c, \widehat{Cu}\right) = \begin{Bmatrix} 0\ ; & \text{for } \tau_{\text{exposure(EFPY)}} < \left(\tau_{peak}/20\right) \\ \dfrac{\ln\left(20 \times \tau_{\text{exposure(EFPY)}} / \tau_{peak}\right)}{\ln(20)}\ ; & \text{for } \left(\tau_{peak}/20\right) \le \tau_{\text{exposure(EFPY)}} < \tau_{peak} \\ 1\ ; & \text{for } \tau_{\text{exposure(EFPY)}} \ge \tau_{peak} \end{Bmatrix}$$

$$\widehat{\tau}_{peak} = \frac{10^{\left[\frac{10684}{T_{c(K)}} - \left(15.3 - \frac{0.3}{\widehat{Cu}}\right)\right]}}{1 + \dfrac{\widehat{\phi} \times 10^{-32}}{\exp\left(-\dfrac{\widehat{E}}{kT_{c(K)}}\right)}} \qquad \widehat{E} = \begin{Bmatrix} \widehat{E}_0\ ; & \text{for } \widehat{\phi} < \phi_{LIM} \\ \widehat{E}_0 - 0.03\ln\left(\dfrac{\widehat{\phi}}{\phi_{LIM}}\right)\ ; & \text{for } \widehat{\phi} \ge \phi_{LIM} \end{Bmatrix}$$

$$\widehat{E}_0 = -kT_{c(K)} \ln\left\{\frac{\phi_{LIM} \times 10^{-32}}{\dfrac{10^{\left[\frac{10684}{T_{c(K)}} - \left(15.3 - \frac{0.3}{\widehat{Cu}}\right)\right]}}{\tau_{peak}^{Cu_{\max}}} - 1}\right\}$$

$$\tau_{peak}^{Cu_{\max}} = \frac{10^{\left[\frac{10684}{T_{c(K)}} - \left(15.3 - \frac{0.3}{Cu_{\max}}\right)\right]}}{1 + \dfrac{\phi_{LIM} \times 10^{-32}}{\exp\left(\dfrac{-2.8}{kT_{c(K)}}\right)}}$$

$$Cu_{\min} = 0.03 \text{ wt\%};\ Cu_{\max} = 0.425 \text{ wt\%};\ \phi_{LIM} = 6\times10^{12}\ \left[\text{n/cm}^2/\text{sec}\right];\ k = 8.617\times10^{-5}\ [\text{eV/K}]$$

$$\text{neutron flux: } \phi = \frac{\widehat{f_0}(r)}{3600\tau_{\text{exposure}}}\left[\frac{\text{neutrons}}{\text{cm}^2-\text{sec}}\right];\ T_{c(K)} = \frac{T_c - 32}{1.8} + 273\ \ [\text{K}]$$

<u>**Phosphorous Rich Precipitation**</u>

$$\Delta\widehat{YS}_{(PRP)} = \begin{cases} 0\ ; & \text{for } \widehat{P} \le 0.012 \\ \min\left[\max\left(\dfrac{\log_{10}\left(\widehat{f_0}(r)\right)-16}{3},0\right),1\right]\left(44470.5-70T_{c(K)}\right)\left(\widehat{P}-0.012\right)\ ; & \text{for } \widehat{P} > 0.012 \end{cases}$$

where in all of the above correlations $\widehat{Cu}$ is the sampled copper content in wt%, $\widehat{Ni}$ is the sampled nickel content in wt%, $\widehat{P}$ is the sampled phosphorous content in wt%, $\widehat{Mn}$ is the sampled manganese content in wt%, $\hat{f}_0(r)$ is the sampled and then attenuated neutron fluence in neutrons/cm^2, *r* is the position from the inner surface of RPV wall, $\tau_{\text{exposure}(EFPY)}$ is the exposure time in effective-full-power-years (EFPY), τ_{exposure} is the exposure time in hours (calculated from $\tau_{\text{exposure}(EFPY)}$), and T_c is coolant temperature in $°F$. The fast-neutron fluence at the inner surface of the vessel, $f_0(0)$, is sampled. The sampled neutron fluence for the flaw is then attenuated (but not resampled) as the crack grows through the wall.

The uncertainty in the sampled CVN transition shift values, $\widehat{\Delta T}_{30}$, is treated as *epistemic*. Having used information concerning composition and irradiation conditions to estimate the CVN transition temperature shift, it is necessary to transform these $\widehat{\Delta T}_{30}$ values into shifts in the fracture-toughness transition temperature. Figure 21 provides an empirical basis for the following least-squares fits for $\widehat{\Delta RT}_{NDT}$ using data extracted from the literature.

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

One additional model in FAVPFM includes 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/cm^2; $E > 1$ MeV] attenuated from the inner surface to the clad/base metal interface

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

Note that the $\widehat{\Delta RT}_{NDT}$ based on 10CFR50.61 is not corrected by 0.99 or 1.10.

Following the modularization effort, these correlations have been consolidated into module radiation_shift_m and submodule(radiation_shift_m) and supporting modules trend_curve_m and submodule(trend_curve_m), except for subroutine EWO1998.

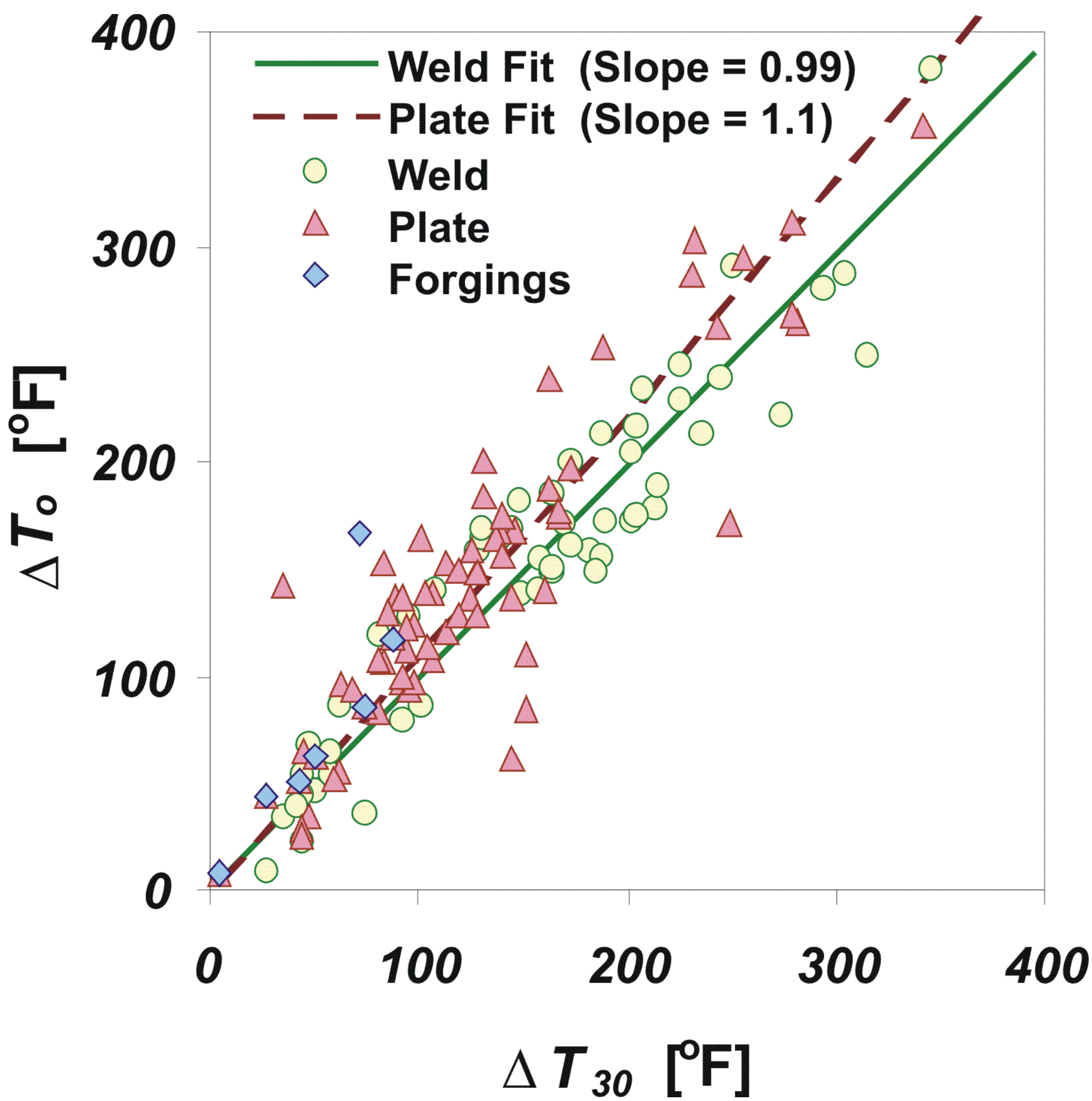

Figure 21: Relationship between the change in the fracture-toughness index temperature ($\Delta T_0 \approx \Delta RT_{NDT}$) change in the 30 ft-lbf CVN transition temperature (ΔT_{30}) for welds and plates/forgings produced by irradiation. The difference in the best-fit slopes is statistically significant.

Design 12 For probabilistic fracture analyses, the determination of conditional probability of crack initiation, CPI, is calculated as follows:

$CPI_{(i,j,k)} = \left\| \{cpi(\tau^m)\}_{(i,j,k)} \right\|_\infty$ for $1 \leq m \leq n$, 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 is assumed to occur such that the conditional probablity of CPI is evaluated. For combining multiple flaws, the CPI for the i[th] transient and j[th] RPV trial is calculated as:

$$CPI_{RPV(i,j)} = 1 - \prod_{k=1}^{nflaw} (1 - CPI_{(i,j,k)})$$
$$= 1 - \left[\left(1 - CPI_{(i,j,1)}\right)(1 - CPI_{(i,j,2)}) \ldots (1 - CPI_{(i,j,nflaw)}) \right]$$

Subroutine PFM contains the logic using the above equations to calculate CPI for each RPV trial.

Design 13 For the VFLAW based flaw input, a flaw propagation model uses the following assumptions for initial flaw orientation:

Table 16: 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*

Where:

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 $\frac{3}{8}t$, and

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

The above orientations (Table 16) are set in Module Procedure FLAW within modules flaw_m and submodule flaw_s. The assignment is done through the variable iflaw.

Values of iflaw values from 1 to 8 are for regions for which the load does not include through-wall weld residual stress, i.e., plate or forged regions.

For internal surface axially oriented flaws, iflaw=1 through iflaw=4 (**NOT USED DOWNSTREAM**),

- iflaw=1 ==> axial orientation, aspect ratio=99 (infinite length)
- iflaw=2 ==> axial orientation, aspect ratio=2
- iflaw=3 ==> axial orientation, aspect ratio=6
- iflaw=4 ==> axial orientation, aspect ratio=10

For internal surface circumferentially oriented flaws,

- iflaw=5 ==> circum. orientation, aspect ratio=99 (continuous)
- iflaw=6 ==> circum. orientation, aspect ratio=2
- iflaw=7 ==> circum. orientation, aspect ratio=6
- iflaw=8 ==> circum. orientation, aspect ratio=10

iflaw 9 through 16 are applied to regions for which the load does include through-wall weld residual stress, i.e., weld regions.

For internal axially oriented flaws, iflaw=9 through iflaw=12 (**NOT USED DOWNSTREAM**),

- iflaw=9 ==> axial orientation, aspect ratio=99 (infinite length)
- iflaw=10 ==> axial orientation, aspect ratio=2
- iflaw=11 ==> axial orientation, aspect ratio=6
- iflaw=12 ==> axial orientation, aspect ratio=10

For internal circumferentially oriented flaws,

- iflaw=13 ==> circum. orientation, aspect ratio=99 (continuous)
- iflaw=14 ==> circum. orientation, aspect ratio=2
- iflaw=15 ==> circum. orientation, aspect ratio=6
- iflaw=16 ==> circum. orientation, aspect ratio=10

Values of iflaw values from 17 to 24 are for regions for which the load does include through-wall weld residual stress, i.e., weld.

For external surface axially oriented flaws,

- iflaw=17 ==> axial orientation, aspect ratio=99 (infinite length)
- iflaw=18 ==> axial orientation, aspect ratio=2
- iflaw=19 ==> axial orientation, aspect ratio=6
- iflaw=20 ==> axial orientation, aspect ratio=10

For external surface circumferentially oriented flaws,

- iflaw=21 ==> circum. orientation, aspect ratio=99 (continuous)
- iflaw=22 ==> circum. orientation, aspect ratio=2

- iflaw=23 ==> circum. orientation, aspect ratio=6
- iflaw=24 ==> circum. orientation, aspect ratio=10

iflaw 25 through 32 are applied to regions for which the load does not include through-wall weld residual stress, i.e., plate or forged regions.

