

**SIMMER-III: A Computer Program for LMFR Core
Disruptive Accident Analysis**

- Version 3.A Model Summary and Program Description -

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O-arai Engineering Center
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SIMMER-III: A Computer Program for LMFR Core Disruptive Accident Analysis

- Version 3.A Model Summary and Program Description -

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ABSTRACT

An advanced safety analysis computer code, SIMMER-III, has been developed to investigate postulated core disruptive accidents in liquid-metal fast reactors (LMFRs). SIMMER-III is a two-dimensional, three-velocity-field, multiphase, multicomponent, Eulerian, fluid-dynamics code coupled with a space-dependent neutron kinetics model. By completing and integrating all the physical models originally intended at the beginning of this code development project, SIMMER-III is now applicable to integral reactor calculations and other complex multiphase flow problems. A systematic code assessment program, conducted in collaboration with European research organizations, has shown that the advanced features of the code have resolved many of the limitations and problem areas in the previous SIMMER-II code.

In this report, the models, numerical algorithms and code features of SIMMER-III Version 3.A are described along with detailed program description. Areas which require future model refinement are also discussed. SIMMER-III Version 3.A, a coupled fluid-dynamics and neutronics code system, is expected to significantly improve the flexibility and reliability of LMFR safety analyses.

This study was performed under the Agreement between JNC and FZK/CEA/IRSN on the SIMMER-III code.

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高速炉炉心損傷事故解析コード SIMMER-III - Version 3.A モデル概要及びプログラム記述 -

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要 旨

核燃料サイクル開発機構（サイクル機構）では、高速炉の仮想的な炉心損傷事故を評価するために新たな安全解析コード SIMMER-III の開発を進めてきた。SIMMER-III は、2次元、3速度場、多相多成分、オイラー座標系の流体力学モデルを中核として、物質配位及びエネルギー状態に対応した空間依存の核計算モデルを有機的に結合したコードである。現在までに、本コード開発プロジェクトの当初に計画していた全てのモデル開発を終了したことになり、いよいよ実機の安全解析や複雑な多相流解析に本格的に適用できる段階に達した。また、コード開発と併行して、体系的なモデル検証研究を欧州研究機関と共同で進めており、その結果、モデルの高度化により従来の SIMMER-II コードで問題とされた適用限界の多くが解消できるとの見通しを得つつある。

本報告書では、SIMMER-III Version 3.Aの詳細なプログラム解説に加えて、各要素物理モデル、数値計算アルゴリズム及びコードの特徴について述べる。今後さらにモデル改良を行うことが望まれる分野についてもとりまとめた。新たに完成した SIMMER-III Version 3.Aにより、高速炉の安全解析における信頼性と適用範囲が飛躍的に向上できるものと期待されている。

本研究は、核燃料サイクル開発機構がドイツ FZK 及びフランス CEA/IRSN との間の SIMMER-III コードに関する協力協定に基づいて実施した研究の成果である。

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CHAPTER 1

INTRODUCTION

1.1. Objectives and Perspective

The consequences of postulated core disruptive accidents (CDAs) have been one of major concerns in the safety of liquid-metal fast reactors (LMFRs). Complexities in evaluating the transition phase of CDAs, together with limited direct experimental data in comparison with the initiating phase of CDAs, tend to introduce relatively large uncertainties in the safety analysis [1, 2]. In the past, the SIMMER-II code was developed at the Los Alamos National Laboratory (LANL) [3], and has been used in many experimental and reactor analyses [4]. The code has played a pioneering role, especially in studying the transition phase phenomenology. However, extensive application also revealed several serious limitations in virtually all the major areas of fluid dynamics, particularly in: heat, mass and momentum constitutive relationships; the multiphase-flow numerical solution methods; the multicomponent equation-of-state (EOS) formalism; and the fuel-pin and structure models. For the neutronics model, neutron flux shape calculations sometimes had difficulty in obtaining a converged solution under an extreme fuel configuration. These deficiencies and shortcomings have limited the code applicability and reliability, and have motivated a new code development project.

The development of a next-generation code, SIMMER-III, was initiated in the late 1980s at the Japan Nuclear Cycle Development Institute (JNC), formerly called Power Reactor and Nuclear Fuel Development Corporation (PNC), initially in collaboration with LANL under the agreement with the United States Nuclear Regulatory Commission (USNRC). This joint SIMMER-III program between JNC and the USNRC was terminated soon and the subsequent development effort was taken over solely by JNC in 1990. The program was later joined, starting from 1992, by AEA Technology, United Kingdom, until 1993, Forschungszentrum Karlsruhe (FZK), Germany, and Commissariat à l'Energie Atomique (CEA), France. The CEA partner had also included Institute de Radioprotection et de Sûreté Nucléaire (IRSN), formerly called Institute de Protection et de Sûreté Nucléaire (IPSN), until 1998. Since 2002, IRSN has participated again. The present code development and assessment program is being carried out based on the agreement between JNC and FZK/CEA/IRSN.

The purpose of SIMMER-III is to alleviate some of the above limitations in the previous code and thereby to provide the next-generation tool for more reliable analysis of the transition phase. SIMMER-III is a two-dimensional, three-velocity-field, multiphase, multicomponent, Eulerian, fluid-dynamics code coupled with a space- and energy-dependent neutron kinetics model. The scope of the code development effort is determined primarily from the needs on the accident-analysis point of view and is optimized so as to utilize either existing or achievable technologies. The outcome and experience gained in course of the AFDM development [5-8] are used to maximum extent.

The advanced features of the code can resolve many of the problems and limitations associated with SIMMER-II, as summarized in **Tables 1-1** and **1-2**. SIMMER-III is intended to be a generalized code that is useful for analyzing relatively short-time-scale multiphase flow problems with or without neutronics. Although the original objective of SIMMER-III is primarily to resolve some of the key LMFR CDA issues, its flexible framework enables us to apply the code to various areas of interest which are consistent with the SIMMER-III modeling framework. It is believed, therefore, that the application of the code will possibly include: accident analyses of any types of future or advanced fast reactors, steam-explosion problems in current- and future-generation light water reactors, and general types of multiphase flow problems.

The development of the SIMMER-III code has successfully reached the milestone that integrated code application can be initiated [9]. Major physical models were completed and integrated into a fluid-dynamics code system, that is Version 1, which was released in 1993. The coupling of the neutronics model to the fluid-dynamics model has been completed for the release of Version 2. The Phase 2 assessment has been completed and documented in 2000 [10-12] and SIMMER-III is now used for reactor applications as well [13]. The originally intended scope of the code is now completely available, and in addition far more sophisticated features are made available. The latest version of the code is Version 3.A which is documented in the present report.

One of the major limitations of SIMMER-III is the geometric framework that allows only one- or two-dimensional calculations. Needs for a three-dimensional version of SIMMER have long been discussed, because extension of the SIMMER technology to three dimensions is rather straightforward. Such an effort has been actually taken at JNC since several years ago, with completing the first version of SIMMER-IV in 2000. Version 1 of SIMMER-IV couples the three-dimensional fluid dynamics, a direct extension of SIMMER-III, with two-dimensional neutronics. The latest version of SIMMER-IV, Version 2.A, is documented in Ref. [14]. In this version, coupling with a three-dimensional neutronics model has been completed under collaboration between FZK and JNC.

The partners of the SIMMER-III project (JNC, FZK, CEA and IRSN) are conducting a systematic and comprehensive validation of the code. This effort, termed more generally as “the assessment program”, consists of two phases: Phase 1 for fundamental or separate-effect code assessment of individual models; and Phase 2 for integral code assessment for key physical phenomena relevant to LMFR safety. The Phase 1 assessment has been completed in 1996 and the achievement of the study is summarized in Ref. [10]. The Phase 2 assessment has been completed, with a full synthesis report published in 2000 [12].

The development and assessment of SIMMER-III is still an on-going program. Recent code applications to reactor safety analyses and the Phase 1 and 2 assessment studies have identified the several modeling areas that require further improvement in the future. There are several active safety experimental programs being conducted or planned, and they are expected to provide valuable data for further code validation and improvement. These desired future studies are discussed in Ref. [12]. Thus the SIMMER-III code is considered to represent an evolving technological project. It should be noted that the international collaboration in this project between JNC and FZK/CEA/IRSN has been extremely successful and productive, and hence the continuation is highly desired.

1.2. Structure of Documentation

This report is intended to serve as a user’s manual of SIMMER-III Version 3.A, and provides the information necessary for code users who run the code. It should not be expected that the use of SIMMER-III is easy to use for beginner users and hence should not be used as a black box. Using such complex codes as SIMMER-III and SIMMER-IV requires sufficient phenomenological understanding on physical processes being calculated; otherwise there will be a certain risk to produce non-physical results.

In the rest of this report, the summary description of SIMMER-III models and methods are given in **Chapter 2**. The program description in **Chapter 3** presents the minimum programming information for users. **Chapter 3** also explains the standard sample problems released with the code and defined for testing various parts of SIMMER-III. Furthermore **Appendices** to this report provide: the description of: Comdecks and Decks (**Appendix A**), system-dependent routines/functions (**Appendix B**), equation-of-state functions (**Appendix C**), thermophysical-property functions (**Appendix D**), constants and default data used in SIMMER-III (**Appendix E**), post-processing (plot) files (**Appendix F**), the full input manual (**Appendix G**), and sample input data listings (**Appendix H**). A useful and powerful post-processing program, BFSCAN, was developed at JNC and is released with SIMMER-III. The minimum information needed to use BFSCAN is given in **Appendix I**.

Table 1-1. Previous Limitations and SIMMER-III Improvements.

Models and Methods	SIMMER-II (Limitation/Problem areas)	SIMMER-III (Improved models)
Dimensions	2	2
No. of velocity fields	2	3
No. of pin fuel nodes	1	2 (surface and interior) and optionally multi-node
Fuel-to-clad gap conductance	No	Yes
Distinction of left and right structures	No (1 crust fuel and 1 can wall)	Yes (left/right crust fuels and can walls; surface/interior nodes for each wall)
Fission gas in pin fuel	Intra-/inter-granular gases and release from pin fuel	One fission gas in pin fuel and no release from solid
Fission gas in liquid field	No	Fission gases in liquid fuel and solid particles and release
Control material	Pin control or liquid	Pin control or solid particles
No. of EOS materials	5 (for all the system)	5 (different sets in different regions)
EOS model	Analytic EOS with simple (or temperature-independent) functions	Accurate analytic EOS with consistent functions over wide temperature ranges
Thermophysical properties	Mostly constant (except for liquid density and speed of sound)	Most properties expressed by accurate analytic functions
Gas EOS	Ideal gas	Non-ideal gas (MRK EOS)
Spatial differencing	First-order donor cell	Higher-order scheme (van Leer)
Convection algorithm	Combined explicit/implicit method from KACHINA	Semi-implicit method
Viscous (momentum diffusion) terms	No	Yes
Mass and energy source terms and intra-cell updates	Exchange rates determined at the beginning of cycle	Four-step algorithm (from AFDM) to update source terms separately
Multi-phase flow regimes	Dispersed (droplet) flow regime only	Multiple flow regimes with smooth transition for both pool and channel flows
Interfacial areas	Instantaneous; no convection	Convection with flow; time-dependent source terms

Table 1-1. (cont).

Models and Methods	SIMMER-II (Limitation/Problem areas)	SIMMER-III (Improved models)
Melting and freezing (M/F)	Only equilibrium path; non-equilibrium path for fuel crust formation	Both equilibrium and non-equilibrium M/F transfers for all the dominant paths
Fuel freezing model	Particle (bulk) and crust (conduction) formation	Fuel caps freezing model for generalized modeling
Vapor state in single-phase cells	No explicit treatment (abrupt change in phase transition)	Consistently treated with two-phase cells
Vaporization and condensation (V/C)	Only at liquid/vapor interface and same material	Allow phase transition for all the paths at liquid/vapor and liquid/liquid interfaces
Diffusion-limited phase transition	Modeling attempted but not used.	A model for multi-component available
Film boiling heat transfer	No	Yes
Drag coefficient of hot droplet with film boiling configuration	No	Yes
Cell-dependent B.C.	No	Yes
Virtual walls	No	Yes
Fluid particle distortion	No	Cap-shape bubbles in MXF; internal circulation in HTC
Cross-section models	No up-scattering	A full scattering matrix
Neutron flux shape method	Diffusion or TWOTRAN	TWODANT
External neutron source and sub-critical treatment	No	Yes
Time-step control	Automatic control based on physics	Automatic control with fluid time-step re-calculations
Plot files for post-processing	Standard but limited	Plus extensive and flexible features added
Programming language and standard computer	FORTRAN-IV and Los Alamos CDC and CRAY	FORTRAN-77 and IBM compatible or Unix EWS
Other programming technique	Designed for CDC, no vector programming, and limited modularization	Designed for modular and vector programming, and NAMELIST input

Table 1-2. Accident Analysis Aspects of Advanced SIMMER-III Features.

Key Accident Phenomena (Formerly Identified Problem Areas)	Advanced SIMMER-III Features (Improvement from SIMMER-II)
Pool boil-up exaggerated due to instantaneous interfacial areas	Interfacial area convection with time-dependent source terms
Liquid interface smeared due to numerical diffusion	Higher-order differencing for better interface resolution
No fuel/steel separation nor fuel penetration into coolant	Three-velocity-field treatment allows relative motion between liquids
Liquid/vapor coupling over-estimated in low void fraction flows	Modeling a bubbly flow with smooth transition between flow regimes
Inconsistency with initiating phase code (SAS-series)	Detailed pin modeling allows better connection from SAS
Instantaneous fission gas release upon pin fuel breakup	Accommodate fission gas in liquid/particle fuel and model its release
Can wall melt-out treated inappropriately	Separated left/right walls with two-node representation
Discontinuity or instability upon single to two phase transition	Consistent treatment of single-phase cells with much accurate analytic EOS
Pressure drop along a pin bundle underestimated	Modeling channel flow regimes as well with smooth transition in-between
No fuel or steel vapor condensation on coolant	Modeling all the important mass-transfer processes
Instabilities of vaporization/condensation and EOS at high temperature	A new and stable solution procedure
Poor conservation of mass and energy	Much improved by semi-implicit method, and consistent treatment of single-phase cells and missing components
Convergence difficulties in flux shape under come conditions (TWOTRAN)	More stable and efficient solution method available (TWODANT)
Cross-section model only for fast neutron spectrum	Allowing up-scattering for modeling thermal neutron spectrum as well
Limited boundary condition treatment	Flexible and versatile specifications
Code assessment limited and not systematic	Code assessment in parallel with development for systematic and comprehensive validation

CHAPTER 2

SUMMARY OF MODELS AND METHODS

2.1. SIMMER-III CODE FRAMEWORK

2.1.1. Code Framework and Geometry

The conceptual overall framework of SIMMER-III is shown in **Fig. 2-1**. The entire code consists of three elements: the fluid-dynamics model, the structure (fuel pin) model, and the neutronics model. The fluid-dynamics portion, which constitutes about two thirds of the code, is interfaced with the structure model through heat and mass transfer at structure surfaces. The neutronics portion provides nuclear heat sources, based on the time-dependent neutron flux distribution in consistent with mass and energy distributions calculated by the other code elements. Without the neutronics, nuclear heat source can still be provided by power-versus-time table, based on input specification and specific power density distribution.

To increase the computational efficiency, an optimized hierarchy of three-level time-step control is implemented; that is, the fluid-dynamics, reactivity (and fuel pin heat transfer), and flux-shape time steps in the order from the smallest. This time-step control scheme is shown in **Fig. 2-2**, and the overall computational flow in **Fig. 2-3**.

The basic geometric structure of SIMMER-III is a two-dimensional R-Z system as shown in **Fig. 2-4**, although optionally an X-Z or one-dimensional system can also be used for various fluid-dynamics calculations. A domain of a neutronics calculation, implicitly assumed an R-Z cylinder, is a sub-region of the fluid-dynamics computational mesh, and each neutronics radial ring can be sub-divided into smaller nodes. In each fluid-dynamics mesh cell, the structure-field volume fraction, α_s , is defined for the sum of the volume fractions for fuel pin and can wall components, which are stationary and provides walls containing fluid flow. Unlike SIMMER-II, the can walls with refrozen crust fuel attached on them are distinguished between left and right cell boundaries for improved simulation of a core melt-out behavior. In addition, the structure surface nodes are separated from the interior nodes to improve thermal response from contact with the fluid.

The remaining volume ($1-\alpha_s$) is occupied by fluid having three velocity fields. When the cell vapor volume fraction falls below a certain non-zero value (α_0), the mesh cell is regarded as single phase. This treatment is necessary, even in SIMMER-III, for the numerical reason that a vapor state is explicitly treated even in a single-phase liquid cell.

The treatment of single-phase cells consistent with two-phase cells eliminates such problems observed in SIMMER-II as vapor mass non-conservation and unphysical pressure behavior upon phase transition. The value of α_0 can be made reasonably small (for example, 10^{-4} , with the default value in SIMMER-III being 10^{-2}), compared with the former codes, such that any errors associated with this approximation are negligible.

2.1.2. SIMMER-III Components

The complete lists of the structure-, liquid- and vapor-field components are shown in **Tables 2-1** through **2-3**. In these tables, the lower-case subscripts denote density components while the upper-case subscripts denote energy components commonly used throughout SIMMER-III. The fuel components are divided into fertile and fissile in their mass (density components) to represent different enrichment zones in the core. However, the two materials are assumed to be mixed intimately, and hence the single temperature is assigned as an energy component. Namely, the macroscopic (smeared) densities of a fuel component for example for the pin fuel surface node, $\bar{\rho}_{s1}$, has the following equivalence:

$$\bar{\rho}_{s1} = \bar{\rho}_{s1} + \bar{\rho}_{s2}. \quad (2-1)$$

Since the component specific volumes (not microscopic densities) ν_M are used in the SIMMER-III EOS model, macroscopic densities $\bar{\rho}_M$ are converted to volume fractions α_M , for the above example, by:

$$\alpha_{s1} = \bar{\rho}_{s1} \nu_{s1}. \quad (2-2)$$

The pin fuel interior component is not included in **Table 2-1**, because it is treated only in the fuel-pin model. The pin interior is modeled by one-point temperature node in a standard simple model (SPIN), whereas an optional detailed model calculates the radial temperature distribution (DPIN). The pin models are listed in **Table 2-4**. The intra-granular and inter-granular fission gas components in the pin fuel are not distinguished in SIMMER-III, because such detailed treatment is judged to be beyond the scope of this code. Improvement exists, however, in the modeling of fission gas in the liquid-field fuel components (see **Table 2-2**) and this eliminates a problem of instantaneous release and unphysical pressurization observed in SIMMER-II.

The default assignment of fluid components to the three velocity fields is also shown in **Tables 2-2** and **2-3**. The present selection is made such that the relative motion of fuel with either steel or coolant can be simulated. This assignment can be changed through user-specified input. Finally the vapor species are assumed to be completely mixed and a single energy is assigned to the vapor field.

The direction-related variables are listed in **Table 2-5**. The radial velocity in the R direction is denoted as U with radial node index as I . The axial velocity in the Z direction is denoted as V with axial node index as J .

Table 2-1. SIMMER-III Fluid-Dynamics Structure-Field Components.

Density Components (MCSR)		Energy Components (MCSRE)	
$s1$	Fertile Pin Fuel Surface Node	$S1$	Pin Fuel Surface Node
$s2$	Fissile Pin Fuel Surface Node		
$s3$	Left Fertile Fuel Crust	$S2$	Left Fuel Crust
$s4$	Left Fissile Fuel Crust		
$s5$	Right Fertile Fuel Crust	$S3$	Right Fuel Crust
$s6$	Right Fissile Fuel Crust		
$s7$	Cladding	$S4$	Cladding
$s8$	Left Canwall Surface Node	$S5$	Left Canwall Surface Node
$s9$	Left Canwall Interior Node	$S6$	Left Canwall Interior Node
$s10$	Right Canwall Surface Node	$S7$	Right Canwall Surface Node
$s11$	Right Canwall Interior Node	$S8$	Right Canwall Interior Node
$s12$	Control	$S9$	Control

Table 2-2. SIMMER-III Fluid-Dynamics Liquid-Field Components.