For external axially oriented flaws,

- iflaw=25 ==> axial orientation, aspect ratio=99 (infinite length)
- iflaw=26 ==> axial orientation, aspect ratio=2
- iflaw=27 ==> axial orientation, aspect ratio=6
- iflaw=28 ==> axial orientation, aspect ratio=10

For external circumferentially oriented flaws,

- iflaw=29 ==> circum. orientation, aspect ratio=99 (continuous)
- iflaw=30 ==> circum. orientation, aspect ratio=2
- iflaw=31 ==> circum. orientation, aspect ratio=6
- iflaw=32 ==> circum. orientation, aspect ratio=10

iflaw is used in subroutine pfm to assign appropriate K_I for internal and external surface breaking flaws using the SELECT CASE construct and assigning the appropriate FAVLoad calculated K_I arrays .

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. For VFLAW based flaw input, all internal surface breaking flaws are assumed to be circumferentially oriented and thus become 360° circumferential flaws when crack initiation in cleavage fracture occurs. Whereas, 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.

Any external surface-breaking flaws or embedded flaws in the outer half of the RPV wall are assumed to propagate through the entire wall thickness causing RPV failure upon initiating in cleavage fracture.

Regarding the as-found flaw approach, K_I follows a different method than the VFLAW Case assignments. Within the main FAVPFM program, subroutine calls to AMNKSE , AMNK99, or KEMB are done to calculate K_I (variable akflaw), depending on the type of user specified flaw. If the flaw is a semi-elliptical internal surface breaking flaw, subroutine AMNKSE calculates the appropriate $K_I(t)$ - depending on the flaw's orientation, material (weld or plate) and aspect ratio. For flaws that are an infinite internal surface breaking flaw, subroutine AMNK99 calculates the appropriate $K_I(t)$ – depending on orientation and material (weld or plate). For flaws that are embedded, subroutine KEMB calculates the appropriate $K_I(t)$ – depending on orientation, material (weld or plate), and aspect ratio. It should be noted that the current version treats all aspect ratios as integers.

Following crack initiation, flaw geometries are set as follows:

Table 17: Post-Initiation Flaw Geometries and Orientations

FLAW TYPE & GEOMETRY	LOCATION	ORIENTATION	AFTER INITIATION
surface-breaking (semi-elliptical)	RPV internal surface	*circumferential*	360^0 internal surface breaking flaw
surface-breaking (semi-elliptical)	RPV external surface	*axial*	failure of RPV
		circumferential	failure of RPV
embedded flaw (elliptical)	crack tip between (0 – λ.t) where: λ = 3/8 for flaw population 1; λ = ½ for flaw population 3	*axial*	surface-breaking infinite length flaw with nearly same depth as original crack-tip
		circumferential	surface-breaking 360º flaw with nearly same depth as original crack-tip
embedded flaw (elliptical)	crack tip between (λ.t – t) where: λ = 5/8 for flaw population 2 λ = ½ for flaw population 3	*axial*	failure of RPV
		circumferential	failure of RPV

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

- The fraction of flaws that would fail the RPV are determined (at each time step for each flaw) by performing a Monte Carlo analysis of through-wall propagation of the infinite-length flaw. See Design 9.
- This propagation sub model as described in the previous design descriptions have 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 is determined using a random number drawn from a uniform distribution on the open interval (0,1).
- The nested-loop structure precludes the introduction of a bias in the results regardless of how the transients are ordered by the user. 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 is 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 is drawn from sets of random number sequences created in the second sampling block (e.g., get_grab_bag function and the use of the grab_bag array of saved random numbers used in snorm2a). These set-aside random number sequences (i.e., grab_bag array) 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.

- In each analysis, the infinite-length flaw is incrementally propagated through the RPV wall until it either fails the RPV or experiences a stable arrest.
- For the given flaw, subjected to the current transient, the change in cpi with respect to time is checked and if $\mathrm{dcpi}/\mathrm{dt} > 0$, then the flaw becomes a candidate for propagation through the wall.
- Any flaw that is propagated is assumed that the propagation occurs instantaneously; i.e., the time station remains fixed during flaw growth. Time only advances if the flaw is in a state of arrest.
- In each propagation, a K_{Ia} curve is sampled from the lognormal K_{Ia} distribution by using the P_f sampled value as the sampled percentile.
- The applied K_I for the growing infinite-length flaw is 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 advances by another small fixed increment, and again a check is made for arrest. If the crack does arrest ($K_I \leq K_{Ia}$), the simulation continues 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) is determined based on 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.

Design 9, provides the detailed FAVOR flowcharts describing the Monte Carlo looping and flaw propagation that incorporates the software design elements in Design 12. Subroutines and modules are also presented in that section.

Design 14 When the ductile-tearing model is used, values of CPI produced by FAVOR are unaffected. Counters are used to determine if ductile tearing maybe a potential issue for crack initiation.

Design of subroutine PFM precludes the impact of ductile tearing on conditional probability of crack initiation. Logic, as laid out in subroutine Prop and calls to subroutine ductile_tearing (see flowcharts in Design 9 for further details), shows that ductile tearing is only applied in crack propagation. The major result from the subroutine call to ductile_tearing is whether flaw propagation is stable ductile tearing or not and if vessel failure occurs whether ductile tearing was stable or unstable. This is done through logical statements using the following variables:

- FAIL_UDT = .TRUE. or .FALSE.
- STABLE_DT = .TRUE. or .FALSE.

With respect to the counters, ductile tearing is checked in subroutine PFM through the following FORTRAN logic:

```
if (CHECK_DUCTILE_INI) then
  IF (AKSLOPE.GT.ZERO) THEN
    IF ( ITYPE .EQ.  0 ) THEN
      SFLOW   =  FLWSTR + 0.112d0*DT30
    ELSE
      SFLOW   =  FLWSTR + 0.131d0*DT30
```

```
    ENDIF
    P_T0   = p_rtepi
    P_JIc = PFTHWL(1,1,3)
    P_m   = PFTHWL(1,1,4)
    JIc       = get_JIc(sflow,P_T0,P_JIc,P_m, &
                  TEMP(L,ITRAN,NTSTEP),C_DT,m_DT,Emod_ksi)
    Japplied = ((one-Nu**2)/Emod)*(AKICHEK**2)
    if ((Japplied.GT.JIc).AND.(TEMP(L,ITRAN,NTSTEP).GE.T_DT)) &
         then
      IF (ITEST.EQ.1) THEN
        NUM_INI_DT(ITRAN,2) = NUM_INI_DT(ITRAN,2) + ONE
      ELSE
        NUM_INI_DT(ITRAN,3) = NUM_INI_DT(ITRAN,3) + ONE
      ENDIF
    ENDIF
  ENDIF
ENDIF
```

The counter NUM_INI_DT is used to count the number of ductile tearing events but not used in determining CPI.

Design 15 For probabilistic fracture analyses, the determination of conditional probability of vessel failure, CPF, is performed as follows:

First the $\Delta cpi(\tau^n)$, which is the incremental change in instantaneous conditional probability of initiation between timesteps, is calculated based on Design 12 for all vessels, transients, and flaws;

The P(F|I) is based on the number of flaws that propagated through the wall thickness divided by the total number of initiated flaws.

$$cpf(\tau^n) = \sum_{m=1}^{n_{max}} P(F|I) \times \Delta cpi(\tau^m)$$

$$= \sum_{m=1}^{n_{max}} \Delta cpf(\tau^m)$$

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(τ) occurred; and

The sup-norm of the vector $\{cpf(\tau^n)\}$, CPF, occurs at the same time step as the CPI.

Similar to CPI, the modeled thermal-hydraulic transients are assumed to occur such that the conditional probablity of CPF is evaluated. In addition, CPF is calculated over many flaws as CPI is done.

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

The above calculations and summations are done in subroutine PFM after supporting calls to subroutine Prop, ductile_tearing, and Account. The FAVPFM flowcharts and logic are shown in Figure 13, Figure 15, and Figure 17, along with Table 13, Table 14, and Table 15.

Design 16 Output files are created based on values of conditional 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.

Following the calculation of PFMI(i,j) and PFMF(i,j) in subroutine PFM (based on Design 12 and Design 15), calls are made to subroutines OUTCPI and OUTCPF to write out the values of conditional of crack initiation (i.e., PFMI(i,j)), and the values of the conditional probability of vessel failure (i.e., PFMF(i,j)) for each modeled transient for each vessel simulation, respectively. These output files are "initiate.dat" (Fortran Unit 86) and "failure.dat" (Fortran Unit 87). These files are used as input to FAVPost in order to generate discrete distributions of crack initiation frequency per reactor operating year.

Design 17 User input of the distribution of transient initiating frequencies (typically obtained from Probabilistic Risk Analyses) is combined with conditional probability of crack initiation from Design 16 to generate discrete distributions of crack initiation frequency per reactor operating year, F*I*, and

Design 18 User input of the distributions of transient initiating frequencies (typically obtained Risk Analyses) are combined with values of the conditional probability of vessel failure from Design 16 to generate discrete distributions of through-wall crack (i.e., vessel failure) per reactor operating year, FF, similar to FI.

Design 17 and Design 18 are handled within FAVPost, which is the post-processor program module in the FAVOR package. Since these design descriptions are handled similarly by FAVPost logic, they are being described together. As these descriptions are the first that are related to FAVPost, an overview is presented in the following paragraphs.

18.1 FAVPost Overview

The inputs to the FAVPOST program are: (1) user input transient initiating frequency distributions in the form of probability density functions, which are typically obtained from probabilistic risk analysis (e.g., those from SAPHHIRE), and (2) the FAVPFM generated matrices of conditional probability of fracture (PFMI) and conditional probability of RPV failure (PFMF). The PFMI and PFMF arrays are previously discussed in Design 16. Following the input processing, FAVPost then combines the distributions of conditional probabilities of initiation (PFMI) and failure (PFMF) with initiating frequency distributions for all of the transients under study to create discrete distributions of the frequency of vessel initiation, $\Phi(I)$, and frequency of vessel failure, $\Phi(F)$. This process is described by the following *pseudo code*:

In order for FAVPost to perform the computational and statistical analysis to determine FCI and TWCF, FAVPost first requires user input and preparation of data arrays in a format compatible with ordered statistics.

For j = 1, N_{SIM} vessel simulations run in FAVPFM, increment by 1

For i = 1, N_{TRAN} transients, increment by 1

Sample the discrete cumulative distribution function of the transient initiating frequency for this transient to generate a sample initiating frequency (in events per reactor year).

$\widehat{\emptyset(E)}_{(i)} \leftarrow CDF_{(i,j)}$ of transient-I initiating frequency

End of Transient Loop

The above loop generates a vector of transient-initiating frequencies for this vessel simulation, $\{\widehat{\emptyset(E)}\}_{(1xN_{TRAN})}$ That is, (Φ_1, Φ_2, Φ_3 ……… Φ_{MTRAN})

For the jth vessel, take the dot-product of the transient initiating frequencies vector times the jth column-vectors in the $PFMI$ and $PFMF$ matrices.

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

That is, FAVPost variable array FRQPIE (vessel) = Φ_1 x CPI(vessel, 1) + Φ_2 x CPI(vessel, 2) + ... + Φ_{MTRAN} x CPI(vessel, MTRAN)

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

That is, FAVPost variable array FRQPFE (vessel) = Φ_1 x CPF (vessel, 1) + Φ_2 x CPF(vessel, 2) + ……..+ Φ_{MTRAN} x CPF(vessel, MTRAN)

End of Vessel Simulation Loop

Folllowing the vessel simulation loop, FAVPost then transforms the array FRQPIE (NSIM) to a probability distribution function (PDF) and reports descriptive statistics for this PDF (this is frequency of crack initiation - FCI). Simarly, for vessel failure, FAVPost transforms the array FRQPFE(NSIM) to a probability distribution function (PDF) and reports descriptive statistics for this PDF (this is thru-wall crack frequency – TWCF).

As showed by the above pseudo code, the dot-product of the row-vector of the sampled transient initiating frequencies and the j^{th} column vector of PFMI produces the frequency of crack initiation for the j^{th} vessel simulation, $\Phi(I)_{(j)}$. Likewise, the dot-product of the row-vector of sampled transient initiating frequencies and the j^{th} column-vector of PFMF results in the frequency of vessel failure for the j^{th} vessel simulation, $\Phi(F)_{(j)}$. The (i, j) entry in matrix PFMI represents the conditional probability of crack initiation of the j^{th} vessel simulation subjected to the i^{th} transient. The units are *crack initiations per event*. Therefore, the frequency of crack initiation, as determined from the dot-product of the transient initiating frequency and the conditional probability of crack initiation, is the number of *crack initiations per reactor year*. Likewise, the frequency of vessel failure, as determined from the dot-product of the transient-initiating frequency and the conditional probability of vessel failure is the number of vessel *failures per reactor year*.

At the end of this process, there are discrete distributions of sample size N_{SIM} for the frequency of crack initiation, $\{\Phi(I)\}_{(\text{Nsim } x\ 1)}$, and the frequency of vessel failure, , $\{\Phi(F)\}_{(\text{Nsim } x\ 1)}$. The above process is illustrated in Figure 22.

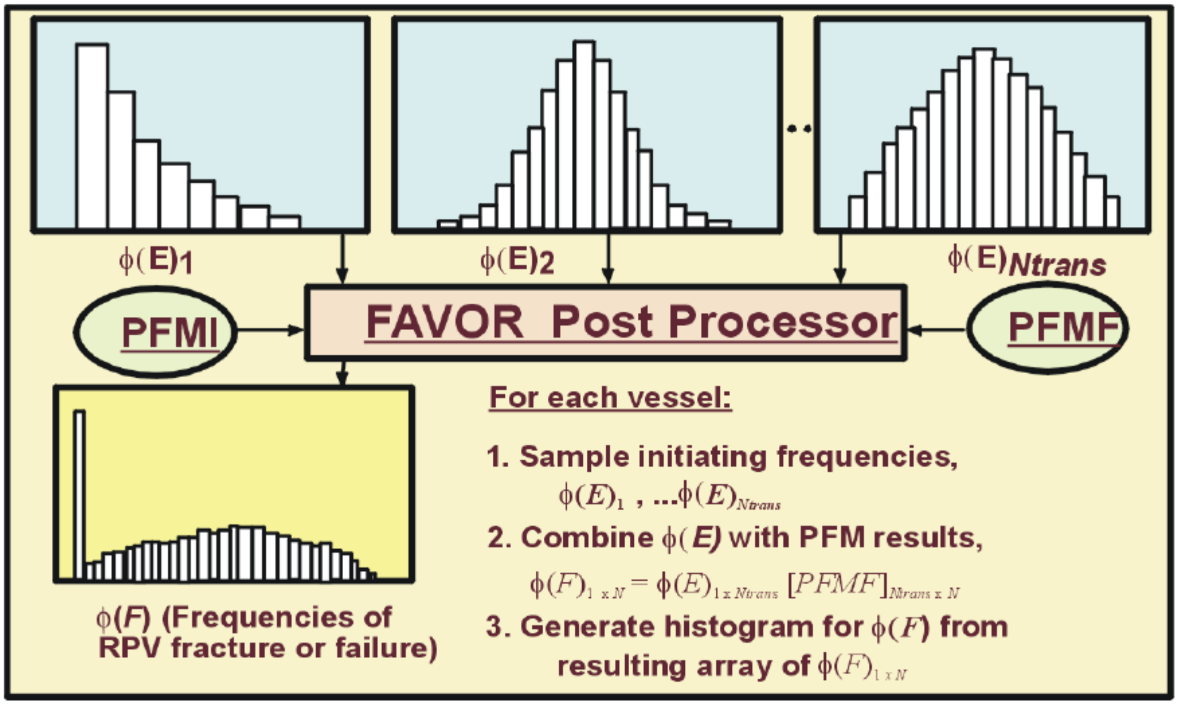

Figure 22: FAVPost Calculation of RPV Fracture and Failure Frequency Distributions

18.2 High-Level Overview of Main Computational Part of FAVPOST source code

This primary computational function of FAVPost in Figure 22 is performed in subroutine GENFRQ. The following general coding logic is used:

SUBROUTINE GENFRQ:

For each vessel (NVESS = 1 to NSIM) – Handled by Do Loop 2005

For each transient ITRAN = 1, MTRAN - Handled by Do Loop 2006

Sample an initiating frequency for each transient ITRAN and store in array SFRQI {ITRAN}:

Handled by Do Loop 2007 (also see Figure 23 below - how transient frequency is sampled)

Multiply the sampled frequency for each transient by the conditional probability of initiation PFMI of this vessel when it is subjected to this transient and the conditional probability of failure PFMF of this vessel when it is subjected to this transient, respectively.

do 2008 I = 1, MTRAN

CONTI (I) = SFRQI(I) * PFMI(I)

CONTF(I) = SFRQI(I) * PFMF(I)

FSUMI = FSUMI + PFMI(I)

FSUMF = FSUMF + PFMF(I)

Additional bookkeeping necessary to generate specific reports fractionalization (allocation) requested by USNRC staff:

Fractionalization of FCI by material (weld or plate)

Fractionalization of FCI by flaw category (1, 2, or 3)

Fractionalization of TWCF by material (weld or plate)

Fractionalization of TWCF by flaw category (1, 2, or 3)

Fractionalization of FCI by RPV major beltline region

Fractionalization of TWCF by RPV major beltline region

2008 Continue (end of transients)

FRQPIE(NVESS) = FSUMI

FRQPFE(NVESS) = FSUMF

2005 Continue (end of vessels)

END GENFRQ

After calling GENFRQ, the main program executes the following call sequence prior to ending the run:

- CALL POSTCPI – generates and outputs (to PDFCPI.out) PDF and descriptive statistics for CPI for each transient
- CALL POSTCPF – generates and outputs (to PDFCPF.out) PDF and descriptive statistics for CPF for each transient
- CALL POSTINIT – generates and outputs (to user-named FAVPOST output file) PDF and descriptive statistics for FRQPIE – frequency of crack initiations (cracked vessels per operating year)
- CALL POSTFAIL – generates and outputs (to user-named FAVPOST output file) PDF and descriptive statistics for FRQPFE – thru-wall crack frequency (failed vessels per operating year)
- CALL POSTSTAT – generates and outputs fractionalization (allocation) reports requested by the USNRC

18.3 Details of the above important called FAVPost subroutines follow:

SUBROUTINE RDPRA - prepares user-named FAVPOST input file to numeric file f83 to be read by SUBROUTINE PRA

- Strips FAVPOST user-named input file (F85) of all comment cards that contain * in column 1
- Writes the results to file 84
- Rewinds file 84

- Call subroutine STRIP which strips F84 it of all non-numeric data
- Writes the all-numeric file to file F83 (will be read by SUBROUTINE PRA)

SUBROUTINE PRA – reads file F83 which contains the numerical PDFs for transient initiating frequencies and generates a cumulative distribution function CDF for each transient such that it can be sampled

```
DO 10 I=1,MTRAN ! j = loop on transient numbers 1…MTRAN
READ (83,*) J, NHIST(I), ISQPRA(I)
       ! NHIST = no of points in PDF, ISQPRA – transient sequence number
       WRITE (82,657) I,NHIST(I) ! write to output file
       SUM = ZERO
       READ (83,*) TFREQ1(I,1),TFREQ2(I,1)
! {PDF pairs:  transient frequency, percent of total}
       CDFQ(I,1) = (TFREQ2(I,1)/100.0d0) ! (convert from % to decimal)
       DO 20 J=2,NHIST(I) ! (loop on number of points in PDF)
              READ (83,*) TFREQ1(I,J),TFREQ2(I,J)
              CDFQ(I,J) = CDFQ(I,J-1) + TFREQ2(I,J)*0.01d0 ! create CDF
              WRITE (82,654) J,TFREQ1(I,J),TFREQ2(I,J),CDFQ(I,J)
              ! write (PDF,CDF) pair-to  output file
       20     CONTINUE
10   CONTINUE
```

SUBROUTINE POSTCPI – called from MAIN PROGRAM for each transient – operates on array CPI(NSIM) – generates and outputs PDF, CDF, and summary statistics of CPI(NSIM) - to file name PDFCPI.out

```
Do 777 IRPV = 1, NSIM
       CPI(IRPV) = PFMI(IPPFM(ITRAN),IRPV)
777 CONTINUE
Call DSORT (CPI, DUMY, NSIM, 1)
! SORT array CPI(NSIM) in ascending order –
! necessary to create a PDF of CPI (NSIM)
Vlow =  CPI(1)
Vhigh = CPI(NSIM)
! Determine the number of bins (ANUM) to be used – usually 99 –
! for purpose of creating / writing out PDF
DEL      = (VHIGH - VLOW)/ANUM
ALEFT    = VLOW
! Perform BINNING process of array CPI (NSIM) divide interval DEL
! into equal intervals of sorted array of CPI  determine the number
! of values of CPI that reside in each interval.
IDIVIDE = ANUM      IDIVIDE + 1
! = number of bins for constructing PDF (usually 100)
DO 150 I=1,IDIVIDE+1
! increment bin
ARIGHT = ALEFT + DEL
DO 160 J=1,NSIM
       IF (CPI(J).GT.ARIGHT) GOTO 75
       IF (CPI(J).GT.ALEFT.AND.CPI(J).LE.ARIGHT) THEN
              HISTIN(I,2) = HISTIN(I,2) + 1.0d0
              ! increment number of events in this bin
       ENDIF
```

```
160 CONTINUE

75 AMID = (ALEFT+ARIGHT)*0.5d0
HISTIN(I,1) = AMID
ALEFT = ARIGHT
! move to next bin
150 CONTINUE
! Create and output PDF and CDF of array CPI(NSIM) TO PDFCPI.OUT (in percentages)
! For a given interval - writes out only if the interval (bin)
! has nonzero percentage
DO 80 I = IDIVIDE + 1
       REL = (HISTIN(I,2) / NSIM) * 100
       ! (note: this is calculation of relative percentage for each interval)
       CDF= get_emp_cdf(nsim,nk,histin(i,1),cpi)*100.0d0
       IF (REL.GT.ZERO) WRITE ((78,768) HISTIN(I,1),REL,CDF
80 CONTINUE
Call STATS
! calculates and writes out summary statistics for array CPI(NSIM) to PDFCPI.out
RETURN
END
```

SUBROUTINE POSTCPF – called from MAIN PROGRAM for each transient – operates on array CPF(NSIM) – generates and outputs PDF, CDF, and summary statistics of CPF(NSIM) - to file name PDFCPF.out

Uses same structure and logic (SORT, BIN, REPORT, and CALL STATS) as SUBROUTINE POSTCPI)

SUBROUTINE GENFRQ – combines transient initiating frequencies with results of PFM analysis

Sample an initiating frequency for each transient and store as a row vector in array SFRQI

```
Do 2005 NVESS= 1,nsim
       Do 2006 ITRAN = 1, MTRAN
              R = rndu- ( )
              Do 2007 j = 1, NHIST(IPPOST(ITRAN))
                     If (R.LE.CDFQ (IPPOST(ITRAN),J)) THEN
                            SFRQI (IPPFM(ITRAN)) = TFREQ1(IPPOST(ITRAN),J)
                            GOTO 2006
                     ENDIF
              2007 CONTINUE
       2006 CONTINUE
```

For the current vessel (NVESS) , combine vector of initiating frequencies SFRQI (MTRAN) with vector of conditional probability of initiation PFM(IPPFM(NVESS)) and vector of conditional probability of failure PFMF(IPPFM(I),NVESS).

```
FSUMI = ZERO
FSUMF = ZERO
DO 2008 I = 1, MTRAN
       CONTI (IPPFM(I)) = SFRQI (IPPFM(I)) * PFMI(IPPFM(I),NVESS)
       CONTF (IPPFM(I)) = SFRQI (IPPFM(I)) * PFMF(IPPFM(I),NVESS)
       FSUMI = FSUMI + CONTI(IPPFM(I))
```

```
        FSUMF = FSUMF + CONTF(IPPFM(I))
        ! Additional bookkeeping necessary to generate specific
        ! reports fractionalization (allocation) requested by USNRC staff:
        ! Fractionalization of FCI by material (weld or plate)
        ! Fractionalization of FCI by flaw category (1, 2, or 3)
        ! Fractionalization of TWCF by material (weld or plate)
        ! Fractionalization of TWCF by flaw category (1, 2, or 3)
        ! Fractionalization of FCI by RPV major beltline region
        ! Fractionalization of TWCF by RPV major beltline region
2008 Continue
! (end of transients)
FRQPIE(NVESS) = FSUMI
! (vector of FCI)
FRQPFE(NVESS) = FSUMF
! (vector of TWCF)
2005 CONTINUE
! (end of vessels)
RETURN
END
! (GENFRQ)
```

SUBROUTINE POSTINT – called one time from MAIN PROGRAM – operates on array FRQPIE (NSIM) - generates and output, PDF, CDF, and summary statistics of Frequency of Crack Initiation (FCI) to user-named FAVPOST output file.

Uses same structure and logic (SORT, BIN, REPORT, and CALL STATS) as SUBROUTINE POSTCPI and POSTCPF

SUBROUTINE POSTINIT also calculates the fractionalization of FCI per transient (the percentage each transient contributed to FCI).

```
TOTI = ZERO
Do 2011 ITRAN = 1, MTRAN
        TOTI = TOTI* + SUMTI(IPPM(ITRAN))
        ! SUMTI is sum of products freq X CPI  for ITRAN
        ! was calculated and stored in GENFRQ
        ! TOTI is summation over all transients
2011    CONTINUE
        DO 2012 ITRAN = 1, MTRAN
                IF (TOTI.GT.ZERO) THEN
                        TIFRAC(IPPM(ITRAN)) = SUMTI(IPPFM(ITRAN)) / TOTI) * PERCENT
                        ! (percent = 100)
                ELSE
                        TIFRAC(IPPFM(ITRAN)) = PERCENT
                ENDIF
        2012    CONTINUE
```

SUBROUTINE POSTFAIL - called one time from MAIN PROGRAM – operates on array FRQPFE (NSIM) - generates and outputs PDF, CDF, and summary statistics of Thru-Wall Crack Frequency (TWCF) to user-named FAVPOST output file.