Density Components (MCLR)		Energy Components (MCLRE)		Velocity Fields
$l1$	Liquid Fertile Fuel	$L1$	Liquid Fuel	$q1$
$l2$	Liquid Fissile Fuel			$q1$
$l3$	Liquid Steel	$L2$	Liquid Steel	$q2$
$l4$	Liquid Sodium	$L3$	Liquid Sodium	$q2$
$l5$	Fertile Fuel Particles	$L4$	Fuel Particles	$q1$
$l6$	Fissile Fuel Particles			$q1$
$l7$	Steel Particles	$L5$	Steel Particles	$q1$
$l8$	Control Particles	$L6$	Control Particles	$q2$
$l9$	Fertile Fuel Chunks	$L7$	Fuel Chunks	$q2$
$l10$	Fissile Fuel Chunks			$q2$
$l11$	Fission Gas in Liquid Fuel			$q1$
$l12$	Fission Gas in Fuel Particles			$q1$

113 Fission Gas in Fuel Chunks

 q_2 **Table 2-3. SIMMER-III Fluid-Dynamics Vapor-Field Components.**(All Vapor Components Have the Same Temperature and Assigned to the Velocity Field q_3)

Density Components (MCGR)		Material Components (MCGM1)	
g_1	Fertile Fuel Vapor	G_1	Fuel Vapor
g_2	Fissile Fuel Vapor		
g_3	Steel Vapor	G_2	Steel Vapor
g_4	Sodium Vapor	G_3	Sodium Vapor
g_5	Fission Gas	G_4	Fission Gas

Table 2-4. SIMMER-III Fuel-Pin Components.

Simple Model (standard)		Detailed Model (optional)	
a	Pin Fuel Interior Node	(NP)	Pin Fuel Radial Nodes
b	Pin Fuel Surface Node (= S_1)	(NPB)	Pin Fuel Surface Node (= S_1)
c	Cladding (= S_4)	($NPB+1$)	Cladding
	Fission Gas in Pin Fuel	(NP)	Fission Gas in Pin Fuel
Fuel-Pin Cavity (MCCR)			
		c_1	Fertile Cavity Fuel
		c_2	Fissile Cavity Fuel
		c_3	Dissolved Fission Gas in Cavity
		c_4	Free Fission Gas in Cavity

Table 2-5. SIMMER-III Velocity Fields.

Direction	Index	Velocity Variable	Cartesian	Cylindrical
Radial	I	U	X	R
Axial	J	V	Z	Z

2.2. Fluid-Dynamics Model

2.2.1. Fundamental Differential Equations

In SIMMER-III, conservation equations are written for independent variables in a unit volume. Thus the mass and energy are represented by macroscopic density and specific

internal energy, respectively. The conservation equations involving fluid mass, momentum and internal energy are, in abbreviated form:

$$\frac{\partial \bar{\rho}_m}{\partial t} + \nabla \cdot (\bar{\rho}_m \mathbf{v}_q) = -\Gamma_m, \quad (2-3)$$

$$\begin{aligned} \frac{\partial \bar{\rho}_q \mathbf{v}_q}{\partial t} + \sum_{m \in q} \nabla \cdot (\bar{\rho}_m \mathbf{v}_q \mathbf{v}_q) + \alpha_q \nabla p - \bar{\rho}_q \mathbf{g} + K_{qS} \mathbf{v}_q - \sum_{q'} K_{qq'} (\mathbf{v}_{q'} - \mathbf{v}_q) - \mathbf{VM}_q \\ = -\sum_{q'} \Gamma_{q'q} [H(\Gamma_{qq'}) \mathbf{v}_q + H(-\Gamma_{qq'}) \mathbf{v}_{q'}], \text{ and} \end{aligned} \quad (2-4)$$

$$\begin{aligned} \frac{\partial \bar{\rho}_M e_M}{\partial t} + \sum_{m \in M} \nabla \cdot (\bar{\rho}_m e_m \mathbf{v}_q) + p \left[\frac{\partial \alpha_M}{\partial t} + \nabla \cdot (\alpha_M \mathbf{v}_q) \right] \\ - \frac{\bar{\rho}_M}{\bar{\rho}_m} \left[\sum_{q'} K_{q'q} (\mathbf{v}_q - \mathbf{v}_{q'}) \cdot (\mathbf{v}_q - \mathbf{v}_{q'}) + K_{qS} \mathbf{v}_q \cdot (\mathbf{v}_q - \mathbf{v}_{qS}) - \mathbf{VM}_q \cdot (\mathbf{v}_q - \mathbf{v}_{GL}) \right] \\ = Q_N + Q_M(\Gamma_M) + Q_H(h, a, \Delta T). \end{aligned} \quad (2-5)$$

In the above equations, the density components are subscripted by m , the energy components by M , the velocity components by q , and $\bar{\rho}_m \equiv \alpha_M / \nu_M$. Similar to the former codes, SIMMER-II and AFDM, the component mass and energy are represented by macroscopic density and specific internal energy in SIMMER-III, such that the equations are written for a unit volume. The mass and energy equations for the fuel-pin and can-wall components, which are stationary, have similar expressions but do not involve the convection terms.

The momentum treatment in Eq. (2-4) for the vapor field includes a virtual mass term to provide a significant stability improvement. The AFDM manual [8] discusses this effect and other conceptual assumptions of these basic equations. Although not explicitly written in Eq. (2-4), the viscous term (momentum diffusion term) is actually coded in the later versions of SIMMER-III. In addition to the above equations, a model for convective interfacial areas is attempted in SIMMER-III to better follow phenomenological histories, as described in **Section 2.2.4**.

2.2.2. Overall Solution Procedure

The overall fluid-dynamics solution algorithm is based on a time-factorization approach, called the four-step method developed for AFDM, in which intra-cell interfacial area source terms, heat and mass transfer, and momentum exchange functions are determined separately from inter-cell fluid convection (see **Fig.2-5**).

Step 1 of the fluid-dynamics algorithm solves Eqs. (2-3) - (2-5) for intra-cell transfers whilst ignoring the convection terms. The computational flow through Step 1 has the following parts:

1. Perform energy and mass transfer operations associated with fuel-pin or can-wall breakup whenever the break-up criterion is satisfied.
2. Determine structure configuration and calculate structure heat-transfer coefficients.
3. Update convective interfacial areas with source terms and determine binary contact areas between components.
4. Calculate momentum-exchange functions.
5. Calculate fluid heat-transfer coefficients.
6. Update internal energies due to nuclear heating.
7. Calculate fission-gas release from liquid and particulate fuel.
8. Perform heat and mass transfer operations due to non-equilibrium melting/freezing and vaporization/condensation.
9. Calculate can-wall heat transfer.
10. Calculate heat and mass transfer due to equilibrium melting/freezing.
11. Update velocities and interfacial areas based on mass transfers.
12. Update the cell state through EOS.

This extremely complex procedure of Step 1 operations is the central reason why the intra-cell transfer is decoupled from the inter-cell convection.

2.2.3. Fluid Convection Algorithm

Steps 2, 3 and 4 of the fluid-dynamics algorithm are to solve fluid convection by integrating Eqs. (2-3) - (2-5) whilst ignoring the source terms on the right hand sides. First Step 2 explicitly estimates the end-of-time-step variables to initialize for the pressure iteration. While the first-order donor-cell differencing scheme is optionally used, a higher-order spatial differencing is the standard scheme to reduce numerical diffusion. The latter was based on the AFDM formulation [8].

Step 3 performs the so-called pressure iteration that obtains consistent end-of-time-step velocities and pressure using a multivariate Newton-Raphson method. During the pressure

iteration, selected sensitive variables are allowed to change from the Step 2 estimates to reduce their residuals to zero. These variables are: the total density of liquid 1, the density of steel, the density of sodium (and control particles), the total density of vapor mixture, the vapor temperature, and the difference between EOS pressure and cell pressure. In addition, an advantage over the previous AFDM approach is the elimination of an inefficient internal EOS iteration to obtain mechanical equilibrium among compressible fluid components. This is done by defining the EOS pressure as a function of the cell pressure, and the latter is related to the amount of liquid compression.

The matrix solution methods currently used for the pressure iteration are: a direct inversion method (in subroutine BNDSOL) and an incomplete LU-decomposition bi-conjugate gradient method (in subroutine PCGSOL). The latter is more advantageous for larger problems, typically with more than 1000 mesh cells. For one-dimensional calculations, a simpler solver of the Gaussian elimination method is automatically selected (in subroutine TRDSOL).

Finally, Step 4 performs consistent mass, momentum and energy convection based on the semi-implicit algorithm. The interfacial areas are also convected consistently in this step. A summary of the above four step updates of variables is schematically shown in **Table 2-6**, where a parenthesized number denotes the corresponding step in which a variable is updated.

Although this modularized, four-step method is advantageous and flexible enough to allow future improvement or exchange of different intra-cell models, problems can arise from decoupling intra-cell mass transfer from the inter-cell fluid convection. Practically this is known to introduce time-step-size sensitivity problems, when the fluid convection is strongly driven by the intra-cell source terms. A completely integrated fully-implicit approach is obviously impractical in a complex multiphase, multicomponent framework of SIMMER-III. However an additional time step control has been implemented by monitoring the pressure change between the intra- and inter-cell transfers, and it was shown that this problem is partially, but reasonably, mitigated.

Table 2-6. Update Procedure in Four-step Algorithm.

Step 1: Calculate intra-cell transfers.

$$(\bar{\rho}^{(1)}, \mathbf{v}^{(1)}, e^{(1)}) \leftarrow (\bar{\rho}^n, \mathbf{v}^n, e^n)$$

Step 2: Estimate end-of-time-step values $(\bar{\rho}^{(2)}, \mathbf{v}^{(2)}, e^{(2)})$ without intra-cell source terms.

$$\frac{\bar{\rho}^{(2)} - \bar{\rho}^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} \mathbf{v}^{(1)}) = 0$$

$$\frac{\bar{\rho}^{(2)} \mathbf{v}^{(2)} - \bar{\rho}^{(1)} \mathbf{v}^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} \mathbf{v}^{(1)} \mathbf{v}^{(1)}) + \nabla p^n = 0$$

$$\frac{\bar{\rho}^{(2)} e^{(2)} - \bar{\rho}^{(1)} e^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} e^{(1)} \mathbf{v}^{(1)}) + p^n \mathbf{v}^{(1)} = 0$$

Step 3: Solve for $(\bar{\rho}^{(3)}, \mathbf{v}^{(3)}, e^{(3)})$ by pressure iteration.

$$\frac{\bar{\rho}^{(3)} - \bar{\rho}^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} \mathbf{v}^{(3)}) = 0$$

$$\frac{\bar{\rho}^{(2)} \mathbf{v}^{(3)} - \bar{\rho}^{(1)} \mathbf{v}^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} \mathbf{v}^{(1)} \mathbf{v}^{(1)}) + \nabla p^3 = 0$$

$$\frac{\bar{\rho}^{(2)} e^{(3)} - \bar{\rho}^{(1)} e^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} e^{(1)} \mathbf{v}^{(1)}) + p^3 \mathbf{v}^{(3)} = 0$$

Step 4: Calculate final end-of-time-step values $(\bar{\rho}^{n+1}, \mathbf{v}^{n+1}, e^{n+1})$.

$$\frac{\bar{\rho}^{(3)} \mathbf{v}^{(4)} - \bar{\rho}^{(1)} \mathbf{v}^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} \mathbf{v}^{(1)} \mathbf{v}^{(3)}) + \nabla p^3 = 0$$

$$\frac{\bar{\rho}^{(3)} e^{(4)} - \bar{\rho}^{(1)} e^{(1)}}{\Delta t} + \nabla \cdot (\bar{\rho}^{(1)} e^{(1)} \mathbf{v}^{(3)}) + p^3 \mathbf{v}^{(3)} = 0$$

$$(\bar{\rho}^{n+1}, \mathbf{v}^{n+1}, e^{n+1}) \leftarrow (\bar{\rho}^{(3)}, \mathbf{v}^{(4)}, e^{(4)})$$

2.2.4. Interfacial Area Model

The interfacial area modeling successfully attempted in AFDM [8] was extended to the SIMMER-III multicomponent system, with a slightly simpler but more comprehensive representation of flow topologies. To obtain the mass, momentum, and energy transfer terms, the binary contact areas must be determined for 52 possible contact interfaces among seven fluid energy components and three structure surfaces (a fuel pin, left can wall and right can wall). Such binary contact areas are determined based on the convective interfacial areas and a flow regime, which describes the topology of the multiphase flow.

Flow regimes are modeled for both pool flow, in which the effect of the structure is negligible, and channel flow, which is confined by structure. The present flow-regime representation is rather simple; for instance, only bubbly, dispersed and in-between transition flow regimes are modeled for the pool flow (see **Fig. 2-6**) [15]. The upper limit of the bubbly regime and the lower limit of the dispersed regime are defined by user-specified void fractions, α_B and α_D , respectively, the typical values being 0.3 and 0.7. In the SIMMER-III flow-regime modeling, it is generally assumed that a cell consists of two local regions: a bubbly and a dispersed regions, as schematically illustrated in **Fig. 2-7**. In **Fig. 2-6**, the

transition regime is defined as a combination of the two regions, which always have the void fractions α_B and α_D . This means that the transition regime, more commonly called a churn-turbulent flow regime, is defined non-mechanistically as a kind of interpolated flow regime. However, this treatment is very advantageous because the flow characteristics can be determined continuously over the entire void fraction range, without abrupt change upon flow-regime transition.

The modeling approach taken for the channel flow regimes is essentially the same, but special flow characteristics resulting from the effects of channel walls also have to be considered. The channel flow-regime map is shown in **Fig. 2-8** for the nine flow regimes modeled as the functions of the vapor volume fraction and the liquid entrainment fraction. The latter is related to the inter-phasic velocity difference, taking into account a flooding criterion for a liquid film on a solid structure. Since we cannot distinguish a liquid film on a fuel-pin surface from one on a can wall, there remain some uncertainties. No geometric picture is given for the interpolated flow regime, where the quantities are estimated purely by mathematical interpolation.

This multiple flow-regime treatment significantly improves the code applicability to reactor and experiment analyses over the previous SIMMER-II, in which only a dispersed droplet flow is modeled. It is also intended to provide a consistent framework of the flow regime map, over the entire range of void fraction, with smooth and stable transitions between flow regimes.

The interfacial area convection model improves the flexibility of SIMMER-III by tracing transport and history of interfaces, and thereby better represents physical phenomena. Ishii [16] proposed a convection equation for the interfacial areas per unit volume (interfacial area concentration) in a general form:

$$\frac{\partial A_M}{\partial t} + \nabla \cdot (A_M \mathbf{v}) = \sum_k S_{M,k} \quad , \quad (2-6)$$

where A_M is the interfacial area of component M per unit volume and $S_{M,k}$ denotes the source terms of the interfacial area. This formulation is difficult to be implemented into an Eulerian code such as SIMMER-III because the real velocity of an interface cannot be determined easily. Therefore, we made a compromise that a convective interfacial area is defined as a surface area of an energy component and is convected with the same velocity. A total of nine interfacial areas associated to moving energy components are presently defined. These are: the surface areas of real liquids (fuel, steel and sodium) in the bubbly region; the surface areas of real liquids in the dispersed region; the surface areas of fuel and steel particles; and the surface area of bubbles in the bubbly region. A special treatment is modeled to avoid abrupt changes in such situations when the area convection occurs into a

cell having a different void fraction. This is done by additional local convection (diffusion) terms between the bubbly and dispersed regions:

$$\frac{\partial A_{M,B}}{\partial t} + \nabla \cdot (A_{M,B} \mathbf{v}) = \sum_k S_{M,B,k} - A_{M,B \rightarrow D} \quad , \text{ and} \quad (2-7)$$

$$\frac{\partial A_{M,D}}{\partial t} + \nabla \cdot (A_{M,D} \mathbf{v}) = \sum_k S_{M,D,k} - A_{M,D \rightarrow B} \quad , \quad (2-8)$$

where $A_{M,B}$ and $A_{M,D}$ are the convective interfacial areas of component M in the bubbly and dispersed regions, respectively. The second term on the right side denotes the diffusion between the two regions. The changes of interfacial areas due to hydrodynamic breakup, flashing, turbulence-driven breakup, coalescence, and production of droplets or bubbles are treated as "source terms" in the interfacial area convection equation.

The binary contact areas are then calculated using the convective interfacial areas, structure surface areas, component volume fractions, physical properties, etc. The present model basically calculates the contact areas based on the volume fractions of the fluids and a "summation rule" that the sum of binary contact areas over a component should be equal to the convective interfacial area (surface area) of the component. For the fluid-fluid contacts between moving discontinuous components, a theory developed for SIMMER-II is used.

2.2.5. Momentum Exchange Functions

Since both theoretical and experimental knowledge is limited for a multicomponent three-velocity flow, the developed formulations are based on engineering correlations of steady-state two-velocity flow. Fluid-structure, fluid-fluid drag and liquid-vapor virtual mass effects are formulated.

The momentum exchange function between velocity fields q and q' , $K_{qq'}$, in the momentum equation is a function of the drag coefficient and interfacial areas. Between the continuous and the discontinuous fields, the momentum exchange function consists of laminar and turbulent terms. The laminar term is described by Stoke's law, and the turbulent term is proportional to the inter-phase velocity difference with the drag coefficient based on Ishii's drag similarity hypothesis [17]. It is noted a treatment of bubbly flow regime was recently improved to include the consideration of bubble shape change from round to cap-shape in the momentum exchange functions [18].

Since standard two-phase pressure drop correlations are not applicable in the three-field situations, the momentum exchange functions between continuous fluids and the structure are calculated separately by Reynolds number correlations. Here the effective hydraulic diameters are defined by the respective binary contact areas and the fluid volume fractions.

The validity of this treatment was confirmed by comparing the two phase pressure drop in a bubbly flow in a pipe with the traditional treatment using Lockhart-Martinelli multiplier. For the momentum exchange function between two discontinuous velocity fields or between a discontinuous field and the structure, only a turbulent term is considered and a constant drag coefficient is employed.

The momentum exchange functions are defined separately for the bubbly and dispersed regions. To smooth the transition between liquid and vapor continuous flows, these two values are averaged logarithmically, since the momentum exchange function may differ by several orders of magnitude between the two regions [15].

Solid mobile particles in a flow require a special consideration, since the presence of particles, depending on their volume fraction, should significantly increase the hydrodynamics resistance of the flow. Therefore the concept of effective particle viscosity is introduced to particle components as a function of particle volume (packing) fraction and it is used in defining the total viscosity of each liquid velocity field. This model is crucial when the fuel blockage formation due to particle jamming is simulated.

2.2.6. Heat-Transfer Coefficients

Heat-transfer coefficients (HTCs) are required to perform the heat and mass transfer calculations. The heat and mass transfer paths between the fluid energy components are illustrated in **Fig. 2-9**. HTCs are defined for 52 binary contacts between the energy components and contribute to 33 vaporization/condensation (V/C) paths and 22 melting/freezing (M/F) paths. The coefficients control heat transfer between the bulk and interface temperatures for each liquid energy component and for the gas/vapor mixture.

The HTCs are based on quasi-steady state heat transfer correlations. The correlations take account of the Prandtl number range of the interacting fluids, which is particularly important when calculating heat transfer in liquid metals.

Solid particles are treated as rigid spheres, and heat transfer is controlled by conduction. Liquid droplets and gas bubbles were also treated as rigid spheres but the effects of internal circulation and oscillation of fluid particles are also treated. In the latter case conduction is augmented by convection in the fluid particles. In the dispersed flow regime the heat transfer between moving droplets can be calculated as a function of the contact times.

Forced convection heat transfer from continuous phase liquids or gas to solid particles is calculated using correlations obtained from forced flow over spheres. Fluid spheres are treated as rigid spheres at low Reynolds number, but at higher Reynolds numbers alternative correlations are used to take account of internal circulation in the fluid particles. When the

velocity difference between the continuous and dispersed phases is low the forced convection heat transfer can be augmented by natural convection heat transfer.

Heat transfer between continuous phase liquid or gas and structure is calculated using correlations obtained for forced convection single-phase flow in pipes.