Uses same structure and logic (SORT, BIN, REPORT, and CALL STATS) as SUBROUTINE POSTCPI, POSTCPF, and POSTINT

SUBROUTINE POSTFAIL also

(1) Calculates and stores the fractionalization of TWCF per transient (the percentage each transient contributed to TWCF).
(2) Writes to user-named FAVPost output file the fractionalization of FCI and TWCF weighted by transient initiating frequency.

```
TOTI = ZERO
Do 2011 ITRAN = 1, MTRAN
       TOTF = TOTF* + SUMTF(IPPM(ITRAN))
       ! SUMTF is sum of products freq X CPF for ITRAN
       ! was calculated and stored in GENFRQ
       ! TOTF is summation over all transients.
2011   CONTINUE
       DO 2012 ITRAN = 1, MTRAN
              IF (TOTI.GT.ZERO) THEN
                     TFFRAC(IPPM(ITRAN)) = SUMTF(IPPFM(ITRAN)) / TOTF) * PERCENT
              ELSE
                     TFFRAC(IPPFM(ITRAN)) = ZERO
              ENDIF
              ! Write for each transient:
              ! transient SEQ no % of FCI % of TWCF
              WRITE(99,761)
ISEQI(IPPFM(ITRAN),TIFRAC(IPPFM(ITRAN)),TFFRAC(IPPFM(ITRAN))
2012   CONTINUE
```

SUBROUTINE POSTSTAT - called one time from MAIN PROGRAM – generates and outputs following fractionalizations (allocations of FCI and TWCF).

7980 Fractionalization of FCI and TWCF by material and flaw category – weighted by transient initiating frequencies – by parent region.

7981 Fractionalization of FCI and TWCF by RPV beltline – by parent region - weighted by % contribution of each transient to FCI and TWCF.

7982 Fractionalization of FCI and TWCF by material, flaw category, and orientation – weighted by transient initiating frequency – by parent region.

17980 Fractionalization of FCI and TWCF by material and flaw category – by child subregion.

17981 Fractionalization of FCI and TWCF by RPV beltline major region - by child subregion - weighted by % contribution of each transient to FCI and TWCF.

17982 Fractionalization of FCI and TWCF by RPV beltline – by material, flaw category, and orientation – weighted by transient initiating frequencies – by child subregion.

7001 Fractionalization of FCI and TWCF by material, flaw category, and flaw depth - weighted by % contribution of each transient to FCI and TWCF.

7011 Fractionalization of FCI and TWCF by material, flaw category, and flaw depth (axial orientation) weighted by % contribution of each transient to FCI and TWCF.

7021 Fractionalization of FCI and TWCF by material, flaw category, and flaw depth (circumferential orientation) - weighted by % contribution of each transient to FCI and TWCF.

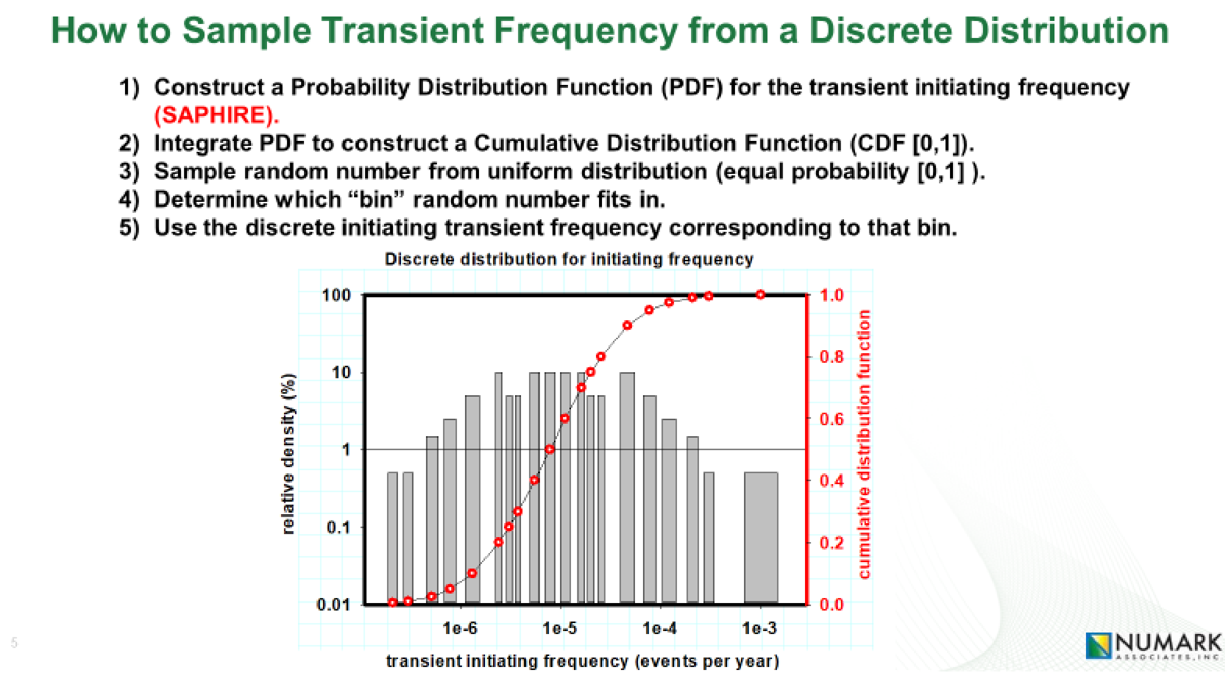

Figure 23: Illustration of how transient frequency is sampled in FAVPOST

Note that the CDF for each transient is created in SUBROUTINE PRA

Design 19 Statistical data in the form of relative densities, cumulative probabilities, and estimated percentiles for vessel failure and crack initiation are developed and later presented in tabulated histograms and summary tables for the various discrete distributions using standard empirical distribution functions on ordinal data.

The cumulative distribution function, CDF, $\boldsymbol{F(x)}$, for $\boldsymbol{F(F)}$ and $\boldsymbol{F(I)}$, is based on the software requirement as

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

where the estimator applied for $F(x)$ shall be based on the Kaplan-Meier estimate, $\hat{F}(x_{(i)}) = i/n$. [8]

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, $\hat{\boldsymbol{F}}(\boldsymbol{x}_{(i)}) = \boldsymbol{i}/\boldsymbol{n}$, a shifted exponential distribution to represent the extreme right tail is used.

In addition, due to Construction of Mixed Empirical/Exponential Distribution Functions, the following process is used.

Data is first ordered by rank such that $X_1 \leq X_2 \leq \cdots \leq X_n$. Then, a piecewise linear CDF is fit to the first $n-k$ ordered data points. Finally, a shifted exponential CDF is fit to the k largest data points.

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

Where:

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

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

The mean of this mixed distribution is $(\mathrm{X}_{(1)} + \mathrm{X}_{(2)} + \cdots + \mathrm{X}_{(\mathrm{n})})/\mathrm{n}$ for $1 \leq \mathrm{k} \leq \mathrm{n}$, thus recovering the original sample mean.

Consistent with the software requirement, the estimator for the variance is determined as follows:

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

Given a specified probability $0 < \mathrm{P_i} < 1$, the corresponding percentile (quantile) is calculated as follows:

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

[8] 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.

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

(2) If $P_i \leq 1 - \frac{k}{n}$, then a piecewise linear interpolation within the empirical distribution is used

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

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

The above calculations and fitting routines are accomplished by calling subroutine STATS and Functions get_emp_Q and get_emp_cdf.

Design 20 An output file is generated that contains all important and critical input and output values for the user to assess and evaluate reactor vessel integrity data.

The subroutine RD79 in FAVLoad, subroutines ECHO_pfm and ECHO2 in FAVPFM, and subroutine ECHO in FAVPost generates an echo of all the user input to output or a *.echo file. All critical input data or in the case of VFLAW based files or As-Found flaw files, only the file names are echoed. The important and critical outputs printed by either FAVLoad, FAVPFM, or FAVPost are:

- temperature as a function of time throughout vessel wall location
- 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
- crack initiation frequency per reactor operating year (Table 3)
- through-wall cracking frequency per reactor operating year

The following design descriptions provide more detailed information on how FAVLoad, FAVPFM, and FAVPost generate this output.

Design 21 Sufficient verifiable information is 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.

FAVLoad, FAVPFM, and FAVPost provide version number and date/time of execution for each user entered run. The following subroutines are used to provide the two outputs: subroutine banner_load for FAVLoad, banner_pfm for FAVPFM (called by subroutine file_init_pfm), and banner_post for FAVPost are used to print out banner pages containing the applicable FAVOR program version number. The common module timedate_m and submodule timedate_s are used to printout date and time of execution.

Design 22 Provide tabular results in 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.

Both FAVPFM and FAVPost use write statements within the main program and various subroutines to print irradiated RT_{NDT}, CPI, and CPF for flaws, transients, material composition (Plate or weld), vessel region, and vessel subregion to assist the user in determining impact of the various input variables.

The main routines of FAVPFM and FAVPost primarily initialize the output files and for FAVPost, also write out the various header information to be later supplied by numerical output from a called subroutine. For FAVPFM, the main subroutines that provide the tabular output to characterize RT_{NDT}, CPI, and CPF by flaws, transients, material composition (Plate or weld), vessel region, and vessel subregion are as follows:

- Subroutine PFM (See write and format statements for Fortran unit 29, which is the output file) Prints out headings for the various tables in the output file.
- Subroutine Report (See write and format statements for Fortran unit 29, which is the output file).

For FAVPost, the main subroutines that provide similar information but factor in the effect of transient initiating frequency are as follows:

- Subroutine PostStat (See write and format statements for Fortran unit 99, which is the output file).
- Submodule post_probability_s reports the % contribution of each transient to the frequency of crack initiation and the frequency of vessel failure (See write and format statements for Fortran unit 99, which is the output file).

Design 23 Provide error messages in the output file(s) to assist the user in diagnosing user input errors or code errors.

Design 3 describes the various subroutines and calling procedures that perform the error reporting logic used for FAVLoad, FAVPFM, and FAVPost. This includes allocation errors and code errors which are handled by the SLATEC error handling procedures.

Design 24 When the user requests a deterministic analysis for surface breaking flaws, provide tabular data results containing time step, transient time, coolant temperature, reactor pressure, hoop stress components of membrane bending for axial flaw (for axial stress for circumferential flaw), applied stress intensity factor, KI, for aspect ratios 2, 6, 10, and infinite.

Design 8 describes the various subroutines and calling procedures that provide the tabular time history data for surface breaking flaws when performing a deterministic analysis.

Design 25 When the user requests a deterministic analysis for embedded flaws, provide tabular data results 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, KI.

Design 8 describes the various subroutines and calling procedures that provide the tabular time history data for embedded flaws when performing a deterministic analysis.

Design 26 When the user requests a deterministic analysis and through-wall analysis, results are in the form of those in Design 24 (surface breaking flaw) or in the form of design 25 (embedded flaw). The tabular data contain time step, transient time, coolant temperature, and reactor pressure are 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.

Design 8 describes the various subroutines and calling procedures that provide the tabular through-wall analysis data for a surface-breaking flaw or embedded flaws when performing a deterministic analysis.

Design 27 For probabilistic LEFM analyses, FAVPFM's software is designed to echo user options 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 or as-found flaw file.

Design 2, Design 3, and Design 20 describe the major FAVPFM subroutines involved in generating key user input. The subroutines FILE_INIT_PFM, RDDET (within submodule read_data_s), RDPFM (with calls to RDBAL and RD17 - within submodule read_data_s), echo_pfm, and echo2 are used to provide (i.e., echo) the user input options in the output file and echo file. Fortran unit 29 is the FAVPFM output file and Fortran unit 30 is the FAVPFM echo file. Subroutine FILE_INIT_PFM, which initiates and opens the input and output files and writes out the names of those files, and then calls RDDET, RDPFM (which then calls RDBAL and RD17), echo_pfm and echo2 subroutines to echo the user input and user options.

Design 28 For probabilistic LEFM analyses, FAVPFM's software is designed to provide the following output values in the output report.

- Initial random seeds used in the analysis,
    - Written to Output (Fortran Unit 29) in subroutine pfm. Variable is current_seed.
- Mean value of CPI for all RPV simulations,
    - Running averages of CPI are written to cpi_history.out (Fortran Unit 71) for all RPV simulations and transients.
    - CPI for each RPV simulation is written to initiate.dat (Fortran Unit 86) for all transients.
    - The mean value of CPI for all RPV simulations is written to the output file (Fortran Unit 29) for all transients.
    - Subroutines pfm and report provide the write statements to provide the header and value, respectively. For Output on Fortan Unit 29, variable is AMNCPI.

- Mean value of CPF for all RPV simulations,
  - Running averages of CPF are written to cpf_history.out (Fortran Unit 72) for all RPV simulations and transients.
  - CPF for each RPV simulation is written to failure.dat (Fortran Unit 87) for all transients.
  - The mean value of CPF for all RPV simulations is written to the output file (Fortran Unit 29) for all transients.
  - Subroutines pfm and report provide the write statements to provide the header and value, respectively. For Output on Fortan Unit 29, variable is AMNCPF.
- 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 <u>parent</u> subregion with totals shown for each column,
  - Subroutine report provides the write statements using the following variables: RTMAX(I), FLAWP, NTFLAW, NIFLAW, SMPCTI, NFCLEV, SMPCTF_CL, NFDUCT, and SMPCTF_DT. Variables used for totals include SUMFL, ITFLW, IITOT, SUMPI, IFTOTCL, SUMPF_CL, IFTOTDT, and SUMPF_DT.
- Mean value of RT_{NDT} at crack tip,
  - Subroutine report provides the write statements. Variable name is SRTMN.
- 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 <u>child</u> subregion with totals shown for each column,
  - Subroutine report provides the write statements using the following variables: RTMAX(I), FLAWP, NTFLAW_C, NIFLAW_C, SMPCTI_C, NFCLEV_C, SMPCTF_CL_C, NFDUCT_C, and SMPCTF_DT_C.
- 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,
  - Subroutine report provides the write statements using the following variables:
    - For weld and ipflaw equal to 1 or 4, variables are iwcat1_i, iiw1_i, w1ipct_i, ifw1_i, w1fpct_i, iwcat2_i, iiw2, w2ipct, ifw2, w2fpct, iwcat3_i, iiw3, w3ipct, ifw3, and w3fpct.
    - For weld and ipflaw equal to 2, variables are iwcat1_e, iiw1_e, w1ipct_e, ifw1_e, w1fpct_e, iwcat2_e, iiw2, w2ipct, ifw2, w2fpct, iwcat3_e, iiw3, w3ipct, ifw3, and w3fpct.
    - For weld and ipflaw equal to 3, variables are iwcat1_i, iiw1_i, w1ipct_i, ifw1_i, w1fpct_i, iwcat1_e, iiw1_e, w1ipct_e, ifw1_e, w1fpct_e, iwcat2_i, iiw2, w2ipct, ifw2, w2fpct, iwcat3_e, iiw3, w3ipct, ifw3, and w3fpct.
    - Totals for weld region use variables IIWT1_T, IIWT2, WTIPCT, IFWT, and WTFPCT.

  - For plate and ipflaw equal to 1 or 4, variables are ipcat1_i, iip1_i, p1ipct_i, ifp1_i, p1fpct_i, ipcat2_i, iip2, p2ipct, ifp2, p2fpct, ipcat3_i, iip3, p3ipct, ifp3, and p3fpct.
  - For plate and ipflaw equal to 2, variables are ipcat1_e, iip1_e, p1ipct_e, ifp1_e, p1fpct_e, ipcat2_e, iip2, p2ipct, ifp2, p2fpct, ipcat3_e, iip3, p3ipct, ifp3, and p3fpct.
  - For plate and ipflaw equal to 3, variables are ipcat1_i, iip1_i, p1ipct_i, ifp1_i, p1fpct_i, ipcat1_e, iip1_e, p1ipct_e, ifp1_e, p1fpct_e, ipcat2_i, iip2, p2ipct, ifp2, p2fpct, ipcat3_e, iip3, p3ipct, ifp3, and p3fpct.
  - Totals for plate region use variables IIPT1_T, IIPT2, PTIPCT, IFPT, and PTFPCT.

- 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,
  - Subroutine report provides the write statements for the child subregions using the following variables:
    - For weld and ipflaw equal to 1 or 4, variables are IWCAT1_Ci, IIW1_C_i, W1IPCT_C_i, IFW1_C_i, W1FPCT_C_i, IWCAT2_Ci, IIW2_C, W2IPCT_C, IFW2_C, W2FPCT_C, IWCAT3_Ci, IIW3_C, W3IPCT_C, IFW3_C, and W3FPCT_C.
    - For weld and ipflaw equal to 2, variables are IWCAT1_Ce, IIW1_C_e, W1IPCT_C_e, IFW1_C_e, IWCAT1_Ce,IIW1_C_e,W1IPCT_C_e,IFW1_C_e, W1FPCT_C_e, IWCAT2_Ce, IIW2_C, W2IPCT_C, IFW2_C, W2FPCT_C, IWCAT3_Ce, IIW3_C, W3IPCT_C, IFW3_C, W3FPCT_C, W1FPCT_C_e, IWCAT2_Ce, IIW2_C, W2IPCT_C, IFW2_C, W2FPCT_C, IWCAT3_Ce, IIW3_C, W3IPCT_C, IFW3_C, and W3FPCT_C.
    - For weld and ipflaw equal to 3, variables are IWCAT1_Ci, IIW1_C_i, W1IPCT_C_i, IFW1_C_i, W1FPCT_C_i, IWCAT1_Ce, IIW1_C_e, W1IPCT_C_e, IFW1_C_e, W1FPCT_C_e, IWCAT2_Ci, IIW2_C, W2IPCT_C, IFW2_C, W2FPCT_C, IWCAT3_Ce, IIW3_C, W3IPCT_C, IFW3_C, and W3FPCT_C.
    - Totals for weld region use variables IIWT1_C, IIWT2_C, WTIPCT_C, IFWT_C, and WTFPCT_C.
    - For plate and ipflaw equal to 1 or 4, variables are ipcat1_ci, iip1_c_i, p1ipct_c_i, ifp1_c_i, p1fpct_c_i, ipcat2_ci, iip2_c, p2ipct_c, ifp2_c, p2fpct_c, ipcat3_ci, iip3_c, p3ipct_c, ifp3_c, and p3fpct_c.
    - For plate and ipflaw equal to 2, variables are ipcat1_ce, iip1_c_e, p1ipct_c_e, ifp1_c_e, p1fpct_c_e, ipcat2_ce, iip2_c, p2ipct_c, ifp2_c, p2fpct_c, ipcat3_ce, iip3_c, p3ipct_c, ifp3_c, and p3fpct_c.
    - For plate and ipflaw equal to 3, variables are ipcat1_ci, iip1_c_i, p1ipct_c_i, ifp1_c_i, p1fpct_c_i, ipcat1_ce, iip1_c_e, p1ipct_c_e, ifp1_c_e, p1fpct_c_e, ipcat2_ci, iip2_c, p2ipct_c, ifp2_c, p2fpct_c, ipcat3_ce, iip3_c, p3ipct_c, ifp3_c, and p3fpct_c.
    - Totals for plate region for child use variables IIPT1_C, IIPT2_C, PTIPCT_C, IFPT_C, and PTFPCT_C.

- 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,
  - Subroutine report provides the write statements for the parent subregions using the following variables:
    - For welds with axial orientation, variables are IWCAT1A, IIW1A, W1IPCTA, IFW1A, W1FPCTA, IWCAT2A, IIW2A, W2IPCTA, IFW2A, W2FPCTA, IWCAT3A, IIW3A, W3IPCTA, IFW3A, and W3FPCTA.
    - Totals for weld region with axial orientation for parent use variables IIWT1A, IIWT2A, WTIPCTA, IFWTA, and WTFPCTA.
    - For welds with circumferential orientation, variables are IWCAT1C, IIW1C, W1IPCTC, IFW1C, W1FPCTC, IWCAT2C, IIW2C, W2IPCTC, IFW2C, W2FPCTC, IWCAT3C, IIW3C, W3IPCTC, IFW3C, W3FPCTC.
    - Totals for weld region with circumferential orientation for parent use variables IIWT1C, IIWT2C, WTIPCTC, IFWTC, and WTFPCTC.
    - For plates with axial orientation, variables are IPCAT1A, IIP1A, P1IPCTA, IFP1A, P1FPCTA, IPCAT2A, IIP2A, P2IPCTA, IFP2A, P2FPCTA, IPCAT3A, IIP3A, P3IPCTA, IFP3A, and P3FPCTA.
    - Totals for plate region with axial orientation for parent use variables IIPT1A, IIPT2A, PTIPCTA, IFPTA, and PTFPCTA.
    - For plates with circumferential orientation, variables are IPCAT1C, IIP1C, P1IPCTC, IFP1C, P1FPCTC, IPCAT2C, IIP2C, P2IPCTC, IFP2C, P2FPCTC, IPCAT3C, IIP3C, P3IPCTC, IFP3C, and P3FPCTC.
    - Totals for plate region with circumferential orientation for parent use variables IIPT1C, IIPT2C, PTIPCTC, IFPTC, PTFPCTC.
- 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,
  - Subroutine report provides the write statements using variable names similar to the parent region as presented above, however the suffix "_C" is added. For example, the parent variable of IWCAT1A is IWCAT1A _c for the child. For simplicity, the child variables will not be all listed, but can be easily determined by adding the suffix "_C" to all the above parent variables for the various attributes (e.g., axial vs circumferential, and weld vs plate).
- 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,

  - Subroutine report provides the write statements for weld using variables RX, IWDEP1(K,1), IWDEP2(K,1,ITRAN), WPCTK1, IWDEP1(K,2), IWDEP2(K,2,ITRAN), WPCTK2, IWDEP1(K,3), IWDEP2(K,3,ITRAN), and WPCTK3.

  - Subroutine report provides the write statements for plate using variables RX, IPDEP1(K,1), IPDEP2(K,1,ITRAN), PPCTK1, IPDEP1(K,2), IPDEP2(K,2,ITRAN), PPCTK2, IPDEP1(K,3), IPDEP2(K,3,ITRAN), and PPCTK3.

- 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,

  - Subroutine report provides the write statements for weld using variables RX, IWDEP1(K,1), IFWDEP2(K,1,ITRAN), WFPCTK1, IWDEP1(K,2), IFWDEP2(K,2,ITRAN), WFPCTK2, IWDEP1(K,3), IFWDEP2(K,3,ITRAN), and WFPCTK3.

  - Subroutine report provides the write statements for plate using variables RX, IPDEP1(K,1), IFPDEP2(K,1,ITRAN), PFPCTK1, IPDEP1(K,2), IFPDEP2(K,2,ITRAN), PFPCTK2, IPDEP1(K,3), IFPDEP2(K,3,ITRAN), and PFPCTK3.

- 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.

  - Subroutine report provides the write statements using the following variables: J, TIME(J), TIFRAC, SUMI, TFFRAC, and SUMF.

- Tabular data showing histogram of the relative density and cumulative density for initiating driving force KI for each transient.

  - Subroutine report provides the write statements using the following variables: KI_Count_X(jbin), KI_bin_value(jbin), and KI_bin_cdf(jbin).

- 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:

  1. Unstable ductile tearing,
  2. Stable ductile tear to plastic instability,
  3. Cleavage propagation to plastic instability,
  4. Stable ductile tear exceeds wall depth failure criteria, and
  5. Cleavage propagation exceeds wall depth failure criteria.

  - Subroutine report provides the write statements using the following variables: KFAIL(ITRAN,1), PCTMECH1, KFAIL(ITRAN,2), PCTMECH2, KFAIL(ITRAN,3), PCTMECH3, KFAIL(ITRAN,4), PCTMECH4, KFAIL(ITRAN,5), and PCTMECH5.

- 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.
  - Subroutine report provides the write statements using the following variables: I, IPFMI2(I), PCENTI, IPFMF2(I), and PCENTF. Printed totals use the variables IMARK1, PTOTI, IMARK2, and PTOTF.

The above detail output is primarily generated by subroutine Report in FAVPFM. Subroutine pfm also is used for the initial random seed output and cpi and cpf data in the cpi_history, cpf_history, initiate.dat, and failure.dat files.

Design 29 For probabilistic LEFM analyses, FAVPFM's software is designed to provide the following output values in two output files, initiate.dat (Fortran Unit 86) and failure.dat (Fortran Unit 87).

An array of values of conditional probability of crack initiation and the values of conditional probability of through-wall cracking (vessel failure) are reported in initiate.dat and failure.dat ouput files for each transient and RPV simulation, respectively. The following data is written by subroutines pfm or report:

- A set of data reporting the source code version number, the number of transients, and the number of RPV simulations.
- A block of data containing the transient sequence number and the user provided unique transient number. Subroutine pfm writes this data.
- Another block of data containing conditional probability of either crack initiation (i.e., initiate.dat) or through-wall cracking (i.e., failure.dat) array by RPV simulation and transient. Subroutines outcpi and outcpf write this data to initiate.dat and failure.dat files, respectively.

For the initiate.dat file containing the conditional probability of crack initiation, the following data blocks is written out:

1. A data block containing the number of major regions and a flag indicating whether child subregions are included in the report. Subroutine Report writes this data to initiate.dat.
2. A data block containing an array of maximum RT_{NDT} and number of flaws by major region. Subroutine Report writes this data to initiate.dat.
3. A data block containing 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. Subroutine Report writes this data (i.e., IWMAX and IPMAX) to initiate.dat.
4. A series of array data containing 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. Subroutine Report writes this data (i.e., variables I, SMPCTI, SMPCTF_CL, and SMPCTF_DT).

5. If the child subregion report was selected, an additional series of array data is provided that mimics the previous output in 4. Subroutine Report writes this data.

6. The next series of data contains 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 index and depth of flaw for the specified transient in previous step 4. Subroutine Report writes this data (i.e., variables K, RX, WPCTK1, WPCTK2, WPCTK3, WPCTK1_1, WPCTK2_1, WPCTK3_1, WPCTK1_2, WPCTK2_2, and WPCTK3_2).