A model to calculate HTC's in the event of film boiling around a hot droplet or particle in a continuous phase coolant liquid is also available in the code. The model can significantly reduce heat fluxes due to the insulating effect of the vapor blanket.

The HTC's are defined for the bubbly, annular and dispersed flow regimes. HTC's in intermediate flow regimes are computed by interpolation between well-defined flow regimes. The interpolation is performed using logarithmic averaging to smooth the transition between flow regimes. In addition the HTC's of two liquid components are interpolated between the continuous and discontinuous phase HTC's when neither liquid forms a dominant continuous phase. This avoids sudden changes in heat transfer caused by small alterations in volume fractions of the components.

2.2.7. Heat and Mass Transfer Model

After the interfacial areas and heat-transfer coefficients are obtained, the conservation equations without convection are solved for intra-cell heat and mass transfer in two steps. The first step calculates the phase transition processes occurring at interfaces, described by a non-equilibrium heat-transfer-limited model. This is a non-equilibrium process because the bulk temperature does not generally satisfy the phase-transition condition when the mass transfer occurs at the interface. The second step of mass and energy transfer is through an equilibrium process occurring when the bulk temperature satisfies the phase-transition condition. At 52 possible interfaces defined in SIMMER-III, all the important non-equilibrium mass-transfer processes are modeled, including 33 V/C paths and 22 M/F paths. Note that in the V/C transfers condensation processes of fuel or steel vapor on other colder liquids are included to avoid the SIMMER-II/AFDM problem of nonphysical presence of subcooled vapor. The mass-diffusion limited model is employed to represent effects of noncondensable gases and multicomponent mixture on V/C processes. The M/F transfers include the crust formation on a can wall that furnishes thermal resistance, and steel ablation and particle formation that contribute to fluid quenching and bulk freezing. In addition, 9 equilibrium M/F transfers are performed to eliminate subcooled liquids or metastable solids as a result of heat transfer and nuclear heating. The mass-transfer processes actually modeled are selected in consideration of their importance in and effects on the behavior of materials in the transition-phase.

The basic concept of the non-equilibrium mass transfer model is illustrated in **Fig. 2-10**, where a binary contact interface of the energy components A and B is shown. This is a heat-transfer-limited process where the phase transition rate is determined from an energy balance at the interface. The heat transfer rates from the interface are:

$$q_{A,B} = a_{A,B} h_{A,B} (T_{A,B}^I - T_A) \text{ in component A, and} \quad (2-9)$$

$$q_{B,A} = a_{A,B} h_{B,A} (T_{A,B}^I - T_B) \text{ in component B.} \quad (2-10)$$

The net energy transfer rate from the interface is defined as:

$$q_{A,B}^I = q_{A,B} + q_{B,A} \quad (2-11)$$

If the net heat flow, $q_{A,B}^I$, is zero, sensible heat is exchanged without phase transition. If $q_{A,B}^I$ is positive, namely the energy is lost at the interface, either a liquid component freezes or a vapor component condenses. Then the mass transfer rate for this case is determined from:

$$\Gamma_{A,B}^I = \frac{q_{A,B}^I}{i_A - i_B^I} \text{ , if the component B is formed by phase transition, or} \quad (2-12)$$

$$\Gamma_{A,C}^I = \frac{q_{A,B}^I}{i_A - i_C^I} \text{ , if a new component C is formed by phase transition.} \quad (2-13)$$

If $q_{A,B}^I$ is negative, on the other hand, namely the energy is gained at the interface, either a solid component melts or a liquid component vaporizes. Then the mass transfer rate for this case is determined from:

$$\Gamma_{B,A}^I = \frac{q_{A,B}^I}{i_A^I - i_B} \text{ , if the component A is formed by phase transition, or} \quad (2-14)$$

$$\Gamma_{B,D}^I = \frac{q_{A,B}^I}{i_D^I - i_B} \text{ , if a new component D is formed by phase transition.} \quad (2-15)$$

In the above four equations, the heat of phase transition (the effective latent heat) is defined as the difference between the enthalpy at the interface and the bulk enthalpy of a component undergoing a phase-transition process.

The physical model to represent the effect of noncondensable gases and multicomponent mixtures on V/C processes is based on a study originally attempted for SIMMER-II. Equations for this model were obtained by considering the quasi-steady, stagnant Couette-flow boundary layer to relate the mass and energy fluxes to the overall forces driving heat and mass transfer. This classical Couette-flow model has been shown to provide a good engineering model for single-component vapor condensation in the presence

of noncondensable gases, thus confirming the adequacy of its theory for incorporation in two-fluid computer codes. In SIMMER-II, the model extended to multicomponent systems was designed to predict not only the suppression of condensation by noncondensable gases such as a fission gas, but also the phase-transition rate for a vapor component condensing on the surface of a different material. However, this previous effort was not successful for the practical use of the code because its solution scheme was incompatible with numerical algorithms applied to SIMMER-II multiphase-flow modeling. In SIMMER-III, extensive model modifications are made as necessary and a new solution scheme is developed to make it suitable for implementation to the multi-fluid code.

In the V/C model, the energy- and mass-conservation equations coupled with EOSs are then solved iteratively using the mass-transfer rates obtained. In the solution procedure, based on a multivariate Newton-Raphson method, five sensitive variables (three condensable vapor densities, coolant energy and vapor temperature) are updated implicitly, whereas the remaining less sensitive variables are updated explicitly following the convergence of the iteration. In a single-phase cell, vapor is assumed to always exist in a non-zero small volume, $\alpha_0(1 - \alpha_s)$, so its density and energy are calculated consistently with two-phase cells to avoid numerical difficulties. The single-phase V/C calculations are performed using the same procedure as two-phase cells except for the energy transfer between liquids. At a liquid/liquid interface, such as fuel/sodium contact in a two-phase cell, vaporization can occur, and in this case the interface temperature is defined as the saturation temperature of a vaporizing material. In a single-phase cell, however, the interface temperature of the liquid/liquid contact is defined so that no vaporization is caused by the energy transfer between the liquids. Instead phase transition occurs only when the liquid temperature increases sufficiently to cause vaporization at a liquid/vapor interface.

The M/F calculation is also based on the two modes: non-equilibrium and equilibrium processes. The former is similar to the V/C processes; however all the variables are updated explicitly except for the coolant energy, which is identified as sensitive. After calculating the heat and mass transfer resulting from non-equilibrium processes and structure heat transfer, the equilibrium M/F rates are determined by comparing the updated component energy with its liquidus energy for freezing or its solidus energy for melting.

The intra-cell heat and mass transfer calculations result in updated component volume fractions and masses. The convective interfacial areas and velocities are then adjusted consistently.

2.2.8. Inter-cell Heat Transfer

SIMMER-III, like its preceding codes SIMMER-II and AFDM, originally calculated only intra-cell heat transfer, and could not transfer energy between cells except for the energy

transfer by convection. However, a treatment of inter-cell heat transfer was essential to analyze small-scale pool boiling behavior correctly and so a new model to calculate the inter-cell heat conduction was developed and implemented into SIMMER-III.

The energy conservation equation including the heat conduction term is:

$$\frac{\partial \bar{\rho}_M e_M}{\partial t} + \nabla \cdot (\bar{\rho}_M e_M \mathbf{v}_q) = Q_{ic} + \nabla \cdot q_c \quad (2-16)$$

The numerical algorithm of SIMMER-III is a fractional time step method which solves Eq. (2-16) by separating the source terms on the R.H.S. and the convection term on the left hand side. In SIMMER-III, the source terms are evaluated in Step 1 and the resultant energy is convected in Steps 2 to 4. Therefore, the evaluation of the conductive heat transfer is to be performed in Step 1 using the temperature at the beginning of time step. The heat flux which appears in Eq. (2-16) is calculated by Fourier's law and includes the turbulent thermal conductivity:

$$q_c = -(k_c + k_T) \cdot \nabla T_M, \quad (2-17)$$

where the turbulent thermal conductivity, k_T , depends on the position, direction, and the nature of the turbulent flow.

The turbulent heat flux is evaluated by a combination of Prandtl's mixing length theory and experimental correlations.

2.2.9. Equations-of-State Model

An EOS model is required to close and complete the fluid-dynamic conservation equations. Moreover it is crucial from the viewpoints of numerical accuracy and stability, and computing efficiency. Neither SIMMER-II nor AFDM were satisfactory from these aspects. Based on past experiences, therefore, an improved analytic EOS model using the flexible thermodynamic functions has been developed for SIMMER-III [19]. The model treats the basic reactor-core materials: mixed-oxide fuel, steel, sodium, control (B₄C) and fission gas. These materials are assumed to be immiscible, such that a unique EOS for each material can be defined.

The functions use polynomial equations for the liquid and solid phases and a modified Redlich-Kwong (MRK) equation for the vapor phase [20]. The MRK EOS has the form:

$$p_{Gm} = \frac{R_M T_M}{v_{Gm} - a_{G1,M}} - \frac{a(T_G)}{v_{Gm}(v_{Gm} + a_{G3,M})}, \quad (2-18)$$

where

$$a(T_G) = a_{G2,M} \left(\frac{T_G}{T_{Cr,M}} \right)^{a_{G4,M}}, \text{ for } T_G < T_{Cr,M}, \text{ and}$$

$$a(T_G) = a_{G2,M} \left[1 + a_{G4,M} \left(\frac{T_G}{T_{Cr,M}} - 1 \right) \right], \text{ for } T_G \geq T_{Cr,M},$$

and $a_{G1,M}$, $a_{G2,M}$, $a_{G3,M}$ and $a_{G4,M}$ are the EOS parameters.

The above equation is similar to the van der Waals equation, but it can be made reasonably accurate especially at high temperatures. It was found, however, that this EOS poorly reproduces the evaluated data [21] of the internal energy and the heat capacity of sodium vapor. Therefore the MRK EOS was extended to a reacting system, which describes the dimerization process of sodium vapor molecules, and thereby satisfactory agreement was obtained.

The EOS functions are fitted using the most up-to-date and reliable data sources available [22, 23]. The present SIMMER-III EOS model has adequate accuracy at high temperature and high pressure and consistently satisfies basic thermodynamic relationships over the wide temperature range from the solid to supercritical state [24].

In the above standard analytic EOS model, determination of fitting parameters in the EOS functions sometimes requires a tedious procedure in advance and it is definitely inevitable to get rid of numerical errors in its results. Then, a fitting-free EOS (FFEOS) model is also available optionally for solving such shortcomings with the standard model. The FFEOS model requires only few EOS parameters because it determines most of state variables numerically, based on thermodynamic relationships instead of using fitted EOS functions. Although the use of the FFEOS model will deteriorate the numerical efficiency, it would be acceptable even for the long-haul calculations because increase of CPU time is estimated to be about 30 % per material. It is noted that FFEOS is applicable only to liquid and vapor components of fuel, structure and coolant materials. This model would be also useful and convenient for us to perform calculations with non-reactor materials.

2.3. Fuel Pin and Structure Model

2.3.1. Fuel Pin Configuration and Heat-Transfer Model

The fuel-pin and can wall model not only represents the stationary structure in the core, but also traces time-dependent disintegration. The standard fuel-pin model is rather simple with a pellet interior modeled by a single temperature node and with breakup modeled only by a thermal (melt fraction) criterion. However the separated treatment of a pellet surface node provides better thermal coupling with the fluid. Because of the relatively large thermal inertia of the pellet interior, the fuel-pin heat-transfer calculation can be performed with time

steps larger than the fluid-dynamics steps. This simplified model (SPIN) is considered to be sufficient for simulating the fuel-pin behavior in a voided channel typical for a loss-of-flow accident. Again a fuel pin exists only within a mesh cell, the modeling is independent of the dimensions.

Radial and axial fuel-pin geometries are represented as shown in **Figs. 2-11** and **2-12**, respectively. The axial blanket and fission-gas plenum regions can be placed both above and below the core region. The heat-conduction equation in a cylindrical geometry is solved implicitly for specific internal energies of up to three fuel-pin components (interior, surface and cladding). Pellet-cladding gap conductance is modeled by an input constant in this simple model. The pin surface node (either pin fuel surface or cladding) exchanges mass and energy with the fluid. In the fission-gas plenum region, the gas temperature is represented by one point and the heat transfer is solved explicitly because of its slow thermal response. For a control subassembly, the pin fuel is replaced by the control material (B_4C), which is modeled by one node.

The breakup of the pin fuel and cladding is determined from input threshold melt fractions, typically 0.5 for pin fuel and the solidus energy for the cladding. The mass and energy transfer upon breakup is instantaneous and this operation is included in fluid-dynamics Step 1. Similar to SIMMER-II, a special model can be selected by user-input to simulate the mobilization of unsupported pin fuel. Namely, the pin fuel is assumed to break up when both the cladding and can walls in a cell are lost, or when the cladding is lost and the pin fuel below is lost. The control is assumed to break up into particles when the cladding is lost. The control particles are only modeled in a liquid field in SIMMER-III.

As explained in **Section 2.2**, the fission-gas components in the liquid-field fuel (liquid and particles) are modeled in SIMMER-III. Upon breakup of the pin fuel, the fission gas mass is transferred to the liquid field and no direct path to the vapor field is allowed. Then later release from the liquid and particulate fuel is modeled based on user-specified release time constants. This significantly improves the modeling of the important effect of fission gas on fuel motion during the transition phase.

A detailed pin model (DPIN) has been made available in latest versions (Version 2.G and later) of SIMMER-III, in which fuel-pin radial temperature distribution, intra-pin cavity and fuel motion are calculated and is more appropriate for simulating overpower transients. Furthermore a model of gas blowdown from fission-gas plena has been incorporated based on the SAS-series initiating-phase analysis code [25].

2.3.2. Can Wall Configuration and Heat-Transfer Model

The can wall model treats separated left and right can walls assumed to be located at the radial mesh cell boundaries. The presence of the can wall at a cell boundary eliminates radial fluid convection. Fuel crust can grow on a can wall when the heat and mass transfer model predicts this. Inter-cell heat transfer is also calculated when one of the two can walls at a cell interface is missing. When the can wall becomes thin, then the two nodes are merged into a single interior node.

The above requires a complex procedure to define the can-wall structure configuration. The detailed structure of a mesh cell with all the can-wall components is shown in **Fig. 2-13**. Let us consider a mesh cell boundary. If this is the left boundary of the first radial cell or the right boundary of the last radial cell, or a boundary where two can-wall interior nodes are present, then the two cells adjacent at this boundary are thermally decoupled. Each can wall is treated separately in each cell. On the other hand, if one of the can walls at this boundary is missing, then the two cells are coupled thermally through the remaining can wall. Four cases exist in this situation depending on whether the can wall is thick (two nodes) or thin (a single interior node), and whether the crust fuel is present or not.

The can-wall heat transfer is modeled considering the above combinations of geometric configuration and heat transfer paths. The calculation is performed implicitly with fluid time steps based on heat conduction in a slab or cylinder geometry between up to five structure-component layers. The can walls undergo heat and mass transfer with the fluid through non-equilibrium and equilibrium M/F processes (see **Section 2.2.7**).

2.4. Neutronics Model

The neutronics model developed for SIMMER-III is based on SIMMER-II Version 12 [3]. The neutron kinetics is modeled by an improved quasi-static method, in which a space- and time-dependent neutron transport equation is factorized into: a shape function that represents the neutron flux distribution but changes only slowly with time, and a amplitude function that accounts for time evolution of the reactor power. The flux shape calculations are based on a multi-group S_n transport theory: the TWODANT model [27] which takes advantage of a diffusion-synthesis acceleration method and improves both the robustness and computational efficiency. The reactivity and other kinetics parameters are calculated from the neutron flux and macroscopic cross sections. Then the amplitude equation is solved for determining the reactor power.

Coupling with the fluid-dynamics part is carefully designed, because the neutronic state of an LMFR core during a CDA is determined primarily from time-dependent mass and energy distribution of the core materials. It is because of this time dependence that the calculations of shielded (effective) macroscopic cross sections are also performed in the code. To connect with the initiating phase calculations, a capability of transient-state neutronics

initialization is available, similar to SIMMER-II. The neutronics calculation provides: the power distributions (specific internal energy generation rates due to nuclear heating) for each of the five heat-source materials (fertile fuel, fissile fuel, steel, sodium and control); and the parabolic fitting coefficients to extrapolate the power amplitude to the subsequent fluid-dynamics time steps. They are then used in STEP1 to update the component internal energies due to nuclear heating.

Additional features included in SIMMER-III but not available in SIMMER-II are: a simple decay heating model, which provides a consistent treatment with the SAS-series initiating-phase analysis code [25]; the treatment of neutron up-scatterings for applications to thermal or epi-thermal reactors; an external neutron source model for transient analyses of ADSs (Accelerator Driven Systems).

2.5. Initial and Boundary Conditions

2.5.1. Fluid-Dynamics Cell Initialization

In SIMMER-III, volume fractions and temperatures of liquid- and structure-field components, vapor temperature, noncondensable gas pressure, and single-phase pressure are ordinarily specified by user-supplied input data. Before starting a calculation, initialization is required to define the thermodynamic state of cell components based on these inputs. For liquid and structure components, the internal energy and the specific volume are defined using the EOS relationships. The thermodynamic state of the vapor field depends on the vapor temperature and the specific volumes of vapor components. In SIMMER-III, the condensable-gas partial pressure is defined to get the specific volume.

Currently the following three options are available:

- (1-a) The condensable-gas pressure is defined as the saturation pressure of liquid which exists in a cell.
- (1-b) The condensable-gas pressure is defined as the pressure of liquid which exists in a cell, assuming that the liquid saturation temperature is the same as the vapor temperature.
- (1-c) All the partial pressures are specified by inputs.

The specific volume of a vapor component is calculated using the $p-v-T$ relationship. Then the macroscopic density is defined by the volume fraction and the specific volume, that is $\bar{\rho} = \alpha / v$.

SIMMER-III has the following two options:

- (2-a) For liquid- and structure-field components, the macroscopic density is defined using

the volume fractions specified by inputs. For a vapor-field component, the effective volume fraction is calculated using the specified liquid- and structure-field volume fractions.

- (2-b) The macroscopic densities of real liquid and vapor are calculated so as to conserve the mass in a cell, which is the real-liquid macroscopic density defined in the same way as described in (2-a). Therefore, the specified volume fraction of real liquid in a two-phase cell is decreased depending on the vapor macroscopic density.

2.5.2. Boundary Conditions

The boundary conditions (BCs) for SIMMER-III have been made much more flexible than the previous SIMMER-II and AFDM codes. For example, in AFDM, the boundary conditions can be set only on the bottom and top surfaces, and the left and right surfaces are fixed to the free slip condition. There are two kinds of BCs in SIMMER-III. One is the BCs specified on the boundary cells and the other is a unique concept of the 'virtual wall' that can be set on any cell boundary.

The boundary conditions which can be specified in SIMMER-III are described below. A more detailed description is available in the input manual in **Appendix G**.

With respect to the BCs on the boundary cells:

- (1) BCs can be set cell-wise on each surface.
- (2) Cell variables can be kept constant at the initial conditions.
- (3) Transient functions can be specified individually according to velocity, pressure, or temperature.

With respect to the virtual wall:

- (4) It has no mass and no volume.
- (5) Flow normal to the wall is set to zero. The free slip condition is assumed along the wall.
- (6) Two cells on both sides of the wall are thermally cut, i.e. adiabatic.
- (7) A cell can exist that is connected with no other cells.

2.6. Time Step Control

2.6.1. Fluid-Dynamics Time Step Control

Selection of time step sizes is a very important element of controlling the fluid-dynamics calculations. This is because a sufficiently strict time step control is essential for

making the numerical calculation accurate and stable. In addition, practical control is always required from the computing-cost point of view. In SIMMER-III, the following time step controls are implemented and they automatically select the most appropriate time step size. Most of them are physics-based, taking advantage of experience in running SIMMER-III and the previous codes. A message is printed at every fluid-dynamics time step along with an ID name denoting what criterion is effective. The list of the currently effective ID names is given in **Section 3.2.2**.