7. The next series contains output data similar to the previous step 6, except for plate material. Subroutine Report writes this data (i.e., variables K, RX, PPCTK1, PPCTK2, PPCTK3, PPCTK1_1, PPCTK2_1, PPCTK3_1, PPCTK1_2, PPCTK2_2, and PPCTK3_2).

8. CPF related data is provided in similar fashion as steps 4 through 7 above, except that percentage of total CPI is replaced with percentage of total CPF. Subroutine Report also writes this information out to initiate.dat. For welds, variables printed include K, RX, WFPCTK1, WFPCTK2, WFPCTK3, WFPCTK1_1, WFPCTK2_1, WFPCTK3_1, WFPCTK1_2, WFPCTK2_2, and WFPCTK3_2. For plates, variable include K, RX, PFPCTK1, PFPCTK2, PFPCTK3, PFPCTK1_1, PFPCTK2_1, PFPCTK3_1, PFPCTK1_2, PFPCTK2_2, and PFPCTK3_2.

For the failure.dat output file, additional through-wall cracking (vessel failure) information is written following the initial output as described in the above first three bullets (e.g., version number, transient identifiers, and conditional probability of through-wall cracking). The additional information contains a series of array data that first contains the transient sequential number and unique user identified transient number, and then the following data results:

- % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material, (Subroutine Report variables W1IPCT and W1FPCT),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material, (Subroutine Report variables W2IPCT and W2FPCT),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material, (Subroutine Report variables W3IPCT and W3FPCT),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material, (Subroutine Report variables P1IPCT and P1FPCT),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material, (Subroutine Report variables P2IPCT and P2FPCT),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material, (Subroutine Report variables P3IPCT and P3FPCT),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Child Subregion, (Subroutine Report variables W1IPCT_C and W1FPCT_C),

- % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Child Subregion, (Subroutine Report variables W2IPCT_C and W2FPCT_C),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Child Subregion, (Subroutine Report variables W3IPCT_C and W3FPCT_C),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Child Subregion, (Subroutine Report variables P1IPCT_C and P1FPCT_C),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Child Subregion, (Subroutine Report variables P2IPCT_C and P2FPCT_C),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Child Subregion, (Subroutine Report variables P3IPCT_C and P3FPCT_C),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Axial Flaws, (Subroutine Report variables W1IPCTA and W1FPCTA),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Axial Flaws, (Subroutine Report variables W2IPCTA and W2FPCTA),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Axial Flaws, (Subroutine Report variables W3IPCTA and W3FPCTA),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Circumferential Flaws, (Subroutine Report variables W1IPCTC and W1FPCTC),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Circumferential Flaws, (Subroutine Report variables W2IPCTC and W2FPCTC),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Circumferential Flaws, (Subroutine Report variables W3IPCTC and W3FPCTC),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Axial Flaws, (Subroutine Report variables P1IPCTA and P1FPCTA),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Axial Flaws, (Subroutine Report variables P2IPCTA and P2FPCTA),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Axial Flaws, (Subroutine Report variables P3IPCTA and P3FPCTA),
- % of total CP and % of total CPF attributable to Category 1 Flaws in Plate Material for Circumferential Flaws, (Subroutine Report variables P1IPCTC and P1FPCTC),
- % of total CP and % of total CPF attributable to Category 2 Flaws in Plate Material for Circumferential Flaws, (Subroutine Report variables P2IPCTC and P2FPCTC),
- % of total CP and % of total CPF attributable to Category 3 Flaws in Plate Material for Circumferential Flaws, (Subroutine Report variables P3IPCTC and P3FPCTC),

- % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Child Subregion for Axial Flaws, (Subroutine Report variables W1IPCTA_C and W1FPCTA_C),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Child Subregion for Axial Flaws, (Subroutine Report variables W2IPCTA_C and W2FPCTA_C),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Child Subregion for Axial Flaws, (Subroutine Report variables W3IPCTA_C and W3FPCTA_C),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Weld Material for Child Subregion for Circumferential Flaws, (Subroutine Report variables W1IPCTC_C and W1FPCTC_C),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Weld Material for Child Subregion for Circumferential Flaws, (Subroutine Report variables W2IPCTC_C and W2FPCTC_C),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Weld Material for Child Subregion for Circumferential Flaws, (Subroutine Report variables W3IPCTC_C and W3FPCTC_C),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Child Subregion for Axial Flaws, (Subroutine Report variables P1IPCTA_C and P1FPCTA_C),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Child Subregion for Axial Flaws, (Subroutine Report variables P2IPCTA_C and P2FPCTA_C),
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Child Subregion for Axial Flaws, (Subroutine Report variables P3IPCTA_C and P3FPCTA_C),
- % of total CPI and % of total CPF attributable to Category 1 Flaws in Plate Material for Child Subregion for Circumferential Flaws, (Subroutine Report variables P1IPCTC_C and P1FPCTC_C),
- % of total CPI and % of total CPF attributable to Category 2 Flaws in Plate Material for Child Subregion for Circumferential Flaws, (Subroutine Report variables P2IPCTC_C and P2FPCTC_C), and
- % of total CPI and % of total CPF attributable to Category 3 Flaws in Plate Material for Child Subregion for Circumferential Flaws, (Subroutine Report variables P3IPCTC_C and P3FPCTC_C).

The 36 additional blocks described above are printed by subroutine Report. The internal variables used in subroutine Report are identified in the above data blocks.

Design 30 FAVPost output (Fortran Unit 99) is designed to provide final meaningful PFM statistics, such as a 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. In addition, the following output data blocks are provided:

For the initial FAVPost output, procedure postcpf in module post_probablity_distribution_s provides the write statements for transient identifier, 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). Variables are ISEQI(IPPFM(ITRAN)), AMEANI, P95I, P99I, AMEANF, P95, P99, and RATIO. Note that the header and number of simulations (NSIM) are written by proceducre rdcpf in module read_probability_data_s.

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

  Procedure postinit in module post_probablity_distribution_s provides the write statements for the histogram. Variables are HISTIN(I,1), REL, and CDF.

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

  - Minimum value,
  - Maximum value,
  - Range of values,
  - Number of RPV simulations used in the analysis,
  - 5^{th} percentile,
  - Median,
  - 95.0^{th} percentile,
  - 99.0^{th} percentile,
  - 99.9^{th} percentile,
  - Mean,
  - Standard deviation,
  - Standard error,
  - Variance (unbiased),
  - Variance (biased),
  - Moment Coefficient of Skewness,
  - Pearson's 2^{nd} Coefficient of Skewness, and
  - Kurtosis.

  Procedure postinit in module post_probablity_distribution_s calls subroutine STATS to write out all the above values. In order of the above, the variable names in subroutine STATS are z(1), z(ncount), (z(ncount)-z(1)), ncount, Q5, Q50, Q95, Q99, Q999, mean, stdev, error, varu, varb, skew1, skew2, and kurtos.

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

Procedure postfail in module post_probablity_distribution_s provides the write statements for the histogram. Variables are HISTIN(I,1), REL, and CDF.

- Similar summary descriptive statistics as described for crack initiation are provided for through-wall cracking per reactor-operating year.

  Procedure postfail in module post_probablity_distribution_s calls subroutine stats to write out all the above values. In similar order as presented for crack initiation, the variable names in subroutine stats are z(1), z(ncount), (z(ncount)-z(1)), ncount, Q5, Q50, Q95, Q99, Q999, mean, stdev, error, varu, varb, skew1, skew2, and kurtos.

- A table showing the contribution by each transient to frequency of crack initiation and through-wall cracking is provided.

  Procedure postfail in module post_probablity_distribution_s writes out the values. The variable names used are ISEQI(IPPFM(ITRAN)), TIFRAC(IPPFM(ITRAN)), and TFFRAC(IPPFM(ITRAN)).

Design 31 FAVPost output includes a breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency by RPV beltline major region (parent).

The breakdown is presented in tabular form containing the following column data:

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

Subroutine poststat writes out the above tabular data for each major parent region. Variables, in the order presented above, are MAJR, RTMAX(MAJR), FLAWP(MAJR), FRACI_C, FRACL_C, FRADT_C, and FRATOT_C. The summary totals are printed out using variables, FLTOT, FITOT, FCLTOT, FDTTOT, and FFATOT.

Design 32 FAVPost output includes a breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency by RPV beltline major region (child), similar to the previous requirement for parent region.

Subroutine poststat also writes out the tabular data for each child region in the same fashion as the above parent regions. Variables are MAJR, RTMAX(MAJR), FLAWP(MAJR), FRACI, FRACL, FRADT, and FRATOT. The summary totals are printed out using variables, FLTOT, FITOT, FCLTOT, FDTTOT, and FFATOT.

Design 33 FAVPost output includes a breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency by material, flaw category, and flaw depth.

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

- Flaw depth,
- % of total frequency of crack initiation for category 1 type flaws,
- % of total frequency of crack initiation for category 2 type flaws,
- % of total frequency of crack initiation for category 3 type flaws,
- % of total through-wall crack frequency for category 1 type flaws,
- % of total through-wall crack frequency for category 2 type flaws,
- % of total through-wall crack frequency for category 3 type flaws, and
- Summary totals are provided, except for Flaw depth.

Subroutine poststat also writes out the tabular data for characterization of flaw category contribution to frequency of crack initiation and through-wall cracking for welds and plates. Variables for welds that are printed, in the above order, are WDEPTH(IDEPTH), FRACWI1, FRACWI2, FRACWI3, FRACWF1, FRACWF2, and FRACWF3. The summary totals for welds are printed out using variables, FWI1TOT, FWI2TOT, FWI3TOT, FWF1TOT, FWF2TOT, and FWF3TOT. Similarly, variables for plates that are printed are PDEPTH(IDEPTH), FRACPI1, FRACPI2, FRACPI3, FRACPF1, FRACPF2, and FRACPF3. The summary totals for plates are printed out using variables FPI1TOT, FPI2TOT, FPI3TOT, FPF1TOT, FPF2TOT, and FPF3TOT.

Design 34 FAVPost output includes a breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency by material, flaw category, and flaw depth for axial orientated flaws.

Similar to the design description 33, a weld and then a plate breakdown is presented in tabular form containing the following column data for axially oriented flaws:

- Flaw depth,
- % of total frequency of crack initiation for category 1 type flaws,
- % of total frequency of crack initiation for category 2 type flaws,
- % of total frequency of crack initiation for category 3 type flaws,
- % of total through-wall crack frequency for category 1 type flaws,
- % of total through-wall crack frequency for category 2 type flaws,
- % of total through-wall crack frequency for category 3 type flaws, and
- Summary totals shall be provided, except for Flaw depth.

Subroutine poststat also writes out the tabular data for characterization of flaw category and contribution to frequency of crack initiation and through-wall cracking for axially oriented flaws in welds and plates. Variables for welds that are printed, in the above order, are wdepth(idepth), fracwi1, fracwi2, fracwi3, fracwf1, fracwf2, and fracwf3. The summary totals for welds are printed out using variables, fwi1tot, fwi2tot, fwi3tot, fwf1tot, fwf2tot, and fwf3tot. Similarly, variables for plates that are printed are pdepth(idepth), fracpi1, fracpi2, fracpi3, fracpf1, fracpf2, and fracpf3. The summary totals for plates are printed out using variables fpi1tot, fpi2tot, fpi3tot, fpf1tot, fpf2tot, and fpf3tot. Note that these are the same variable names used in the previous design. Subroutine poststat overwrites the variable values as it proceeds through its logic.

Design 35 FAVPost output includes a breakdown (fractionalization) of frequency of crack initiation and through-wall cracking frequency by material, flaw category, and flaw depth for circumferentially orientated flaws.

Similar to the design descriptions 33 and 34, a weld and then a plate breakdown is presented in tabular form containing the following column data for circumferentially oriented flaws:

- Flaw depth,
- % of total frequency of crack initiation for category 1 type flaws,
- % of total frequency of crack initiation for category 2 type flaws,
- % of total frequency of crack initiation for category 3 type flaws,
- % of total through-wall crack frequency for category 1 type flaws,
- % of total through-wall crack frequency for category 2 type flaws,
- % of total through-wall crack frequency for category 3 type flaws, and
- Summary totals shall be provided, except for Flaw depth.

Subroutine poststat also writes out the tabular data for characterization of flaw category and contribution to frequency of crack initiation and through-wall cracking for circumferentially oriented flaws in welds and plates. Variables for welds and plates that are printed, in the above order, are the same as those used in design descriptions 32 and 33. Subroutine poststat overwrites the variable values as it proceeds through its logic.

Design 36 FAVPost processing includes the generation of two output files to assess convergence of the frequency of crack initiation and through-wall cracking frequency (per reactor-year).