- (1) Initial time step (ID name: DTSTRT): The initial time step is specified by a user input (DTSTRT) and is maintained for an input number of cycles (NDT0).
- (2) Maximum time step (ID name: DTMAX): The time step size is limited to a maximum size specified by the user (DTMAX).
- (3) Previous time step (ID name: 2*DTP): The time step is limited by twice the previous time step size.
- (4) Courant condition (ID name: COURNT): The semi-implicit differencing method requires a material (not sonic) velocity Courant condition:

$$Rt_{ri} = \left[r \cdot \max(|u_{q1}|, |u_{q2}|, |u_{q3}|) \right]_{\lambda+} \cdot \max\left(\frac{I}{r_i \Delta r_i}, \frac{I}{r_{i+1} \Delta r_{i+1}} \right), \text{ and}$$

$$Rt_{zj} = \frac{\max(|v_{q1}|, |v_{q2}|, |v_{q3}|)_{g+}}{\min(\Delta z_j, \Delta z_{j+1})}.$$

The criterion for predicting the time step size is defined as

$$\Delta t^{n+1} < c_t / \max(Rt_{ri}, Rt_{zj}),$$

where c_t is an input Courant number.

- (5) Optimum pressure iteration (ID name: OPTPIT): The time step size affects the number of pressure iterations required to converge to the end-of-time-step fluid state. The input optimum number of pressure iterations restricts the time step by the criterion :

$$f_{IT} = \frac{OPTPIT}{ITERA + 1} + 10^{-10},$$

$$f_{IT} = CVMGT(f_{IT} \cdot DTINC, f_{IT}^2, f_{IT} \geq 1), \text{ and}$$

$$\Delta t^{n+1} = f_{IT} \Delta t,$$

where OPTPIT and DTINC are specified by the user.

- (6) Source-term decoupling error (ID names: DTSTP1, DTSTP4, DPSTP1 or DPSTP4): The time step can be optionally restricted by monitoring the potential sources of source-term decoupling error. This is done by restricting the fractional changes in: the cell pressure between Step 1 and Step 2, and Step 2 and Step 4; and the vapor temperature between Step 1 and Step 2, and Step 2 and Step 4.
- (7) Excessive V/C iterations (ID name: DTIVC): If the number of the V/C iterations exceeds a maximum specified by the user (HMTOPT(10)), the next time step size is halved.

The minimum time step size of the criteria from (2) to (7) is used to calculate the next cycle. The predicted time step is compared with the following minimum values.

- (8) Minimum time step (ID name: none): The time step is limited to the minimum size specified by the user (DTMIN). A message is printed when DTMIN is taken.
- (9) Fuel-pin heat-transfer (reactivity) time step (ID name: DTHN): The time step size cannot become larger than the next fuel-pin heat transfer time step or neutronics reactivity step.

Furthermore, a capability of re-calculating the same fluid-dynamics cycle is available in SIMMER-III, whenever non-convergence is detected in any iterative operation. The time step is controlled by the following additional conditions. In the following cases, the same cycle is re-calculated with a halved time step size.

- (10) Non-convergence in VXHMT (ID name: VCITMX): Non-convergence occurred in the VCHMT calculation.
- (11) Excessive change in vapor temperature (ID name: VCDTMX): The excessive change in vapor temperature is detected in the V/C iteration.
- (12) Non-convergence of vapor temperature (ID names: S1ITMX or S4ITMX): Non-convergence occurred in EOST called from either STEP1 or STEP4.
- (13) Extremely low vapor temperature (ID names: S1TGMM or S4TGMM): The vapor temperature became lower than the minimum vapor temperature in EOST called either from STEP1 or STEP4.
- (14) Non-convergence in velocity iteration (ID names: S2VELO or S4VELO): Non-convergence occurred in the velocity iteration either in STEP2 or STEP4.
- (17) Non-convergence in velocity iteration (ID name: PIFAIL): Non-convergence occurred in the pressure iteration in STEP3.
- (18) Keeping reduced time step size: This is a special control to avoid oscillatory change in

time step sizes. Once the time step size is reduced by any of the above criteria, the same size can be maintained for a user-specified number of succeeding cycles (ALGOPT(31)).

2.6.2. Fuel-Pin Heat-Transfer Time Step Control

Fuel-pin heat-transfer time steps are controlled based on the changes of specific internal energies of pin fuel and cladding, and the change of the total power (or amplitude). When the neutronics calculation is performed, the time step size is set to be the same as the reactivity step for a standard use, because the reactivity feedback and fuel heat generation are closely related each other. The time steps based on the energy and power changes are estimated by

$$\Delta t_m = 0.9 f_m \frac{e_M^{n'+1}}{|e_M^{n'+1} - e_M^{n'}|} \Delta t_{old}, \text{ and}$$

$$\Delta t_p = 0.9 f_p \frac{P^{n'+1}}{|P^{n'+1} - P^{n'}|} \Delta t_{old},$$

where f_m and f_p are fractional changes of specific internal energy and power allowed in a time step with its default value 0.5. The time step control also considers the user-specified minimum and maximum, the previous time step, the neutronics reactivity step and the fluid-dynamics time step. Finally the new time step is determined from

$$\Delta t_{new} = \max \left\{ \Delta t_{min}, \min \left(\Delta t_{max}, \Delta t_m, \Delta t_p, 4 \Delta t_{old}, \Delta t_f \right) \right\},$$

where Δt_f is the fluid-dynamics time step, such that the heat-transfer does not exceed the fluid-dynamics time step.

When the neutronics is used (URANUS off), the above time step control also takes into account the time-step control of reactivity update steps. This is because of tight relationship of fuel temperature change with power generation and fuel reactivity feedback. In an additional option, the heat-transfer time step control can be independent of the neutronics. For example, the time steps can be forced to be the same as fluid-dynamics time steps.

2.6.3. Neutronics Time Step Control

The time-step controls for the quasi-static method regulate the length of both the reactivity step and the flux-shape step. Important consideration in SIMMER-III is the tightness of the controls, which must take into account a reactivity level of the system. The controls must be made very tight for a reactivity level near prompt critical, but they are relaxed for a reactivity level not near prompt critical. For this reason, taking advantage of

experience in SIMMER-II, two time-step reduction factors (input variables EPS4 and EPS17) are used in several of the individual time-step controls described below. See Ref. [3] for the detailed description of the formulae used.

During transient calculations, the shape time step is predicted or limited by the following ten individual controls. It is noted the controls depend on the model selection of either the flux-shape extrapolation option ($IFXUDL = 0$) or the flux-shape update option ($IFXUDL > 0$). A selected time step is printed along with the shape step control ID number indicated below.

- (1) Previous shape step (ID #: 1): The shape step is limited to 10 times the maximum of the previous two shape time steps.
- (2) Change in leakage (ID #: 2): The shape step is controlled by the rate of change in the neutron leakage contribution to the reactivity. This control is effective only if the flux-shape acceleration option is used ($IFXUDL = 0$).
- (3) Number of reactivity steps (ID #: 5): The shape step cannot extend over more than the number of reactivity steps (LIPSTP) specified by the user.
- (4) Last real time for the current run (ID #: 6): The shape time cannot exceed the last real time for the current run (TWFIN) specified by a user. This control is effective only if $NIOPT(5)=1$.
- (5) Maximum shape step (ID #: 7): The shape step is limited by a maximum size (DTSMAX) specified by a user.
- (6) Change in neutron flux shape (ID #: 8): The tilt (distortion) of the total flux shape is monitored and used to estimate the shape time step using the user-specified criterion (EPS9). This control is effective only if the flux-shape acceleration option is used ($IFXUDL = 0$).
- (7) Change in reactivity (ID #: 9): The shape step is predicted by comparing the estimated change in reactivity and the maximum permissible change per shape step (EPS18). This control is effective only if the flux-shape acceleration option is used ($IFXUDL = 0$).
- (8) Deviation from quasistatic method constraint condition (ID #: 11): The shape step is halved if the deviation from the constraint condition exceeds the user-specified value (EPS10). This control is effective only if the flux-shape update option is used ($IFXUDL > 0$).
- (9) Demand of an external source model (ID #: 12): The shape step cannot exceed the limit restricted by an external source model. This control is effective only if the external source model option is used ($NIOPT(36) > 0$).

- (10) User-specified shape step (ID #: none): The shape step can be forced to a constant value of DTSMAX by user specification (IQUASI = 1 or 3).

The minimum of the controls (1) through (9) is taken, depending on the model option, and checked for the control (10). Finally the adjustment is made to make sure the next shape step matches the current time (ID #: 10).

During the transient neutronics calculations, the reactivity time step is predicted or limited by eight individual controls in the neutronics. A selected time step is printed along with the update (reactivity) step control ID number indicated below.

- (1) Previous reactivity step (ID #: 1): The reactivity step is limited to twice the maximum of the previous two shape time steps.
- (2) Change in reactivity (ID #: 2): The reactivity step is predicted by the maximum reactivity change permitted (EPS5).
- (3) Next shape time step (ID #: 3): The reactivity step cannot exceed the next shape step.
- (4) Maximum reactivity step (ID #: 4): The reactivity step is limited to a maximum size specified by a user (DTHMAX).
- (5) Change in amplitude (ID #: 5): The reactivity step is limited by the rate of change in the amplitude solution by restricting the minimum number of reactivity steps per 10 times change in amplitude (EPS7).
- (6) Maximum inverse period (ID #: 6): The reactivity step is limited by the change in inverse period, using a user-specified maximum change per reactivity step (EPS8).
- (7) Current shape step size (ID #: 8): The length of reactivity step is limited to less than half of shape step interval.
- (8) User-specified reactivity step (ID #: none): The reactivity step can be forced to a constant value of DTHMAX by user specification (IQUASI > 1).

The minimum of the controls (1) through (7) is selected and checked for the control (8). Then the next reactivity step is taken.

It is noted that the reactivity steps are controlled by the fluid dynamics as well, to take into account the influence of change, for example, in fuel mass or temperature on reactivity calculations. For this purpose, the total masses and internal energies for fuel, steel and sodium are summed up over a series of fluid-dynamics time steps. The following seven controls are tested against user-specified criteria, and the minimum is taken as the next reactivity step. A message of this time step control is printed with a selected time step size. Currently, the fluid dynamics control of reactivity steps works independently of the neutronics control of time steps described above.

- (1) Fractional change in the total fuel mass during fluid cycles (EPS14)
- (2) Fractional change in the total steel mass during fluid cycles (EPS15)
- (3) Fractional change in the total sodium mass during fluid cycles (EPS16)
- (4) Fractional change in the total fuel internal energy during fluid cycles (EPS11)
- (5) Fractional change in the total steel internal energy during fluid cycles (EPS12)
- (6) Fractional change in the total sodium internal energy during fluid cycles (EPS13)
- (7) Change in amplitude projected to fluid dynamics (EPS7)

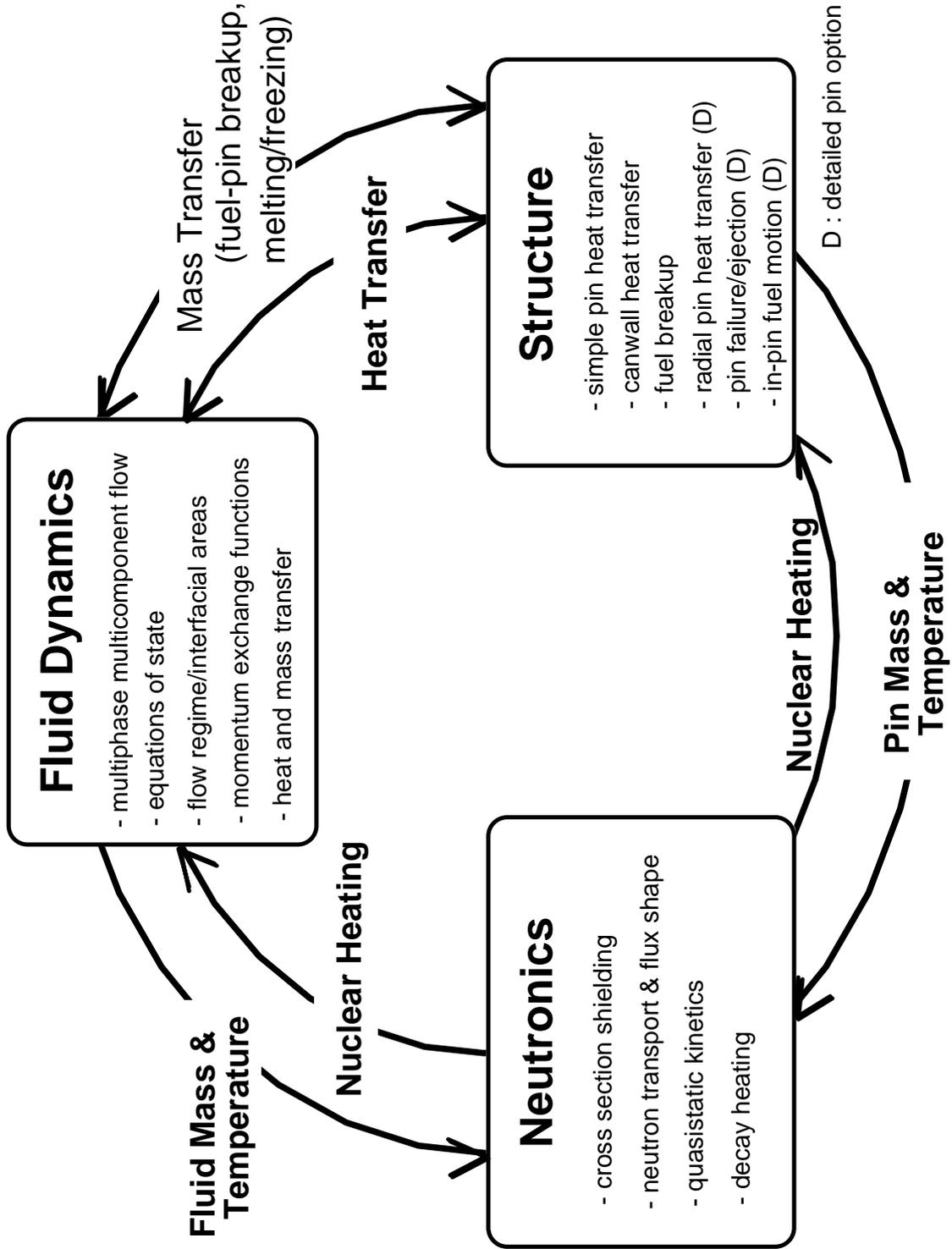


Fig. 2-1-1. SIMMER-III Overall Code Structure.

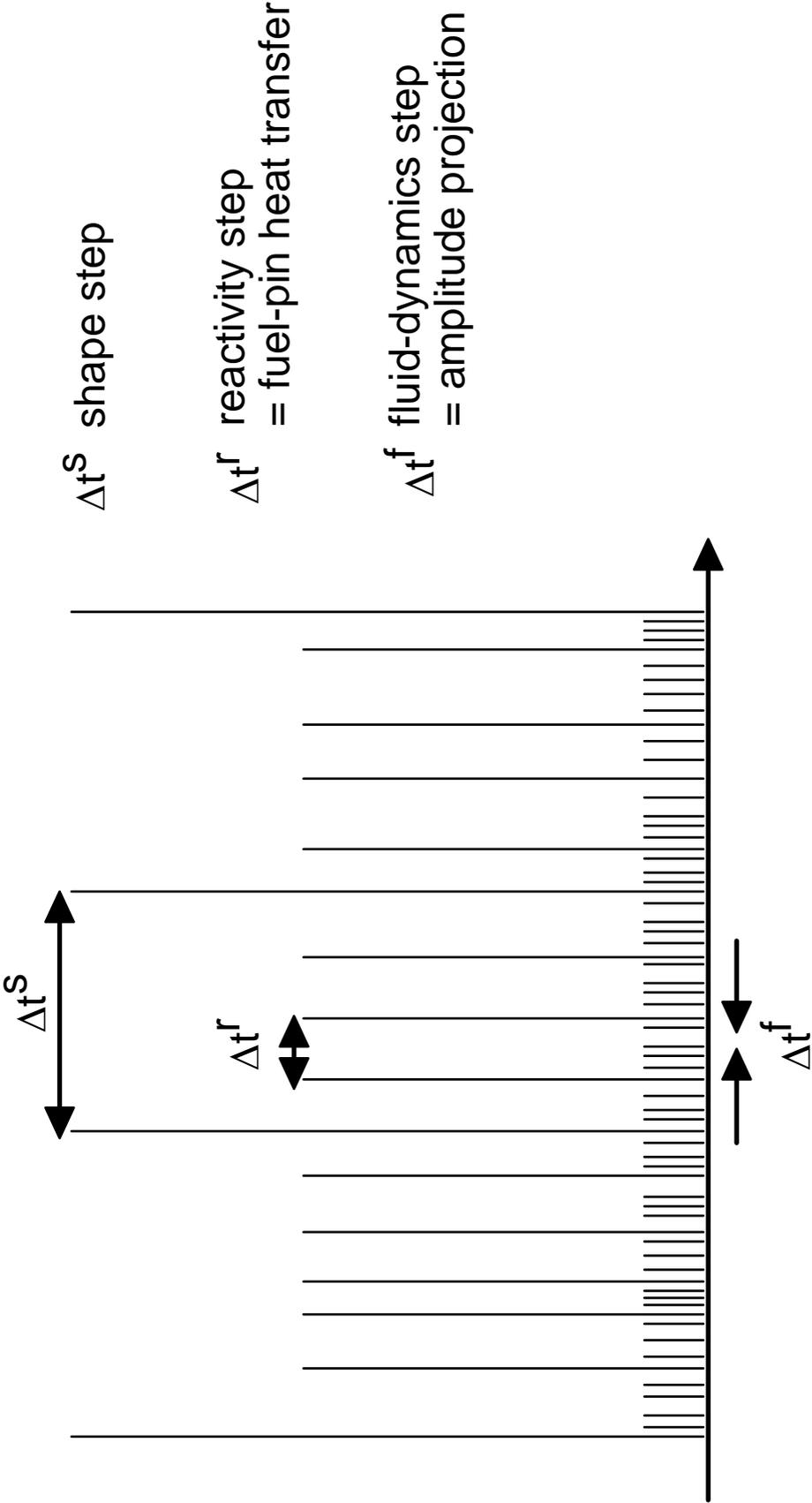


Fig. 2-2. SIMMER-III Time Step Hierarchy.

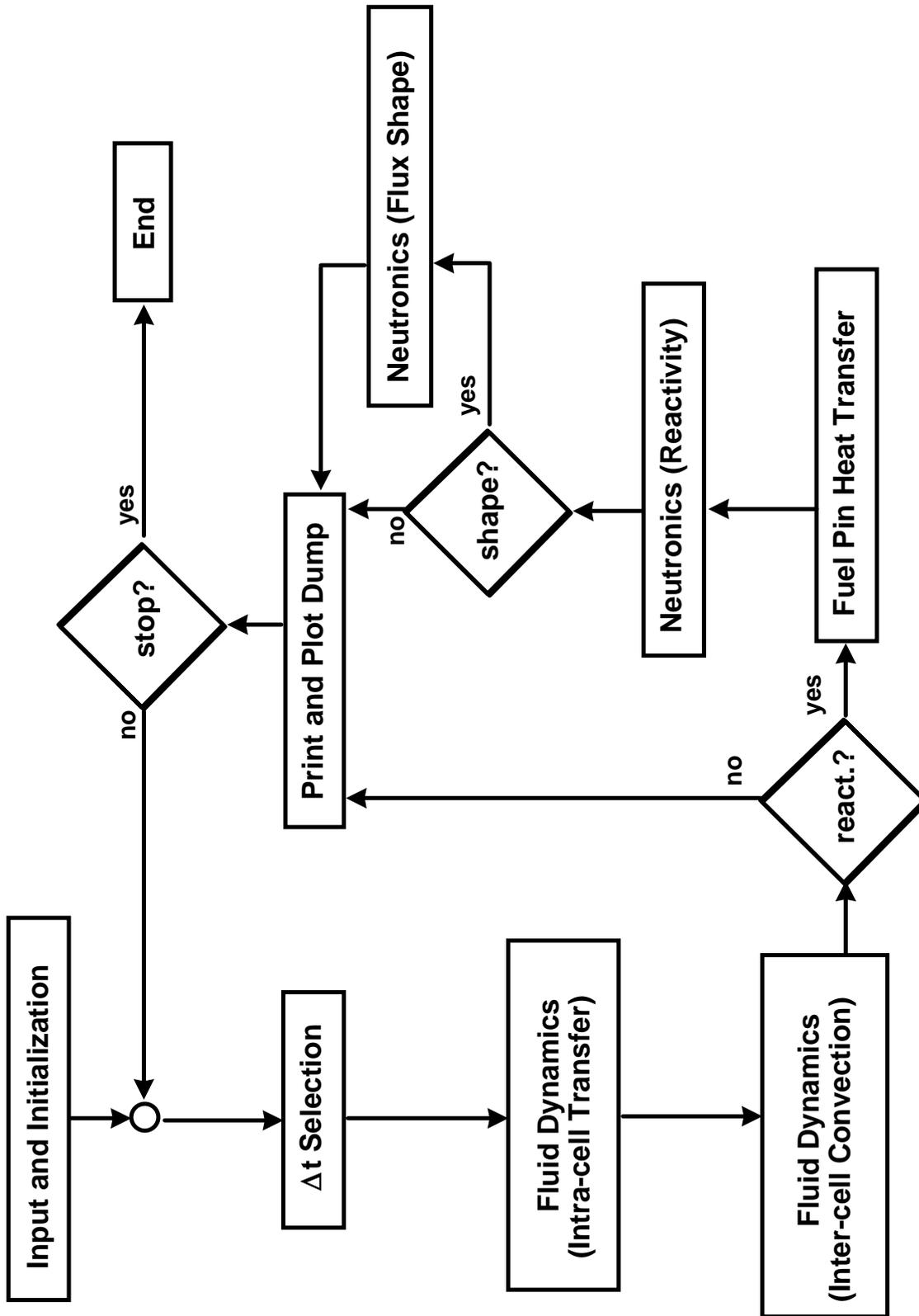


Fig. 2-3. SIMMER-III Calculational Flow.

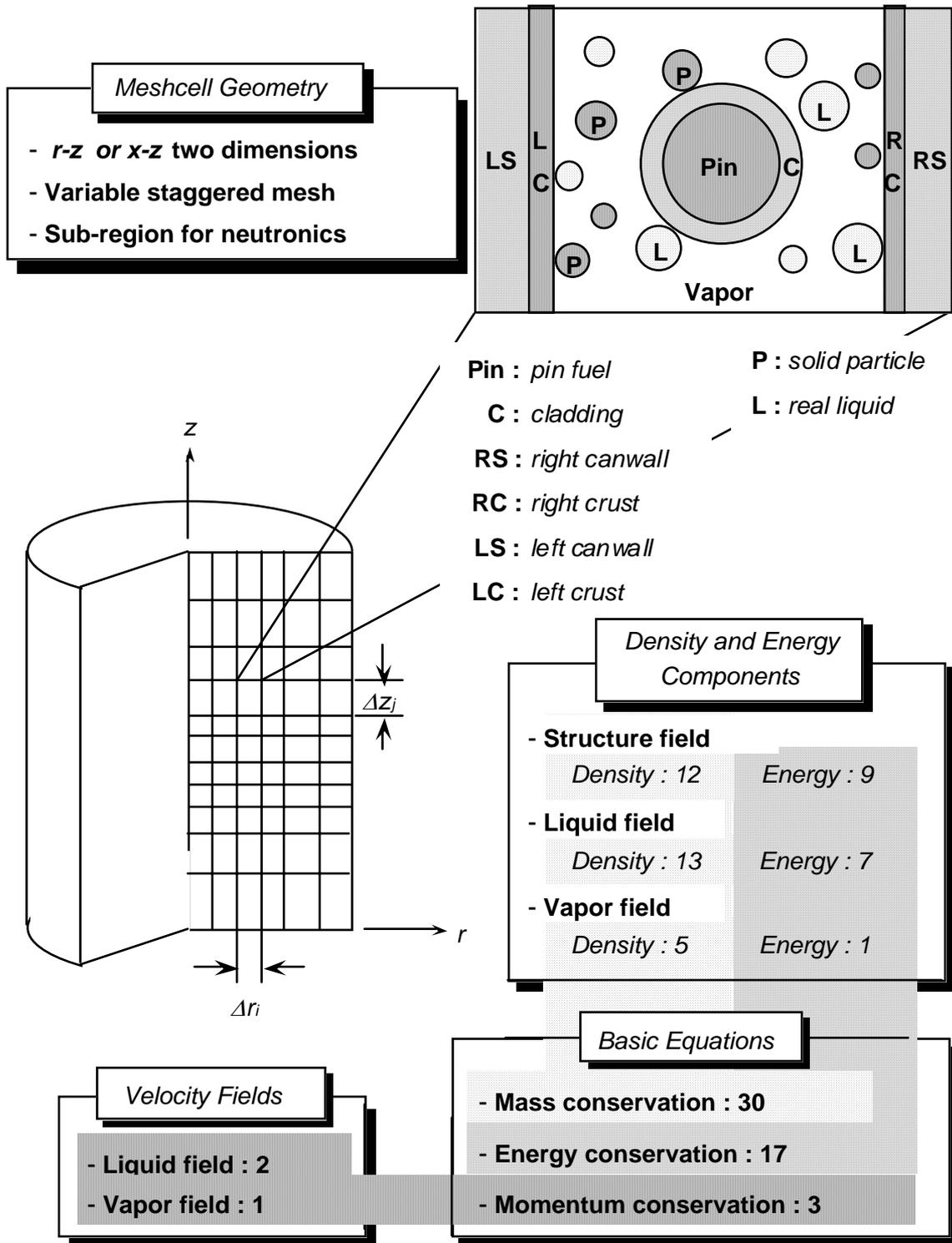


Fig. 2-4. SIMMER-III Geometric Framework.

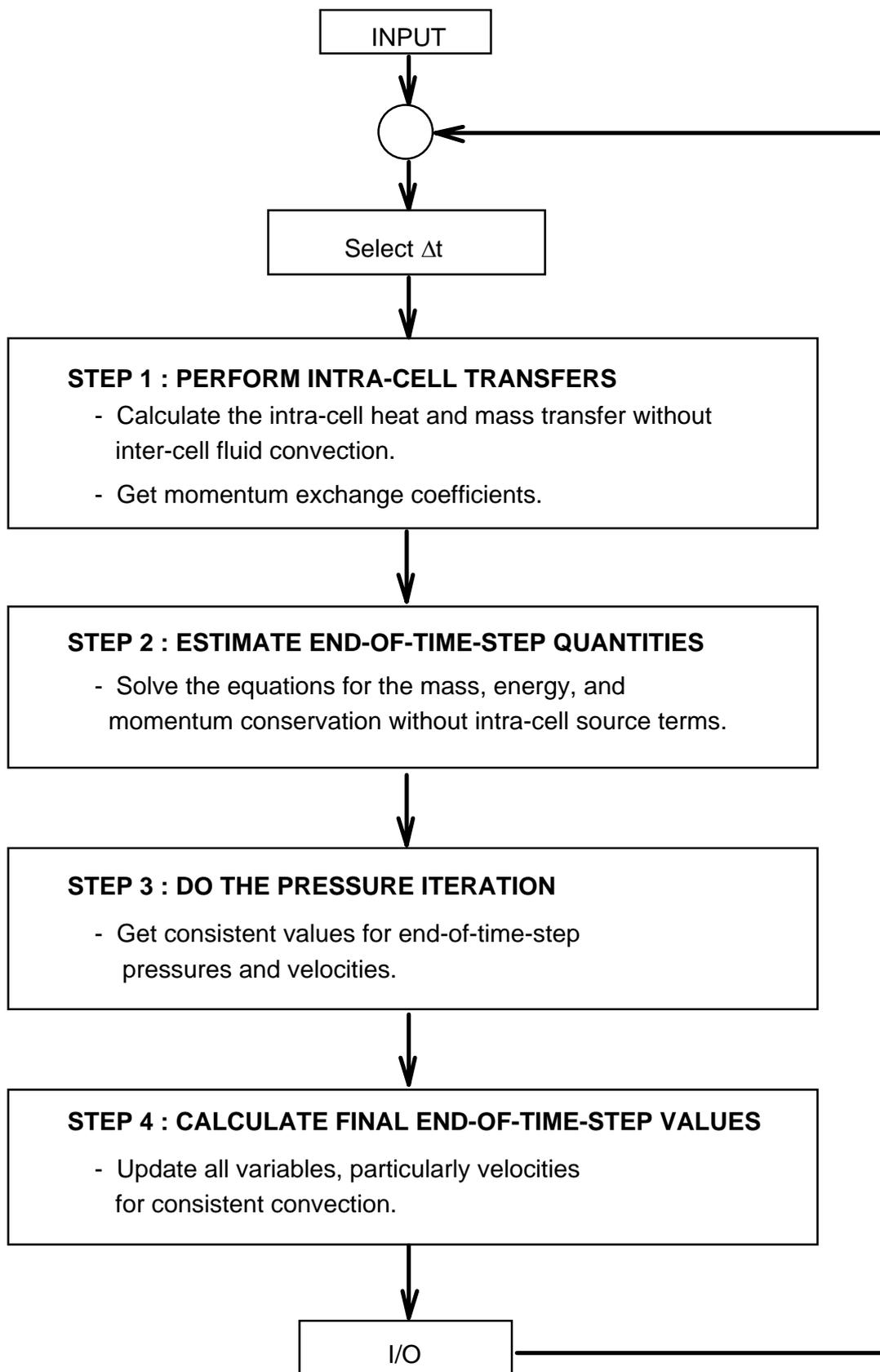


Fig. 2-5. Schematic Diagram of the Four-Step Method.

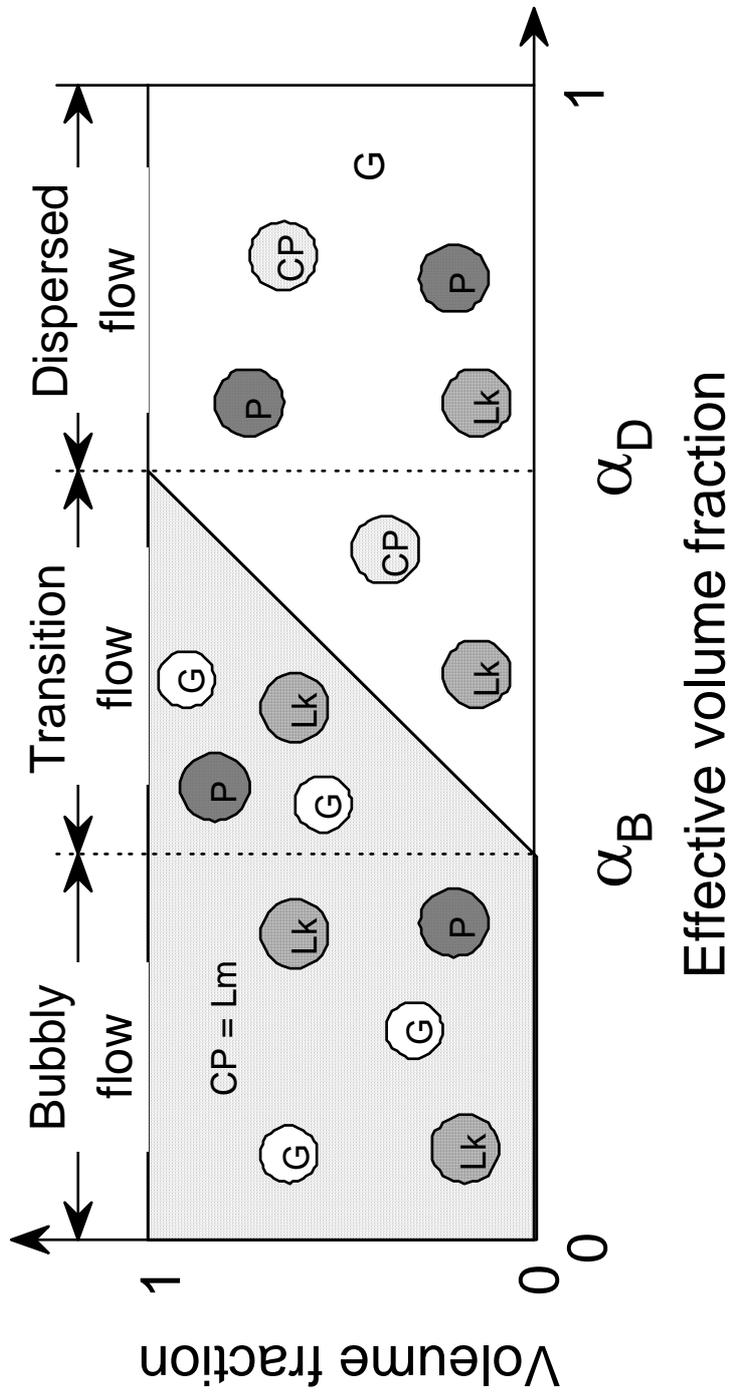


Fig. 2-6. SIMMER-III Pool Flow Regime Map.

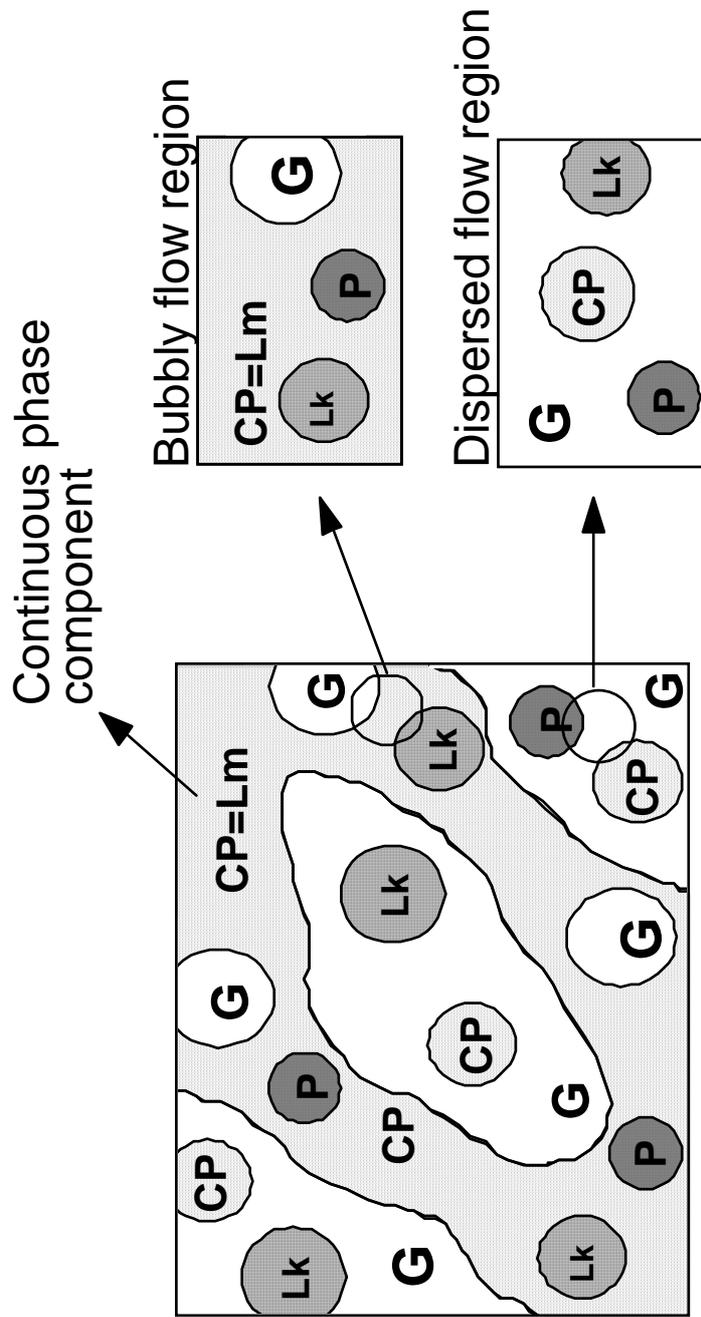


Fig. 2-7. Schematic Concept of Separating Bubbly and Dispersed Regions.

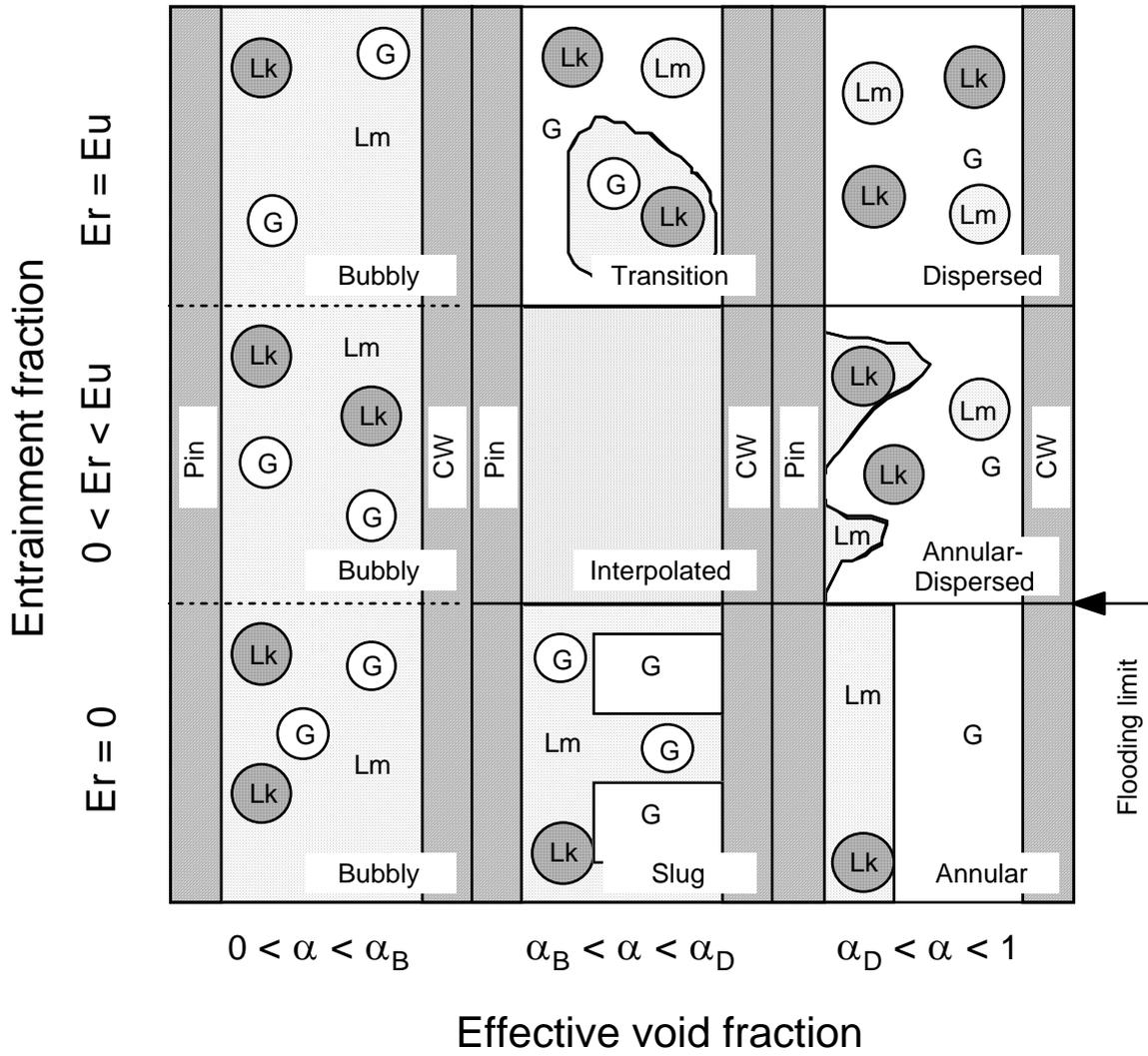
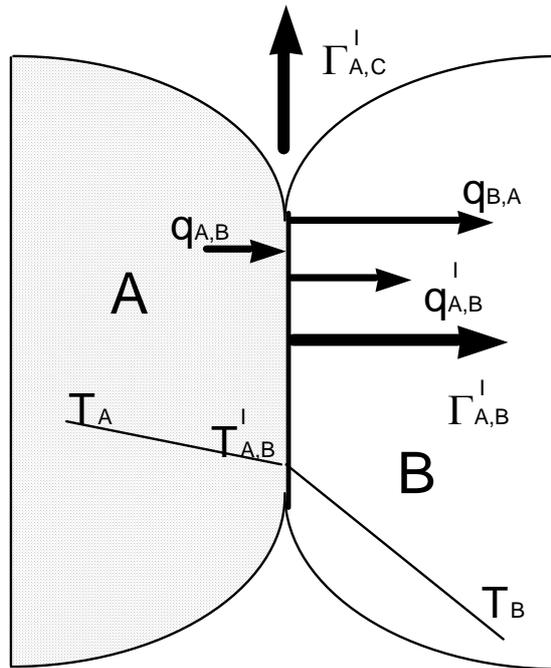


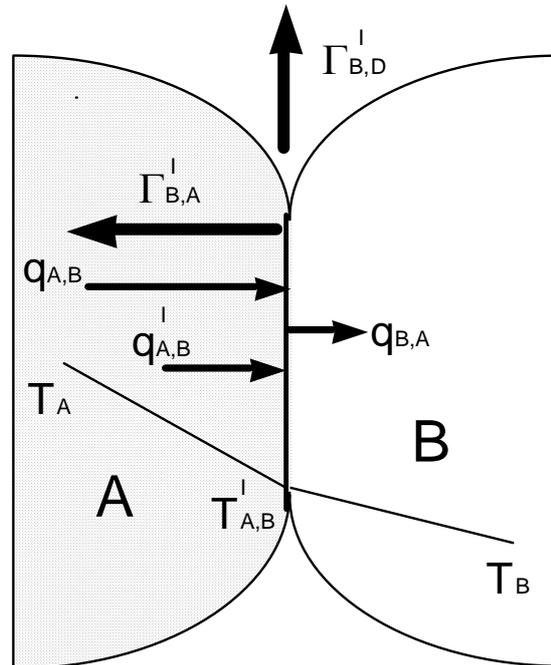
Fig. 2-8. SIMMER-III Channel Flow Regime Map.