The two optional output files (i.e., for CPI and CPF) with a name containing the suffix "convergence_table_ini.out" and "convergence_table_fail.out" are made available to the user that contain the following tabular data:

- The trial number for both files,
- 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,

- The 95th Percentile of the two frequencies, respectively,
- The 99th Percentile of the two frequencies, respectively,
- The 99.9th Percentile of the two frequencies, respectively,
- The covariant mean of the two frequencies, respectively,
- The 95th Percentile of the two frequencies' covariance, respectively,
- The 99th Percentile of the two frequencies' covariance, respectively, and
- The 99.9th Percentile of the two frequencies' covariance, respectively,

If the user selects to build the convergence tables, the main FAVPost program creates the two files, Fortran Unit 79 for the convergence_table_ini.out and Fortran Unit 80 for the convergence_table_fail.out, respectively. The main program also prints the header information in these files. Procedures postinit and postfail in module post_probability_distribution_s generate the data for these files. The variables used are nsim, ntrial_ID(nsim), mean, Q95, Q99, Q999, cov_mean, cov_Q95, cov_Q99, and cov_Q999. The same variable names are used in procedures postinit and postfail.

Design 37 FAVPost processing includes the generation of two output files to assess transient impact on frequency of crack initiation and through-wall cracking frequency (per reactor-year).

The two output files (i.e., for CPI and CPF) with names called "PDFCPI.OUT" and "PDFCPF.OUT" are made available to the user that contain the following tabular data for each transient.

- 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) are provided showing both relative density and cumulative distributions.
- 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:
    - Minimum value,
    - Maximum value,
    - Range of values,
    - Number of RPV simulations used in the analysis,
    - 5th percentile,
    - Median,
    - 95.0th percentile,
    - 99.0th percentile,
    - 99.9th percentile,

- Mean,
- Standard deviation,
- Standard error,
- Variance (unbiased),
- Variance (biased),
- Moment Coefficient of Skewness,
- Pearson's 2nd Coefficient of Skewness, and
- Kurtosis.

The main FAVPost program calls file_init_post, which creates the two files, Fortran Unit 78 for the PDFCPI.OUT and Fortran Unit 77 for the PDFCPF.OUT, respectively. Subroutine file_init_post also prints the user specified input file name, FAVPFM failure.dat and initiate.dat file names, and FAVPost output file name. Procedures postinit and postfail in module post_probability_distribution_s call subroutine STATS to write out the above statistical distribution values following the printing of the number of simulations, number of the transient sequence number, the histogram, and the header information. Variables used in postinit and postfail for transient sequence number and histogram are ISEQI(IPPFM(ITRAN)), HISTIN(I,1), REL, and CDF. In subroutine STATS the summary statistical descriptive values are printed using variables ncount, Q5, Q50, Q95, Q99, Q999, mean, stdev, error, varu, varb, skew1, skew2, and kurtos. The same variable names are used in subroutine Stats to generate the summary statistical descriptive values in PDFCPI.OUT and PDFCPF.out files.

Design 38 FAVOR generates an output file that provides the flaw arithmetic within each vessel region when using the VFLAW based flaw files.

- Tabular data of major region and RPV inner surface area used in establishing the number of surface breaking flaws for each major region are provided.
- Tabular 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 are provided.
- Tabular data of major region and plate volume for each major plate region are provided.
- Tabular data of number of flaws in each major region fractionalized by flaw category are provided for the 1st set of 1000 sets of flaw characterization files, such as:
    - 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,
    - 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,
- A breakdown of total number of flaws for the 1000 sets of flaw characterization files fractionalized by product from and category, such as:

- 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.
- Following this breakdown, average values over the 1000 flaw characterization files of each column data provided in the previous requirement are be provided.
- In addition, a percentage breakdown over the 1000 flaw characterization files of each column data provided in the previous requirement are provided.
- Finally, an aspect ratio check for input flaw densities is performed 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.

In order to generate this information, the main FAVPFM program first creates a file using Fortran Unit 83, called FLAWNO.OUT. The main program also writes out the three VFLAW file names specified by the user, along with the FAVPFM input, FAVLoad output, and FAVPFM output file names associated with the FAVPFM execution. Following a call to subroutine GEOMQA, the tabular data in the first three bullets that represent areas and volumes associated with welds and plates are printed. Variables used in subroutine GEOMQA include MAJ and ARCAT1M for the first set of tabular data. For the second set of tabular data (i.e., weld fusion line areas), variables include MAJ, WLDAREA, TARCAT2, and TARCAT3. For the third set of tabular data (i.e., volume data), variables include MAJ and PVOLs. The set of data describing the flaw characterization is generated in procedure FLWDIS within module flaw_s. FLWDIS is called in the main FAFPFM program. Variables for the number of weld flaws include MAJ, FLSUM1, FLSUM2, FLSUM3, and FLSUM4, and for totals, WSUM(1,IFILE), WSUM(2,IFILE), WSUM(3,IFILE), and WELDTOT(IFILE). Variables for the number of plate flaws include use the same PTOT1(IFILE), PTOT2(IFILE), PTOT3(IFILE), and PLATOT(IFILE). For total weld and plate flaws, the variables are FTOT1, FTOT2, FTOT3, and FLWTOT(IFILE). The number of flaws characterized by product form and category are generated within the same FLWDIS procedure. Variables included are IFILE, WSUM(1,IFILE), WSUM(2,IFILE), WSUM(3,IFILE), WELDTOT(IFILE), PTOT1(IFILE), PTOT2(IFILE), PTOT3(IFILE), PLATOT(IFILE), and FLWTOT(IFILE). Average values over the 1000 flaw characterization files are printed using variables W1AVG, W2AVG, W3AVG, W4AVG, P1AVG, P2AVG, P3AVG, P4AVG, and WPAVG. Percentage breakdown of all flaws by form and category are printed using variables FRAC1, FRAC2, FRAC3, FRAC4, FRAC5,FRAC6, FRAC7, and FRAC8. The last two sets of tabular data are the aspect ratio checks in welds and plates. Subroutine ARATIO, which is called in the main FAVPFM program following the call to FLWDIS, is used to print the final set of data in the FLAWNO.OUT file. For welds, variables printed are K, WFLASPT(IROW,K,IFILE), and WASPCDF(IROW,K,IFILE), and for plates, variables are K, PFLASPT(IROW,K,IFILE), and PASPCDF(IROW,K,IFILE).

Design 39 FAVOR generates a FLAW_TRAC.LOG file that provides the flaw arithmetic within each vessel region when using the VFLAW based flaw files.

FAVPFM reads an input value on the TRAC record, called FLAW_LOG_OPTION, to determine if the log file is generated. When the user sets this variable to 1, a flaw-tracking log table is generated to help put a trace on a particular flaw (KFLAW variable in FAVPFM) as a means to verify the computation of CPI and CPF. This log file (Fortran Unit 15, same as Fortran Unit used for user input file) is used in conjunction with the TRACE.OUT and ARREST.OUT files described in Design Descriptions 42 and 43. The printed logged flaws are the first flaws sampled in the PFM looping structure that meet the different criteria in the tables. Procedure flaw_track within module flaw_s is used to write out the flaw tracking log table. Variables used are ctype(ktype), 1(2)or(3), itran, ntrial, nflaw, nsbr2, and nsbr1. A sample of the output in the FLAW_TRAC.LOG files is shown below:

```
STABLE ARREST :parent circ. plate category 1 flaw: itran=2 irpv=26 kflaw=18 parent
subr=8 child subr=8
VESSEL FAILURE:parent axial weld category 2 flaw: itran=2 irpv=29 kflaw=17 parent
subr=5 child subr=5
STABLE ARREST :parent axial plate category 2 flaw: itran=2 irpv=40 kflaw=52 parent
subr=8 child subr=8
VESSEL FAILURE:parent circ. plate category 1 flaw: itran=1 irpv=43 kflaw=28 parent
subr=12 child subr=12
VESSEL FAILURE:parent circ. plate category 1 flaw: itran=1 irpv=46 kflaw=25 parent
subr=13 child subr=13
```

Design 40 FAVPFM generates CPI_History and CPF_History output files containing the running average (mean) of CPI and CPF, respectively, for the purposes of evaluating convergence.

These files contain tabular data of trial #, mean CPI (or CPF) for transient i, i + 1, through the last transient.

As discussed in 133, the cpi_history.out file captures the running averages (i.e., "mean') of CPI. Subroutines pfm and report provide the write statements to provide the header and value, respectively, and are written to cpi_history.out (Fortran Unit 71) for all RPV simulations and transients. The variable name used is AMNCPI.

Also, the cpf_history.out file captures the running averages (i.e., "mean") of CPF. Subroutines pfm and report provide the write statements to provide the header and value, respectively, and are written to cpf_history.out (Fortran Unit 72) for all RPV simulations and transients. The variable name used is AMNCPF.

Design 41 An RTNDT.out file is generated to contain meaningful and descriptive output for crack tip RT_{NDT} distribution within the vessel. The file contains the following information:

- 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.
- 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.
- 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.

In order to generate this information, the main FAVPFM program first calls subroutine file_init_pfm to create a file using Fortran Unit 85, called RTNDT.OUT. Then FAVPFM calls subroutine pfm, which then calls subroutine Mark. Subroutine Mark writes out the headers and values for the first data block described above (i..e, major region #, product, subregion # with the controlling RT_{NDT}(max) for that major region and actual subregion #, and the RT_{NDT}(max) value) using variables I, ISMAXP, ISMAXC, and RTMAX for welds and variables I, JMAX, and RTMAX for plates and forgings. For the next set of printed data table values, subroutine pfm uses the following variables: I, IRTDT, IRTACC(J,I,1), ISUM1, IRTACC(J,I,2), ISUM2, ISUM3, and ISUM4. In the last table which summarizes all the major regions, subroutine pfm uses the following variables: IRDT, ISUM5, HISTOT, CDFTOT, ISUM6, HSTCPI, and CDFCPI.

Please note that the reported RT_{NDT} values in the RTNDT.OUT file are different than those reported in the output file described in Design 28 on page 133. The RTNDT.OUT file contains the epistemic corrected RT_{NDT} values (see Figure 14 and Reference [16]), whereas the output file (Fortran Unit 29) does not.

Design 42 An ARREST.out file is 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 is generated for each transient and for all transients. In addition to the summary statistics, the following detailed information is provided when the flaw tracking option is selected:

1. Arrest trial # (trial number in IGA model), P_F value, Parent region #, Child region #, depth of flaw, inner crack tip location (relative to inside vessel surface), flaw category #, and aspect ratio,

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 $\widehat{\Delta T_{30}}$ shift due to irradiation), sampled RT_{NDT0}, -DTEPA (sampled $\widehat{-\Delta RT}_{epistemic-arrest}$ epistemic uncertainty term in RT_{Arrest}), DTARR (sampled $\widehat{-\Delta RT}_{Arrest}$), DRTNDX ($\Delta RT_{NDT}$ 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 $\left[ksi\sqrt{in.}\right]$) for driving force for crack, KIC (current value of K_{IC} $\left[ksi\sqrt{in.}\right]$), KIA (current value of K_{Ia} $\left[ksi\sqrt{in.}\right]$), KJIc (current value of J_{IC} converted to K_{IIC} $\left[ksi\sqrt{in.}\right]$), KJR* (current value of J_R^* converted to K_{JR^*} $\left[ksi\sqrt{in.}\right]$), USEI (current value of irradiated upper-shelf CVN energy (ft-lbf), C_DT (coefficient for sampled J_R curve where $J_R = C_{DT}(\Delta a^{m\_DT})$), m_DT (exponent for sampled J_R curve where $J_R = C_{DT}(\Delta a^{m\_DT})$, da0 (accumulated flaw advancement under stable ductile tearing), P_T0 (cumulative probability used in sampling T0), P_JIc (cumulative probability used in sampling for JIc, P_m (cumulative probability used in sampling m_dT, and sflow (sampled flow stress).

3. If a trial results in chemistry being resampled, SCU (sampled copper content), SNI (sampled nickel content), SPHOS (sampled phosphorous), and SMN (sampled manganese content) are provided.

The main FAVPFM program calls subroutine file_init_pfm using Fortran Unit 84 to create the ARREST.OUT file. Following the call to file_init_pfm, the main program then calls subroutine pfm to perform the main probabilistic fracture mechanics calculations, which generates the necessary information for the ARREST.OUT file through the many calls to other subroutines. Subroutine pfm calls subroutine account to write out the first line in the ARREST.OUT file by printing the Arrest trial # (trial number in IGA model), P_F value (sample probability from a uniform distribution), Parent region #, Child region #, depth of flaw, inner crack tip location (relative to inside vessel surface), flaw category #, and aspect ratio for the user selected RPV trial, transient, and flaw number obtained from the previously generated FLAW_TRAC.LOG file (see Design 39 on page 148). Subroutine account variables used are J, PF, NSBR2, NSBR, XDEPTH, XINNER, IFLCAT, and ASPECT.