Energy Component	Energy component which is being interacted with:													Mass Transfer paths:	
	Gas/Vapor G	Liquid Fuel L1	Liquid Steel L2	Liquid Sodium L3	Fuel Particle L4	Steel Particle L5	Control Particle L6	Fuel Chunk L7	Fuel Pin Structure K1	Left Structure K2	Right Structure K3	M/F	V/C		
Gas/Vapor G	V/C	HGLM(1) I1 {1}	HGLM(2) I2 {2}	HGLM(3) I3 {3}	HGLM(4) I4 {3}	HGLM(5) I5 {3}	V/C	V/C	HGS I29 {3}	HGS I37 {3}	HGS I45 {3}	-	27		
Liquid Fuel L1	V/C		HRT(1) I8 {1}	HRT(2) I9 {1}	HRT(3) I10 {1}	HRT(4) I11 {1}	M/F	M/F	HRS(1) I30 {1}	HRS(8) I38 {1}	HRS(10) I46 {1}	6	1		
Liquid Steel L2	V/C			HRT(8) I14 {1}	HRT(9) I15 {1}	HRT(10) I16 {1}	M/F	M/F	HRS(2) I31 {1}	HRS(9) I39 {1}	HRS(11) I47 {1}	4	2		
Liquid Sodium L3	V/C				HRT(15) I15 {1}	HRT(16) I16 {1}	M/F	M/F	HRS(3) I31 {1}	HRS(3) I39 {1}	HRS(3) I47 {1}	-	3		
Fuel Particle L4	V/C					HPT(1) I10 {1}	M/F	M/F	HRS(4) I31 {1}	HRS(4) I39 {1}	HRS(4) I47 {1}	1	-		
Steel Particle L5	V/C						M/F	M/F	HRS(5) I31 {1}	HRS(5) I39 {1}	HRS(5) I47 {1}	2	-		
Control Particle L6	V/C						M/F	M/F	HRS(6) I31 {1}	HRS(6) I39 {1}	HRS(6) I47 {1}	-	-		
Fuel Chunk L7	V/C						M/F	M/F	HRS(7) I31 {1}	HRS(7) I39 {1}	HRS(7) I47 {1}	1	-		
Fuel Pin Structure K1	V/C						M/F	M/F	H/M transfer calculated in V/C routines or M/F routines				2	-	
Left Structure K2	V/C						M/F	M/F	HTC(1) is array name and number of the HTC				3	-	
Right Structure K3	V/C						M/F	M/F	Interface ID {no. mass transfer paths}				3	-	
											Total no. paths =		22	33	

Fig. 2-9 Role of HTCs in SIMMER-III Heat and Mass Transfer.



Mass transfer possibilities at an (A,B) interfaces with net heat flow to the interface from Component A
 - Component A condenses or freezes



Mass transfer possibilities at an (A,B) interfaces with net heat flow to the interface from Component A
 - Component B vaporizes or melts

Fig. 2-10. Interface Treatment in Non-equilibrium Transfer.

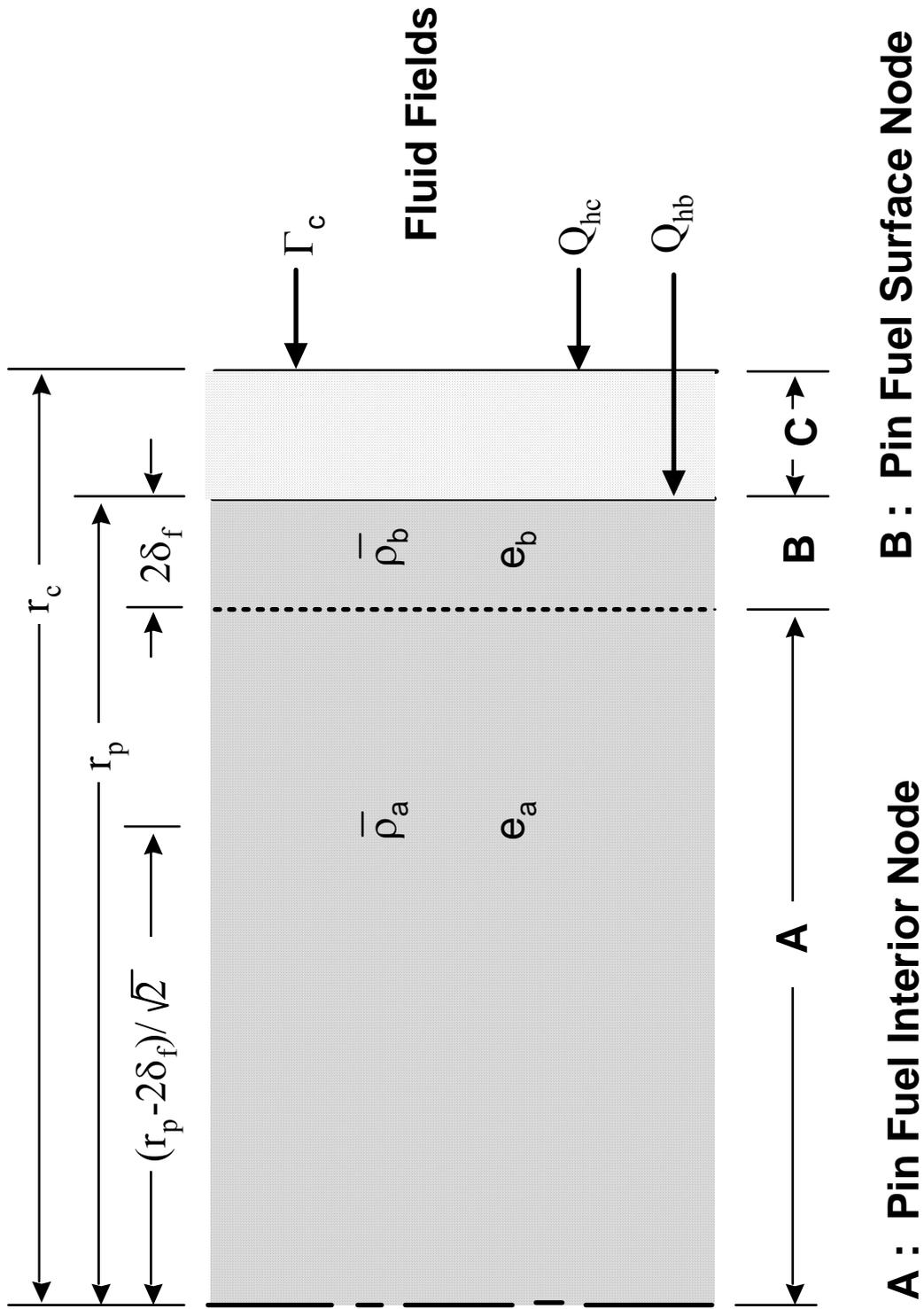


Fig. 2-11. Radial Fuel-Pin Cross Section in SIMMER-III (Simple Model).

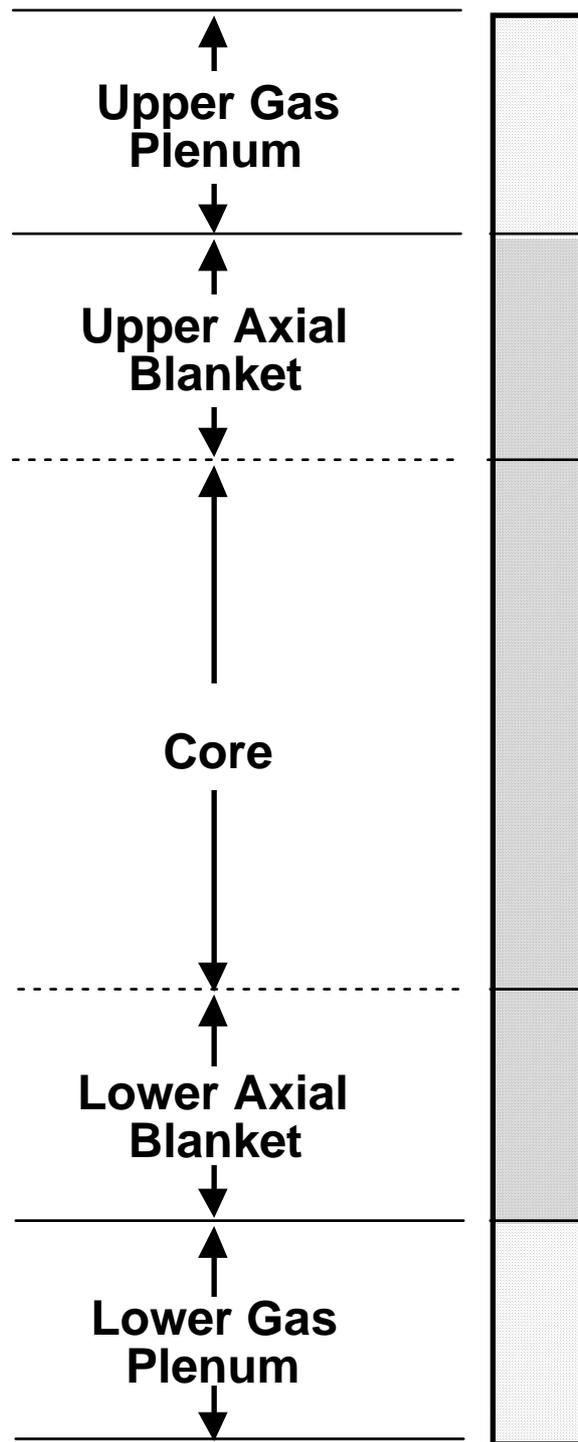


Fig. 2-12. Axial Fuel-Pin Representation in SIMMER-III (Simple Model).

CHAPTER 3

PROGRAM DESCRIPTION AND USE

In this chapter, the programming information of the SIMMER-III code is provided for users of the code. This includes: the description of: Comdecks and Decks (**Appendix A**), system-dependent routines/functions (**Appendix B**), equation-of-state functions (**Appendix C**), thermophysical-property functions (**Appendix D**), constants and default data used in SIMMER-III (**Appendix E**), post-processing (plot) files (**Appendix F**), the full input manual (**Appendix G**) and sample input data listings (**Appendix H**). A useful and powerful post-processing program, BFSCAN, was developed at JNC and is released with SIMMER-III. The minimum information to use BFSCAN is given in **Appendix I**.

3.1. Code Structure

3.1.1. Code Library and Options

The SIMMER-III code was programmed at JNC in standard FORTRAN-77 and is operated on FACOM's mainframe (GS-8800), vector processors (VPP-300), and UNIX engineering workstations (EWSs). The FACOM systems are compatible with IBM mainframes, and the EWSs (IBM RS6000, SUN, HP9000 and DEC-ALPHA) are standard UNIX systems. They are also compatible with Windows NT workstations or LINUX systems. The purpose of programming techniques of SIMMER-III is to provide a vectorized, portable, and easy-to-maintain code. It is for this reason that the code is maintained exclusively using OpCode's HISTORIAN [26] as a special program library file similarly to the former SIMMER-II [3] or AFDM [8]. The user, therefore, must have access to and knowledge of HISTORIAN to maintain the code in the same way as JNC.

In the HISTORIAN code library of SIMMER-III, Fortran source cards are grouped into sets of common decks and decks. A common deck, starting from a `"*COMDECK"` card with a unique name, represents common blocks, equivalences, parameters or other declaration statements. A deck, starting from a `"*DECK"` card with a unique name, corresponds to each subroutine or function. In a deck, common decks are not expanded but they are called using a `"*CALL"` directive. A complete list of common decks and decks are described in **Appendix A**.

In a code library, each card of the source code has a unique line identifier consisting of a DECK (or COMDECK) name and a sequential number. When the card is modified by a correction set, the name is replaced with the correction identification name. Historically, SIMMER-III libraries were re-sequenced three times when Version 1.A, Version 2.A and

Version 3.A were created. This means all the versions later than Version 3.A will retain a history from Version 3.A. Even though there are more than ten thousand cards inserted or replaced since Version 3.A, the library will not be re-sequenced in the near future to avoid confusion for the users who maintain special correction sets separately from the library.

The Gather and Scatter operations for the CRAY machine, which frequently appeared in AFDM, are no longer present. They are simply replaced by using indirect addressing. The conditional vector merge functions CVMGn are still used and included in the library, because they are sometimes useful to simplify a code logical structure.

There are a few system dependent subroutines that may have to be supplied by users depending on the computing system they use. The specifications of the system-dependent routines are described in **Appendix B**.

The HISTORIAN code library allows us to insert various code options using `"*IF DEF"` or `"*IF -DEF"` directives. This is again the same format as the former SIMMER-II and AFDM. In SIMMER-III, however, the use of code options has been reduced in order that most of model or algorithm options can be specified by input data. Therefore the needs for HISTORIAN preprocessing and re-compilation can be minimized. The code options appearing at present in Version 3.A are listed below in **Table 3-1**. It is noted that the former code option CRAY is no longer supported, since no one in the current SIMMER community is using CRAY computers.

Table 3-1. Historian Code Options in SIMMER-III.

1.	FACOM	ON	Use a FACOM system (IBM compatible).
		OFF	Do not use a FACOM system.
2.	RS6000	ON	Use an IBM RS6000 EWS system (UNIX).
		OFF	Do not use an IBM RS6000 system.
3.	SUN	ON	Use a SUN EWS system (UNIX).
		OFF	Do not use a SUN system.
4.	HP9000	ON	Use a HP9000 EWS system (UNIX).
		OFF	Do not use a HP9000 system.
5.	ALPHA	ON	Use an ALPHA-chip EWS system (UNIX).
		OFF	Do not use an ALPHA-chip EWS system.
6.	ALPHANT	ON	Use an ALPHA-chip EWS system (Windows NT).

	OFF	Do not use an ALPHA-chip EWS system.
7.	URANUS	ON Do not use the neutronics model. The fluid-dynamics code with power-vs.-time input available.
	OFF	Use the space- and energy-dependent neutronics (transport theory only) model.
8.	ISOTOPE	ON Use isotope-wise cross section calculations (URANUS off).
	OFF	Use material-wise cross section calculations. Requires use of the MXS neutronics preprocessor before beginning a transient calculation.
9.	DPIN	ON Use the detailed fuel-pin model to calculate heat transfer inside pellet, cavity treatment, in-pin fuel motion and ejection.
	OFF	Use the simple fuel-pin model.
10	BLOW	ON Use the plenum fission-gas blowdown model.
	OFF	Do not use the plenum fission-gas blowdown model.
11	NOMF	ON Do not use the non-equilibrium melting/freezing model.
	OFF	Use the non-equilibrium melting/freezing model.
12	NOVC	ON Do not use the non-equilibrium vaporization/ condensation model.
	OFF	Use the non-equilibrium vaporization/condensation model.
13	DCOM	ON Remove the comment cards of dummy argument lists from the sub-program source files.
	OFF	Do not remove the comment cards.

3.1.2. Code Structure

The overall code structure is shown in **Figs. 3-1** and **3-2**. The meanings of individual subroutines are documented in **Appendix A**. SIIIPR is the main program that calls driver routines for input and initialization (INITIL), fluid dynamics (STPFLO), fuel-pin thermal calculation (SPIN or DPIN), and neutronics (GRIND). It also controls overall computational flow and prints and dumps the results. A restart file is dumped at specified timing or upon termination. A computational flow in SIIIPR is shown in **Fig. 3-3**. The calculation is terminated only in SIIIPR by checking the maximum problem time, the maximum number of fluid-dynamics cycles and remaining CPU time, or by monitoring a flag that indicates a problem during the calculation.

The input driver, INITIL, calls several subroutines to read input and initialize the problem. In addition to the card input, cross-section files are also read when a neutronics calculation is made (the code option URANUS is off).

The fluid-dynamics driver, STPFLO, controls the fluid-dynamics calculation by calling STEP1 for intra-cell transfer operations, and STEP2, STEP3 and STEP4 for inter-cell convection operations. The fluid-dynamics time step size is controlled, and the time and cycle are actually incremented in STPFLO. When non-convergence is observed in one of the steps, a feature is provided to re-calculate the same cycle with a halved time step size.

STEP1 represents the largest portion of SIMMER-III, and calls a series of subroutines to do intra-cell heat and mass transfer operations step by step. This is a level-3 routine (see **Section 3.2.4**) to define a structure of the erasable array, and calls level-4 routines with transferring the array through an arguments list. The computational flow of the STEP1 operations are shown in **Fig. 3-4** in the order of operations.

The structure of the neutronics model (GRIND as a driver) is essentially the same as SIMMER-II except for the flux shape calculation, and users are referred to the SIMMER-II manual [3]. GRIND calls: SHLDXS for cross-section calculations, TWODANT for flux-shape calculations, and PKDRIV for transient neutron kinetics calculations with an improved quasi-static method. Subroutine LINKM reads input and initializes the problem for TWODANT. GRIND controls both the initial stationary and transient neutronics calculations. The interface subroutines exchanging data from and to the fluid dynamics are also called from GRIND.

The fuel-pin heat-transfer driver, SPIN, simply calls routines for fuel-pin heat transfer (PINHTR) and plenum fission gas heat transfer (FGPTHR). SPIN is called at each heat-transfer time step consisting normally of several fluid-dynamics time steps. When the neutronics calculation is performed, it is called at each reactivity step before GRIND is called. This is because fuel temperature updates are essential for determining important Doppler feedback appropriately. This standard treatment of heat-transfer time step control can be flexibly changed by user specification, for example, by forcing the time step sizes to fluid dynamics. The detailed fuel-pin model, DPIN, is available in the latest version of SIMMER-III and it replaces SPIN.

3.1.3. Restart Capability

A restart capability is provided in SIMMER-III. Restart dump files are written at an interval specified by user or upon problem termination. A dump file contains all the common blocks needed to resume a calculation. To facilitate the calculation of word lengths of common blocks, a dummy variable is added at the very end of each common block.

Word lengths are counted during initialization of the problem (INILEN). Therefore special care must be taken when a first or last variable in a common block is to be modified. A restart calculation from a dump file is invoked by specifying "RESTART" in the first input card.

3.2. Programming

3.2.1. Input

The input data of SIMMER-III are described in **Appendix G**. The input for SIMMER-III (S-III) is in a NAMELIST style. In the NAMELIST format, the input variables are divided into classes that correspond to different NAMELISTs. Namely each class is distinguished by a different NAMELIST name. In an input stream, NAMELIST classes can be freely ordered with a few exceptions as noted in **Appendix G**. All the variables, with the exception of the mesh-cell variables, have been given default values. Comment cards may be entered between NAMELIST groups freely, since they are simply ignored. Special input flags to control model and/or algorithm selection and debug printing are provided in NAMELIST classes XCNTL for the fluid dynamics and NCNTL for the neutronics. The input listings of the four sample problems describe in **Section 3.3** are given in **Appendix H**.

3.2.2. Printer Output

The output listing of SIMMER-III can be printed on paper as logical unit 6 or a file name SIM06. Various input options in the program determine and control the amount and kind of printer output. The printed output listing is separated into the following six sections.

1. Code option and problem control card input edit
2. Fluid-dynamics input edit
3. Neutronics input edit
4. Neutronics initial calculation edit
5. Neutronics transient calculation edit
6. Fluid-dynamics transient calculation edit

1. Problem Control Card Input Edit. The first page of SIMMER-III output indicates the SIMMER-III version name, the problem title, the execution date, and time. The following lines indicate the HISTORIAN options selected to create the current load module. Finally, values of option control flags ALGOPT(n), EOSOPT(n), TPPOPT(n), HTCOPT(n), IFAOPT(n), HMTOPT(n), EDTOPT(n), MXFOPT(n), FPNOPT(n), RSTOPT(n), and ERROPT(n) read from the input stream then are edited.

2. Fluid-Dynamics Input Edit. The edit of the fluid-dynamics input consists of some sections which correspond to the NAMELIST classes. These are: the problem geometry, time step control, region-wise input of mesh-cell data, edit control, equation-of-state model parameters, thermophysical properties, interfacial area model inputs, momentum exchange function model inputs, heat transfer coefficient model inputs, boundary conditions, heat source, heat and mass transfer model inputs, fuel pin model inputs, and miscellaneous inputs. Each SIMMER-III input variable is printed with a description of the variable and its effect on the problem.

3. Neutronics Input Edit. The edit of the neutronics input consists of some sections which correspond to the NAMELIST classes. These are: the problem dimensions and control input parameters, time-step and quasi-static method control inputs, edit control, initial conditions, convergence parameters, shielding factor control parameters, definition of mesh cell sub-division and isotopic inventory regions, delayed neutron data, isotopic mixture specifications and cross-section regions, mesh dimensions, isotopic microscopic cross sections (optional), S_n constants, region-wise number density inventories (optional), and external neutron source (optional). Each SIMMER-III input variable is printed with a description of the variable and its effect on the problem.

4. Neutronics Initial Stationary Calculation Edit. After initialization, SIMMER-III does initial stationary neutronics calculations for both the adjoint and real fluxes. For both cases, a summary of the convergence progression is printed at each outer iteration. Before the summary print, region-wise isotopic number densities are printed if $INVPRT > 0$. The amplitude equation parameters are printed at the end of the initial calculations. The initial neutronics edit consists of the following information.

(a) Region-Wise Inventory Edit. The summations of isotopic number densities are printed for user-specified regions. This feature is useful to check the appropriateness of user input specification of specific number densities and fluid-dynamic macroscopic densities.

(b) Outer Iteration Summary Edit. A single line per at each outer iteration indicates: CPU time, outer iteration counter, the numbers of inner and multigroup DSA iterations, the current k-eff estimate, the precision of k-eff, the maximum point-wise changes of flux and fission source, and information on the status of the inners. The format is common to both the adjoint and real flux solutions. If the transient initialization is active ($ITR=1$), a summary of the neutronics data adjustment factors is included in the summary.

(c) Neutronics Time Step Summary Edit. After the convergence in the initial stationary flux shape, a neutronics (reactivity) time step summary is printed in the same format as the transient edit. The summary contains: the current time, power (POWER), amplitude (1.0), and reactivity, and amplitude equation parameters.

5. Neutronics Transient Calculation Edit. For the neutronics transient calculations, the time-step controls are monitored for both the reactivity update steps and flux-shape steps. The time-step control information is printed for both the reactivity update steps and flux-shape steps at each reactivity step for the smallest estimates of the criteria defined in **Section 2.6.3**. If a shape-step calculation is performed, a summary of the flux shape calculation is printed in the similar format as the initial stationary solution. At this time, only the real flux is calculated. The outer iteration summary appears at each reactivity step if the flux-shape update option is used (IFXUDL>0). In addition, a print of region-wise isotopic number densities is given, if INVPRT \geq 2. At reactivity steps, the reactivity and amplitude calculated from the updated amplitude equation solution, based on the current cross sections and flux shape, are printed along with other amplitude equation parameters. The decay power amplitude is also printed. The reactivity projected to the next reactivity step and the corresponding amplitude from the amplitude equation solution follows. Then a summary of the energy conservation imbalance between the neutronics and fluid dynamics solutions is printed. After the flux shape update for the gamma iteration, the outer iteration summary edit is followed by the printing of information of a series of recalculated reactivity steps along with updated amplitude equation parameters. Finally the neutronics time step summary is printed again before taking the next reactivity step.

6. Fluid-Dynamics Transient Calculation Edit. The fluid-dynamics transient calculation has four different kinds of output.

- (a) Time-step edits
- (b) Cell status edits controlled by the input parameter PCGRP
- (c) Variable edits in the whole calculational region controlled by the input parameter LPRGN.

(a) Time-Step Edits. For each EDTOPT(48) time step cycle, a single line is printed to summarize the results. Each line indicates

- (1) time-step number (CYCLE),
- (2) time,
- (3) time step size,
- (4) the mechanism which determines the current time step size,
- (5) the number of pressure iterations (ITERA),
- (6) the number of vaporization/condensation iterations (ITIVC), and
- (7) the amplitude (relative power).

If the post-processing dump and/or restart dump files are written, their sequential numbers are printed in the same line. The mechanism dominating the time step size is indicated by a word which consists of 6 characters. Each word means,

- DTSTRT : Initial time step restriction,
- OPTPIT : The number of pressure iteration exceeded the limit,
- 2*DTP : The time step cannot become larger than twice of the previous time step size,
- COURNT : Courant conditions,
- DTMAX : Maximum time step size,
- VCITMX : Non-convergence occurred in VCHMT calculation and the same cycle is re-calculated with a halved time step size,
- VCDTMX : An excessive change of vapor temperature was predicted in VCHMT calculation and the same cycle is re-calculated with a halved time step size,
- DTIVC : The number of the V/C iterations exceeded a maximum specified by the user and the next cycle is calculated with a halved time step size,
- S1ITMX : Non-convergence of vapor temperature occurred in EOST calculation in Step 1 and the same cycle is re-calculated with a halved time step size,
- S1TGMN : The vapor temperature tended to be lower than the minimum vapor temperature in EOST calculation in Step 1 and the same cycle is re-calculated with a halved time step size,
- S2VELO : Non-convergence of velocity occurred in VITERP calculation in Step 2 and the same cycle is re-calculated with a halved time step size,
- PIFAIL : Non-convergence occurred in the pressure iteration in Step 3 and the same cycle is re-calculated with a halved time step size,
- S4VELO : Non-convergence of velocity occurred in VITER calculation in Step 4 and the same cycle is re-calculated with a halved time step size,
- S4ITMX : Non-convergence of vapor temperature occurred in EOST calculation in Step 4 and the same cycle is re-calculated with a halved time step size,
- S4TGMN : The vapor temperature tended to be lower than the minimum vapor temperature in EOST calculation in Step 4 and the same cycle is re-calculated with a halved time step size,
- DPSTP1 : Time step restriction due to the source term splitting error based on the pressure difference between Step 1 and Step 2,
- DPSTP4 : Time step restriction due to the source term splitting error based on the pressure difference between Step 2 and Step 4,
- DTSTP1 : Time step restriction due to the source term splitting error based on the vapor-temperature difference between Step 1 and Step 2,
- DTSTP4 : Time step restriction due to the source term splitting error based on the vapor-temperature difference between Step 2 and Step 4,
- ALGO31 : The time step cannot increase during ALGOPT(31) cycles since the previous time step reduction, and
- DTHN : The time step cannot become larger than the fuel-pin heat-transfer time step and/or the reactivity time step.

(b) Cell Status Edits. The cell status edits provide a table of values of the major mesh-cell variables for the mesh cells specified by PRCEL.

(c) Whole Region Edits. The whole region edits provides a table of mesh-cell-dependent variables specified by LPRGN in the whole calculational region including the boundary cells.

3.2.3. Programming Techniques

The goal of SIMMER-III programming is to produce a fully vectorized, portable and user-friendly code. The portability of the code is guaranteed by utilizing the OpCode's HISTORIAN to maintain the source files. The separated assignment of integer, real, and character variables to the different common blocks also keeps the portability of the code between 4-byte machines such as FACOM and 8-byte machines such as CRAY. To take advantage of the vector capabilities, the inner-most loop should have the long vector length. Therefore, the inner-most loop is designed to be the cell loop in SIMMER-III programming. In the case that not all the cells are to be processed in a cell loop, the indirect addressing technique is used while the GATHER/SCATTER technique heavily used in AFDM for the CRAY machine was abandoned. However, the CVMGn function (conditional vector merge) originated from CRAY is still utilized because it allows us to reduce the length of the program extensively. It is recommended to make use of the in-line expansion feature of FORTRAN compiler for CVMGn and the other frequently referred functions to reduce the calculational costs in running SIMMER-III. In the FACOM systems, this can be done using the compiler option of in-line expansion by declaring the @FORTRAN statement at the top of the SIMMER-III program as follows:

```
@FORTRAN INLINE(EXP(CVMGT, ICVMGT, XPGM, .....)).
```

3.2.4. Memory Management

The mesh cell storage is divided into common block data and erasable array data. The latter is extensively used to save the memory size necessary to run the code. The common data are passed between the subroutines higher than level 3 and from the current time step to the next time step. The common data are classified into three groups, CELLP, CELLK, and CELLM variables.

CELLP : the beginning-of-time-step (previous time step) values.

CELLK : the end-of-time step (the most up-to-date) values.

CELLM : the end-of-STEP1 values, updated through the intra-cell transfer processes and transferred to inter-cell convection.

An important feature of SIMMER-III is the use of erasable storage. The erasable array is a large block of core memory to which the cell variables are equivalenced at each

time step. The data are not preserved between the subroutines higher than level 3 and between the time steps. All levels 1 to 3 may use all of the erasable storage freely. When a level 3 calls a lower level routine, the cell-storage variables should be assigned to the erasable array in the calling routine and transferred through the argument list. The routine which requires the largest cell storage and serves as the example of the most complex one is STEP1. It is important to minimize the storage size in this routine by overlapping some variables on the same address. There is some trade-off between the core memory size and the flexibility in modifying the code. The basic policy is to minimize the core storage without losing the flexibility. To achieve this, the mesh cell variables are allocated in the reversed order of the appearance of the subroutines which refers these variables last in STEP1 (see **Fig. 3-5**). The concept of the erasable array is also used in the neutronics, but the storage requirement is normally dominated by the fluid dynamics in SIMMER-III.

3.2.5. File Management

The standard files for the fluid-dynamics calculation consist of input data set, output listing, post-processing, restart dump, and restart input. Additional files such as cross-section related files are required to perform space-time dependent neutronics calculation. Two file management ways exist for IBM compatible FACOM systems and UNIX systems. In the FACOM systems, the files must be allocated to the logical file units as shown in **Table 3-2**. In the UNIX systems, the file names in **Table 3-2** are determined in the OPEN statement in the main program. The logical record length for input data set is 80 bytes and for output listing 133.

Table 3-2. File names and logical file units in SIMMER-III.

Variable for Logical File Unit	Logical File Unit	File Name	Description
INPFU	5	sim05	The input data set file.
OUTFU	6	SIM06	The output-listing file.
PPFU	7	SIMPF	The fluid-dynamics post-processing file.
DMPFU	8	SIMDF	The restart dump file
DMPRFU	9	simdf	The restart input file (simrf, if the code option ALPHANT is on).
BFU	77	SIMBF	The fluid-dynamics post-processing file
FFU	78	SIMFF	The post-processing file for detailed pin model.
NPLTPK	3	SIMPK	The neutronics post-processing file for summary and point-kinetics information.

NFPLT	4	SIMNP	The neutronics post-processing file.
ISNCON	11	sncons	The CCCC standard file for Sn constants; read when ISNT<0 (in input class NPAR), otherwise built-in constants are used.
ISOTXS	12	isotxs	The CCCC standard file for infinite-dilute cross sections.
IBRKXS	13	brkoxs	The CCCC standard file for self-shielding factors.
IATFLI	21	atflux	The binary input file of the initial adjoint flux; read when ICOS=2 or 4 (in input class NPAR).
IRTFL1	22	rtflux	The binary input file of the initial real flux; read when ICOS=3 or 4 (in input class NPAR).
IATFLO	23	ATFLUX	The output file for the initial adjoint flux.
IRTFLO	24	RTFLUX	The output file for the transient real flux.
IADJMA	41	adjmac	The binary interface of the macroscopic cross-section file for adjoint calculation.
IMACRX	42	macrxs	The binary interface of the macroscopic cross-section file.
IASGMA	43	asgmat	The binary interface file for the assigning materials to cells.
IGEODS	44	geodst	The binary interface file for the geometry description.
ISOLIN	45	solinp	The binary interface of the SIMDANT-SOLVER module data file.
INP2D	46	inp2d (inp2t)	The TWODANT input data (inp2d). The TWOTRAN-II input data (inp2t).
IMACRX8	47	macrxs-int8	The binary interface of the macroscopic cross-section file (integer*8).

3.2.6. Dimensions and Parameters

Parameter statements are used to dimension the most of the array variables. These parameter statements are gathered in common decks named DIMEN for the fluid dynamics and NDIMEN for the neutronics. This allows the quick change of all dimensions if the problem size is changed. The parameters that define the problem size are IBM and JBM. These are the maximum numbers of fluid-dynamics mesh cell in the radial and axial directions, respectively. The users are free to change these parameters in creating the FORTRAN compiler source by HISTORIAN to optimize the size of a load module for each

problem. The major parameters, their default values, and their meanings are listed below in **Table 3-3** for the fluid dynamics and **Table 3-4** for the neutronics.

Table 3-3. Parameters defined in SIMMER-III: fluid dynamics.

IBM	12	The maximum number of radial cells.
JBM	16	The maximum number of axial cells.
MNMS	1400	The maximum number of real erasable arrays.
MNIMS	250	The maximum number of integer erasable arrays.
MREG	100	The maximum number of regions for region-wise input of mesh cell variables.
MAXTP	40	The maximum number of power vs. time table.
MCSRE	9	The number of structure energy components.
MCLRE	7	The number of liquid energy components.
MCGRE	1	The number of vapor energy components.
MCSR	12	The number of structure density components.
MCLR	13	The number of liquid density components.
MCGR	5	The number of vapor density components.
MNMAT	5	The number of materials
MNMATN	2	The maximum number of sub-materials.
MMOM	3	The number of momentum fields.
MFMAT	7	The number of fuel materials.
MEOSRN	2	The maximum number of EOS regions.
MARL	7	The number of convective interfacial areas for liquid components.
MARV	1	The number of convective interfacial areas for vapor.
MNGRP	50	The maximum number of cells to be edited the status of cell-wise variables.
MNPP	50	The maximum number of variable groups to be written to the post-processing file.
MPBSZ	2048	Not used
MNTEC	10	The maximum number of data points to control the time interval of listing, post-processor dump, and restart dump.
NRPDMP		The number of records written to the restart dump.
	63 (DPIN-off, and URANUS-on)	
	77 (DPIN-off, and URANUS-off, and ISOTOPE-off)	

	79 (DPIN-off, and URANUS-off, and ISOTOPE-on)	
	64 (DPIN-on, and URANUS-on)	
	78 (DPIN-on, and URANUS-off, and ISOTOPE-off)	
	80 (DPIN-on, and URANUS-off, and ISOTOPE-on)	
MHSO	5	The number of components heated by nuclear power.
MULTI	2	The factor of word length by 4 bytes.
MPMAT	6	The number of residual errors in pressure iteration.
NPBM	11 (DPIN-on)	The number of radial nodes in fuel.
MCCR	4 (DPIN-on)	The number of materials in cavity.

Table 3-4. Parameters defined in SIMMER-III: neutronics.

NEI	36	The maximum number of radial neutronics cells.
NEJ	48	The maximum number of axial neutronics cells.
NEIGM	18	The maximum number of neutron energy groups.
NEIGD	6	The maximum number of delayed-neutron precursor groups.
NEISN	4	The maximum order of Sn constants.
NEINV	6	The maximum number of isotopic inventory regions.
NERXS	1	The maximum number of cross-section regions.
NEMT	5	The maximum number of neutronics materials.
NERSTP	10	The maximum number of reactivity steps per shape step.
NETPT	9	The maximum number of temperature table points in shielding factors (BRKOXS).
NEPS0	14	The maximum number of background cross-section table points in shielding factors (BRKOXS).
NEDK	6	The maximum number of decay heat sources.
NEHOMO	160	The maximum number of homogeneous region.
NEMFR	10	The maximum number of neutronics mesh-divisions per neutronics mesh cell.
NEFFB	9	The maximum number of reaction types in shielding factors (BRKOXS).
NEISO	5	The maximum number of isotopes (default: 26, if the code option ISOTOPE is on).

NEISXS	20	The maximum number of isotopic cross-section pointers.
NEIS4C	40	The maximum number of isotope for calculation use.

3.2.7. Constants and Default Data

In the SIMMER-III programming, floating-point values are not directly coded as numerical values, but they are defined by the Fortran variables for which their numerical values are assigned during initialization. All the constants defined and used in SIMMER-III Version 3.A are described in **Appendix E**.

To minimize input errors and user's burden to prepare a large amount of input data, most of the input variables are given their default values internally in the code. They are defined by Block data. The exceptions are the Namelists XMSH, XRGD and XCWD, which define the geometry of the problem, and initial mass, temperature and pressure distributions which must be always supplied by the user. The complete list of the default data currently available in the code is given in **Appendix E**. Despite these default data are available, the users can freely provide the input data, which override the default data during initialization.

3.2.8. Error and Diagnostics Messages

Error and diagnostics messages are printed in the output listing during the calculation. The general format of the message is as follows,

SPNAME-*nnn*L: Messages .

"SPNAME" is the subroutine name which prints this message and "*nnn*" is a serial number of the message in the subroutine. "L" is a one-character flag which identifies the severity level of the error. Currently 4 levels are defined as,

I : Information,
W : Warning,
E : Error, and
S : Serious Error.

The calculation stops if error level "E" or "S" is detected. "Messages" provide the explanation and information about the error.

3.3. Sample Problems

In this report, four sample problems are currently provided. These problems were prepared such that all the code elements of SIMMER-III Version 3.A are tested. The sample problems are also useful to check and confirm that the implementation of the code at different

sites is made correctly. There is no intention to discuss the physical validity or appropriateness of the computed results described in this section. The card input listings of the four test problems are given in **Appendix H**.

3.3.1. Little Work Energy Problem (LWE)

The little work energy (LWE) problem examines, in a simplified form, the partition of energy and the resulting vessel damage potential following an energetic core disassembly. During the post-disassembly expansion phase, the high-pressure and high-temperature fuel can expand into an above-core sodium pool, vaporize sodium and do work on its surrounding environment. Estimating the damage resulting from such a core expansion is a complex problem that has been attempted by the predecessors of SIMMER-III. Since SIMMER is uniquely suited for simulating large-scale motions, it was used to furnish estimates of dynamic loading on core and vessel structures.