A number of subroutines are then called by subroutine pfm to print out the detail flaw characteristics depending on its status (arrest, stable, propagated, initiated, reinitiated, non-reinitiated or failed). First, subroutine pfm calls subroutine Account, which then calls subroutine PROP. Subroutine PROP is the primary routine which controls which subroutine will be called next to write out information to the ARREST.OUT file. Note that subroutine pfm does not have any write statements to ARREST.OUT. A summary of the called subroutines by subroutine PROP and their description include the following (presented in call order of subroutine PROP):

- Subroutine ARRHEAD prints out the headers and first set of detailed flaw status and characteristics for an initiated flaw (i.e., "INITIA"). Variables used include NFLAW, TIME(MTSTEP), L, ZSURF(L), TEMP(L,ITRAN,MTSTEP), DT30, RTNDTO, RTNDTII, an AKICHEK. Note that two different headers will be printed depending on whether the ductile tearing checking option is selected or not.
- Subroutine FAILWR prints out status of flaws that have resulted in vessel failure. The following failure messages are possible:
    - ' FAILURE: UNSTABLE DUCTILE TEARING',
    - ' FAILURE: STABLE DUCTILE TEAR TO PLASTIC INSTABILITY',
    - ' FAILURE: CLEAVAGE PROPAGATION TO PLASTIC INSTABILITY',
    - ' FAILURE: STABLE DUCTILE TEAR PROPAGATION - EXCEEDS WALL DEPTH FAILURE CRITERIA', or
    - ' FAILURE: CLEAVAGE PROPAGATION - EXCEEDS WALL DEPTH FAILURE CRITERIA'.

  Note that unstable ductile tearing occurrences will also print out the detailed flaw characteristics such as NFLAW, TIME(MTSTEP), L, ZSURF(L), TEMP(L,ITRAN,MTSTEP), P, DT30, RTNDTO, -DRTEPA, DRTARR, DRTNDX, RTNDTA, RTNDTII, TEMP(L,ITRAN,MTSTEP)-RTNDTA, TADJII, AKICHEK, SMKIC, SMKIA, KJIc, KJRstar, USEi, C_DT, m_DT, da0, P_T0, P_JIc, P_m, and sflow. These variables match those described in paragraph 2 above.
- Procedure RECHEM in module chemistry_s prints out the resample chemistry values when the flaw enters the next weld layer (i.e., "RECHM" is printed in the output). Variables include SCU, SNI, SPHOS, and SMN.
- Subroutine STABLE prints out the detailed flaw characteristics for a stable ductile tear-related flaw (i.e., "STEAR" is printed in the output). Variables are equivalent to those used in subroutine FAILWR, which are provided above.

- Subroutine PROPA prints out the detailed flaw characteristics for a flaw propagating through cleavage fracture (i.e., "PROPA" is printed in the output). Variables are equivalent to those used in subroutine FAILWR, which are provided above.
- Subroutine ARRT prints out the detailed flaw characteristics for a flaw that was crack arrested (i.e., "ARRES" is printed in the output). Variables are equivalent to those used in subroutine FAILWR, which are provided above.
- Procedure REINI in module write_arrest_data_s prints out detailed flaw characteristics for a flaw that was crack re-initiated by ductile tearing (i.e., "TREINI" is printed in the output). Variables are equivalent to those used in subroutine FAILWR, which are provided above.
- Procedure REINI2 in module write_arrest_data_s prints out detailed flaw characteristics for a flaw that was crack re-initiated by cleavage fracture (i.e., "REINI" is printed in the output). Variables are equivalent to those used in subroutine FAILWR, which are provided above.
- Procedure NREINI in module write_arrest_data_s prints out detailed flaw characteristics for a flaw that has arrested or stopped tearing and is stable for this time step (i.e., "STABLE" is printed in the output). Variables are equivalent to those used in subroutine FAILWR, which are provided above.

Summary statistics are printed by subroutine Report in all PFM cases with the flaw tracking option on or off. A summary of stable arrest and histogram of stable arrest by depth of flaw is generated for each transient and for all transients. Variables used by subroutine Report include I, IATST2(I), ISEQ(ITRAN,1), ISEQ(ITRAN,2), PCTOT.

Design 43 Similar to Design 42 for the ARREST.OUT file, when the user selects the flaw tracking option (i.e., FLAW_LOG_OPTION=1 with ITRAN, IRPV, and KFLAW specified), a TRACE.OUT file is generated which provides verification data for CPI and CPF calculations. A 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 also provided. If the Tracking option is used, the following detailed information is provided:

ITRAN (transient #), IRPV (RPV Simulation), FLAW(Flaw #), Subregion #s (associated with Parent and Child), IPASS (number of flaws in the parent subregion), SCU (sampled $\widehat{\boldsymbol{Cu}}$ content), SNI (sampled $\widehat{\boldsymbol{Ni}}$ content), SPHOS (sampled $\widehat{\boldsymbol{P}}$ content), SMN (sampled $\widehat{\boldsymbol{Mn}}$ content), SFID (sampled/attenuated fluence $\widehat{\boldsymbol{f_0}}(\boldsymbol{r}) \times \mathbf{10^{19}}$ neutrons/cm^2 at the crack tip), RTNDT0 (sampled unirradiated $\widehat{\boldsymbol{RT}}_{\boldsymbol{NDT0}}$), DRTEPI (sampled $\widehat{\boldsymbol{\Delta RT}}_{\boldsymbol{epistemic}}$ epistemic uncertainty term in $\widehat{\boldsymbol{RT}}_{\boldsymbol{NDT0}}$), DRTNDT (sampled $\widehat{\boldsymbol{\Delta T_{30}}}$ CVN shift term from Eason and Wright model), SDRTNDT (sampled $\widehat{\boldsymbol{\Delta RT}}_{\boldsymbol{NDT}}$), 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 $\boldsymbol{K_I}$ [ksi$\sqrt{\text{in.}}$]). TEMP (temperature at crack tip), CPI (current conditional probability of initiation), CDCPI (current Δcpi), 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 Δcpf at this time), and CPFTOT (conditional probability of failure).

The main FAVPFM program calls subroutine file_init_pfm using Fortran Unit 81 to create the TRACE.OUT file. Following the call to file_init_pfm, the main program then calls subroutine pfm to perform the main probabilistic fracture mechanics calculations, which generates the necessary information for the TRACE.OUT file through the many calls to other subroutines. Following the probabilistic fracture mechanics analysis, subroutine pfm calls subroutine account to write out the headers and detailed flaw related information described above. The write statements are located at the end of subroutine account. This data is only written if the user specified ITRAN, IRPV, and KFLAW on the TRAC card results in a calculated CPI > 0. The variables used in writing out the above information are as follows:

- ITRAN for ITRAN (transient #),
- NTRIAL for IRPV (RPV Simulation),
- NFLAW for FLAW(Flaw #),
- NSBR2 and NSBR, respectively for Subregion #s (associated with Parent and Child),
- IPASS for IPASS (number of flaws in the parent subregion),
- STOR2(6) for SCU (sampled $\widehat{\boldsymbol{Cu}}$ content) for cleavage fraction,
- STOR2(7) for SNI (sampled $\widehat{\boldsymbol{Ni}}$ content) for cleavage fraction,
- STOR2(8) for SPHOS (sampled $\widehat{\boldsymbol{P}}$ content) for cleavage fraction,
- STOR2(9) for SMN (sampled $\widehat{\boldsymbol{Mn}}$ content) for cleavage fraction,
- STOR2(10) for SFID (sampled/attenuated fluence $\widehat{\boldsymbol{f_0}}\,(\boldsymbol{r}) \times \mathbf{10^{19}}\ \mathrm{neutrons/cm^2}$ at the crack tip),
- STOR2(6) for SCU (sampled $\widehat{\boldsymbol{Cu}}$ content) for ductile fraction,
- STOR2(7) for SNI (sampled $\widehat{\boldsymbol{Ni}}$ content) for ductile fraction,
- STOR2(8) for SPHOS (sampled $\widehat{\boldsymbol{P}}$ content) for ductile fraction,
- STOR2(9) for SMN (sampled $\widehat{\boldsymbol{Mn}}$ content) for ductile fraction,
- STOR2(1) for RTNDTO (sampled unirradiated $\widehat{\boldsymbol{RT}}_{\boldsymbol{NDT0}}$),
- STOR2(2) for DRTEPI (sampled $\widehat{\boldsymbol{\Delta RT}}_{\boldsymbol{epistemic}}$ epistemic uncertainty term in $\widehat{\boldsymbol{RT}}_{\boldsymbol{NDT0}}$),
- STOR2(17) for DRTNDT (sampled $\widehat{\boldsymbol{\Delta T_{30}}}$ CVN shift term from Eason and Wright model),
- STOR2(5) for DT30,
- STOR2(3) for SDRTNDT (sampled $\widehat{\boldsymbol{\Delta RT}}_{\boldsymbol{NDT}}$),
- STOR2(4) for RTNDT (sampled irradiated at crack tip),
- STOR2(11) for USE0 is printed if ductile tearing is being checked,
- STOR2(12) for USEi is printed if ductile tearing is being checked,

- IFLCAT for FLAW CAT (flaw category),
- XDEPTH for DEPTH (flaw depth),
- XINNER for XINNER (inner crack tip position for embedded flaws),
- ASPECT for ASPECT (flaw aspect ratio),
- IORIENT for IORIENT (axial=1 or circumferential=2 flaw orientation),
- IHEAT for IHEAT (inner surface=1 or outer surface=2 flaw) or IHEAT_EMBEDDED for IHEAT_EMBEDED,
- I for I (time increment counter),
- TIME(I) for TIME(elapsed time in transient),
- STORE(I,1) for KI (applied $\boldsymbol{K_I}$ $[\mathrm{ksi}\sqrt{\mathrm{in.}}]$),
- STORE(I,2) for TEMP (temperature at crack tip),
- CPI(ITRAN,I,NFLAW) for CPI (current conditional probability of initiation),
- CDCPI(I) for CDCPI (current Δcpi),
- FAILCL(I) for FAIL CL (number of trials failing the vessel at this time increment due to cleavage),
- FAILDT(I) for FAIL DT (number of trials failing the vessel at this time increment due to ductile tearing),
- CDCPF(I) for CDCPF (current Δcpf at this time), and
- CPFTOT for CPFTOT (conditional probability of failure).

The associated headers and summary of flaws are printed by the main FAVPFM program if the user sets the FLAW_LOG_OPTION=1. Note that the requirement to have the user specified ITRAN, IRPV, and KFLAW on the TRAC card resulting in a calculated CPI > 0 is not required for the summary report. The summary includes those 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 then provided. For each flaw Category, the values for itran, irpv, kflaw, parent region, and child subregion are printed. The FAVPFM program uses the array iflaw_track(i,j) to print the number of flaws for each category. The iflaw_track(i,j) array is set in procedure flaw_track in module flaw_s. The i indexes correspond to the different material type (plate or weld), axial or circumferential flaw orientation, and Category 1, 2, or 3. The j index from 1 to 5 correspond to itran, irpv, kflaw, parent region, and child subregion, respectively. Note that for Category 1 flaws, only circumferential oriented flaws in weld and plate are presented because these are the most limiting flaws for internal surface breaking flaws.

- Indices j = 1 to 5 and I = 2 to 11 are for flaws experiencing vessel failures.
- Indices j = 1 to 5 and I = 13 to 22 are for flaws experiencing stable arrests.

- Indices j = 1 to 5 and I = 24 to 33 are for flaws experiencing reinitiations.
- Indices j = 1 to 5 and I = 35 to 44 are for flaws experiencing stable ductile tearing.
- Indices j = 1 to 5 and I = 46 to 55 are for flaws experiencing unstable ductile tearing.

Design 44 FAVOR modules are modified such that run times are not degraded.

In order to ensure modifications to not degrade runtimes, FAVOR modules were updated to implement modernization standards. See Design 1. This step has been documented within GitHub through the continous integration and testing. Some examples include replacing non-standard features (e.g., real*), replacing deleted features (e.g., arithmetic-if-stmt), replacing obsolescent features (e.g., common-stmt, block-data-stmt, entry-stmt, character*, alternate-return, and specifically named intrinsic functions), eliminating redundant procedures (e.g., functions and subroutines), and incorporating any parallel processing.

Design 45 FAVOR modules are modified and compiled such that such that FAVOR can run on LINUX, MAC, and Microsoft Windows operating systems.

Consistent with Section 8 of the FAVOR Software Quality Assurance Plan (Ref [3]), modifications are compiled for LINUX, MAC, and MS Windows. The procedure used for compiling the FAVOR module(s), downloading FAVOR module(s), building executables, testing, and installing FAVOR are located and controlled on github.

Here ends the Design descriptions that meet all the design requirements specified in the FAVOR SRD (Reference [4]).

6 Summary

Section 5 of this report provides the software design description for v20.1.12 that meet the software requirements specified in Reference [4]. 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. Consistent with the FAVOR Software Quality Assurance Plan (Reference [3]) , this document captures the computational and logical sequence necessary to meet the software requirements for v20.1.12 (Reference [4]). Applicable software architecture, numerical methods, mathematical models, physical models, control flow, control logic, data model, data flow, process flow, data structures, process structures, and the applicable relationships between data structures and process structures are addressed. The design of the user interface and design of interfaces with other software are also specified. Measures are also discussed to mitigate the consequences of potential user errors or other problems. These potential problems include external and internal abnormal conditions and events that can affect the computer program critical outputs or functionality. Sufficient information in the design has been provided so the code modifications can be passed to a competent programmer for implementation. The Software Design Description Criteria Form FAVOR-SQA-5 (see SQAP [3]) is used as an aide in developing this SDD.