Here, a simplification of such a core expansion is presented as a test calculation. Because of the simplifications that are made in this problem, it is principally useful to assess model performance, code robustness, and stability questions rather than to address directly the post-disassembly energetics question. The configuration chosen for this problem, shown in **Fig. 3-6**, has 36 (3×0.935 m radial and 12×0.9144 m axial) cells. The core is represented by one mesh cell that contains the following materials with the specified volume fractions and temperatures:

$$\begin{aligned} \text{Liquid fuel} & : \alpha_{L1} = 0.626771 \quad T_{L1} = 5966 \text{ K} \\ \text{Liquid steel} & : \alpha_{L2} = 0.18243 \quad T_{L2} = 1754 \text{ K} \end{aligned}$$

This is essentially the same sample problem historically used for SIMMER-II and AFDM. In AFDM, liquid steel was not explicitly treated because it does not allow three liquid components. The material components in the present calculation are therefore specified more realistic than for AFDM. The details of the remaining regions are the same as Ref [8].

The evolution of kinetic energies over the system and the pressure in the cell (3,12) are shown in **Fig. 3-7**, which are the results calculated on the EWS (RS6000).

3.3.2. Little Boiling Pool Problem (LBP)

The little boiling pool (LBP) problem simulates the behavior of an internally heated mixed liquid fuel/steel pool. No neutronics calculation is included (with the URANUS option); instead the constant and uniform heat source is provided. The steel and fuel masses as well as dimensions are typical for an LMFR core of about 1000 MWth. Detailed initial conditions are given in **Fig. 3-8**, which shows the 5×7 R-Z geometry for the SIMMER-III calculations. The liquid volume fractions noted in the figure are the sum of the fuel and

steel volume fractions that are in a ratio of 1.5:1. The walls of the pool are rigid and there is a heat sink along the radial and top boundaries to condense vapor produced in the pool. To test the models for structure disintegration, the fuel pin and can wall structures are included partly in the system. These structures undergo gradual disruption, followed by a gross motion of a fuel/steel boiling pool. Rigid and adiabatic boundary conditions are applied on the boundary of the system. It is noted that the initial component volume fractions and temperatures in **Fig. 3-8** were chosen in such a way that a smooth initial pressure distribution was obtained over the pool.

The volume fractions, temperatures, and pressure are shown in **Figs. 3-9**, which are the results calculated on the EWS (RS6000).

3.3.3. Fuel-Coolant Interaction Problem (FCI)

To test the V/C model of SIMMER-III, a simplified three-cell fuel-coolant interaction (FCI) problem was set up. The geometric model and initial conditions used for this one-dimensional problem are shown in **Fig. 3-10**. The FCI, sodium pool and cover-gas regions are modeled as a one-dimensional cylindrical geometry with three axial mesh cells. The FCI zone is represented by one bottom mesh cell that contains initially a uniform mixture of fuel and sodium. The sodium pool is simulated by liquid sodium and is four times in height of the FCI zone. The top mesh cell, the cover-gas region, is filled with non-condensable gas and a small amount of sodium with a volume fraction of 0.2. This problem has a simple geometry and FCI occurs only in one mesh, so that the code prediction can be easily interpreted. This problem is also adequate for verifying several special case treatments in the V/C model and for testing the robustness of the code.

The vapor volume fraction, the vapor temperature, and the pressure are shown in **Fig. 3-11**, which are the results calculated on the EWS (RS6000).

3.3.4. Space-Time Neutronics Problem (STN)

This sample problem is intended to test the space- and energy-dependent neutron kinetics model and its coupling with the fluid dynamics. The problem setup is a fictitious disrupted LMFR core of an intermediate size for simulating a short-time energetic recriticality event in a model with 12 by 16 meshes. To drive a very rapid reactivity insertion, a slug of molten fissile fuel initially present at the bottom of the core center is moved toward the core midplane with an initial velocity of 100 m/s. The geometric model and initial conditions used for this problem are shown in **Fig. 3-12**. The resultant rapid positive reactivity insertion brings the core to prompt criticality. The power excursion terminates in a short period of several milliseconds due to a negative reactivity feedback mechanism induced by the continued fuel motion in the core center beyond the core midplane.

The calculated histories of the reactor power and reactivity are shown in **Fig. 3-13**, which are the results calculated on the EWS (RS6000). The special code options used in the STN problem are: NOMF and NOVC to eliminate the calculations of material phase transition, with URANUS and ISOTOPE turned off. The input code option NIOPT(32) is set to 1 in order to use extended P0 approximation. The annular core region contains intact fuel pins but the heat-transfer calculation is eliminated by input specification.

3.4. Post-processing

The structures of four different types of post-processing files (PPFs) dumped from SIMMER-III are described in **Appendix F**. User-specified input data flexibly control the PPF dump. Because of an installation dependent nature of computer graphics, no post-processor code is provided with the SIMMER-III code. Since the file format of the main PPFs is compatible with the former SIMMER-II and AFDM, user experience and available tools can be used with minimum changes. To facilitate flexible post-processing at different installations, a special input option is also available for dumping PPFs in a text format.

At JNC, a powerful post-processor, BFSCAN, has been developed for SIMMER-III. This program is available on a UNIX EWS system and is included with the SIMMER-III code. A more detailed description of BFSCAN is given in **Appendix I**.

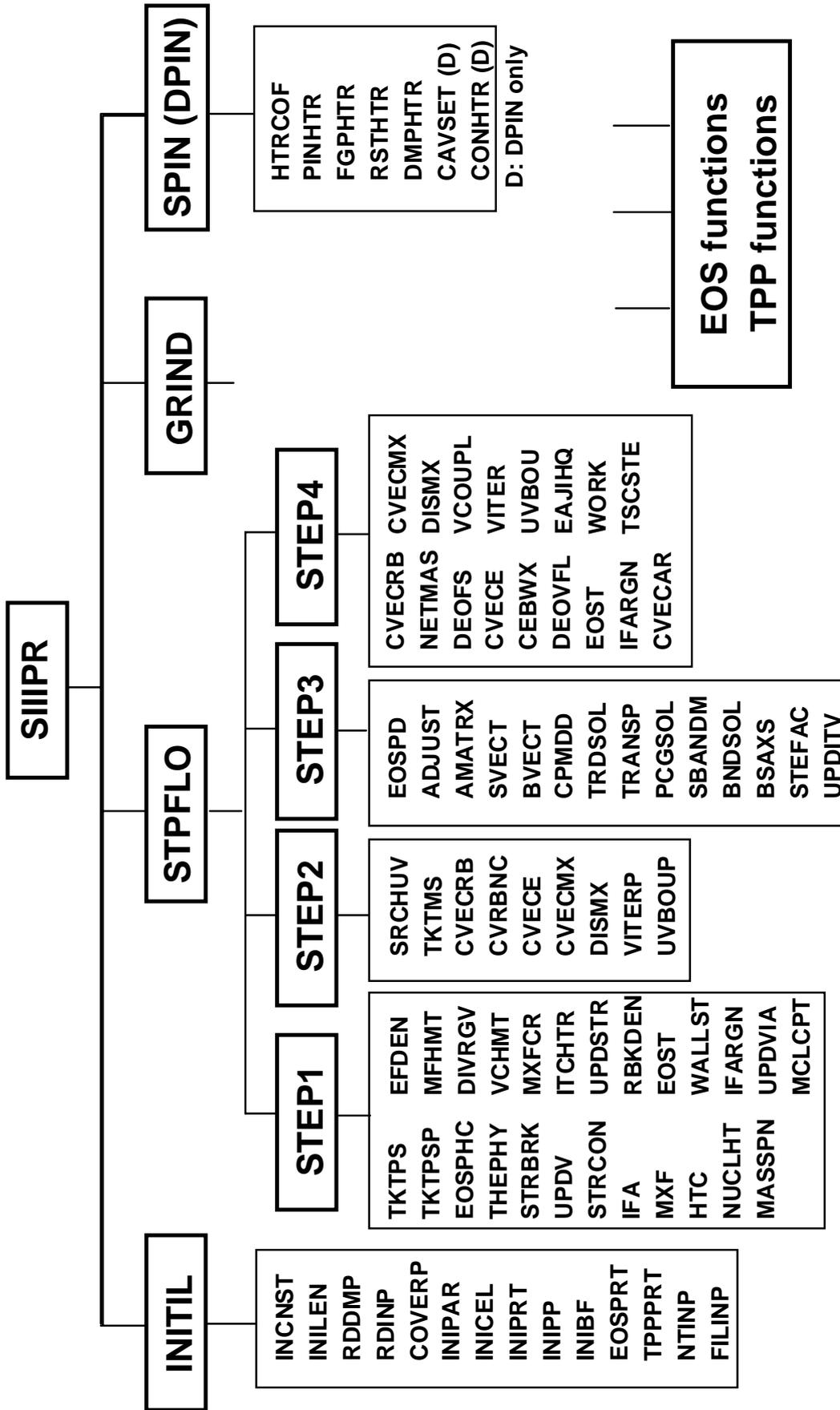


Fig. 3-1. SIMMER-III Overall Code Structure (Fluid-Dynamics and Fuel-Pin Models).

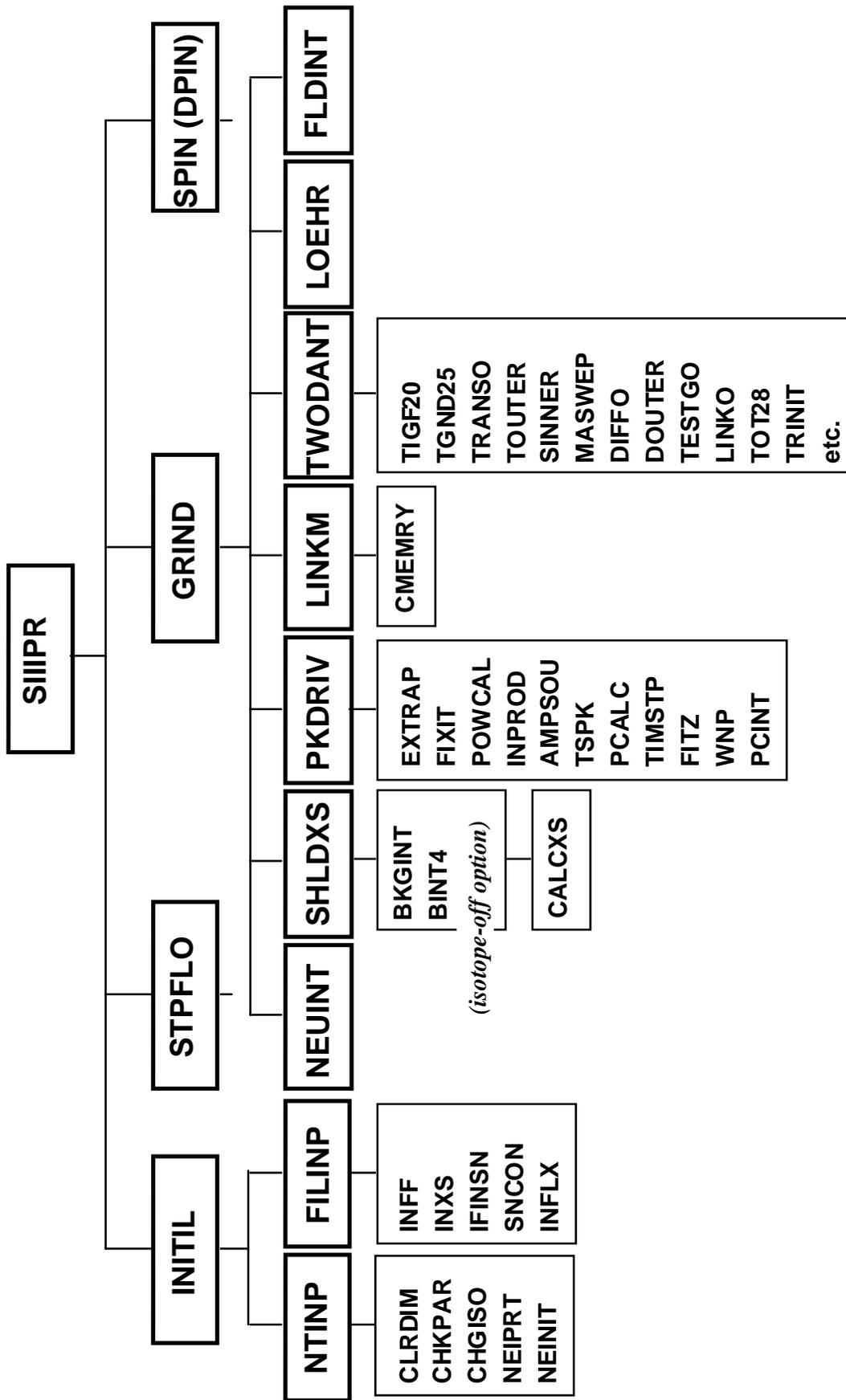


Fig. 3-2 SIMMER-III overall code structure (Neutronics model).

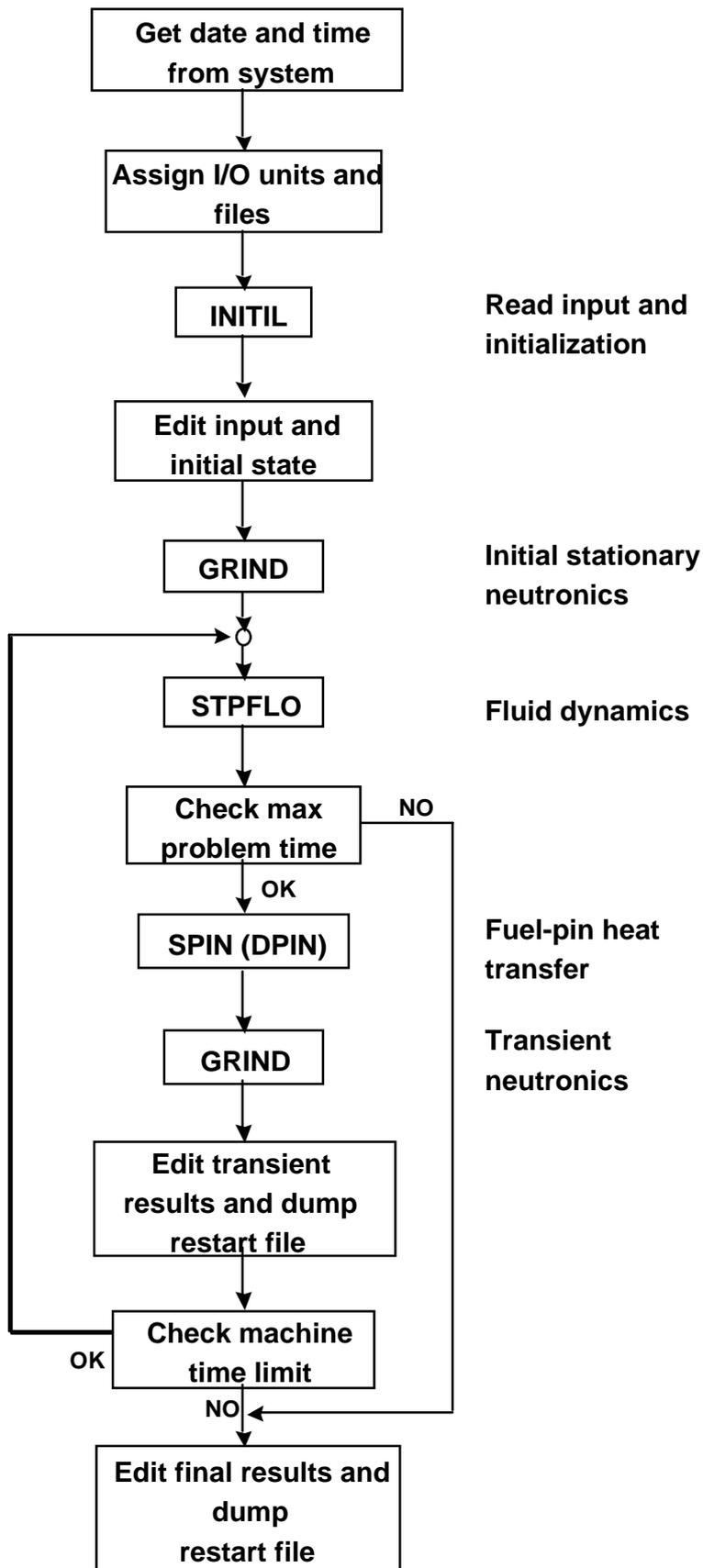


Fig. 3-3. Computational Flow of SIMMER-III Main Program.

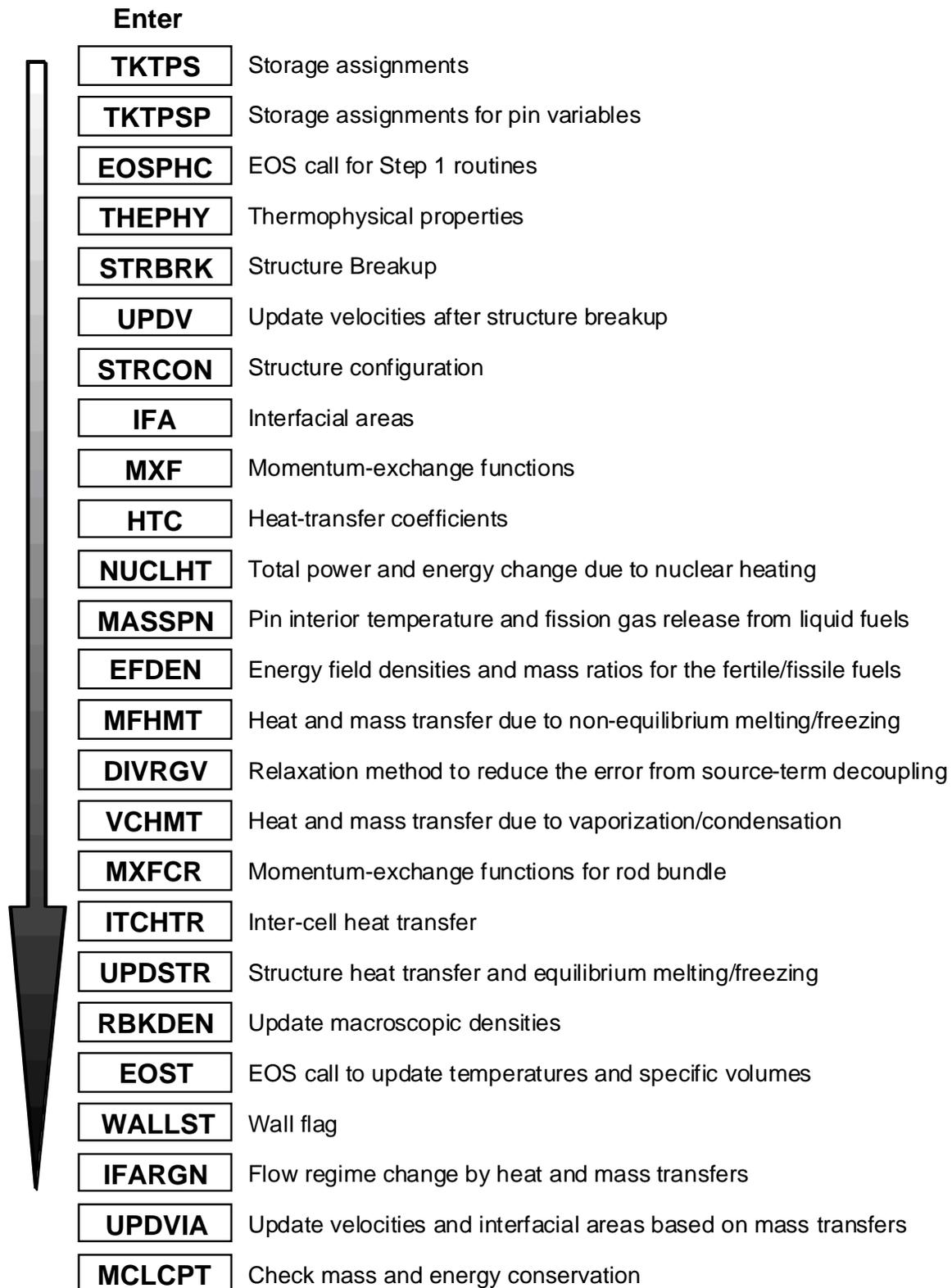


Fig. 3-4. Computational Flow of the STEP 1 Operations.

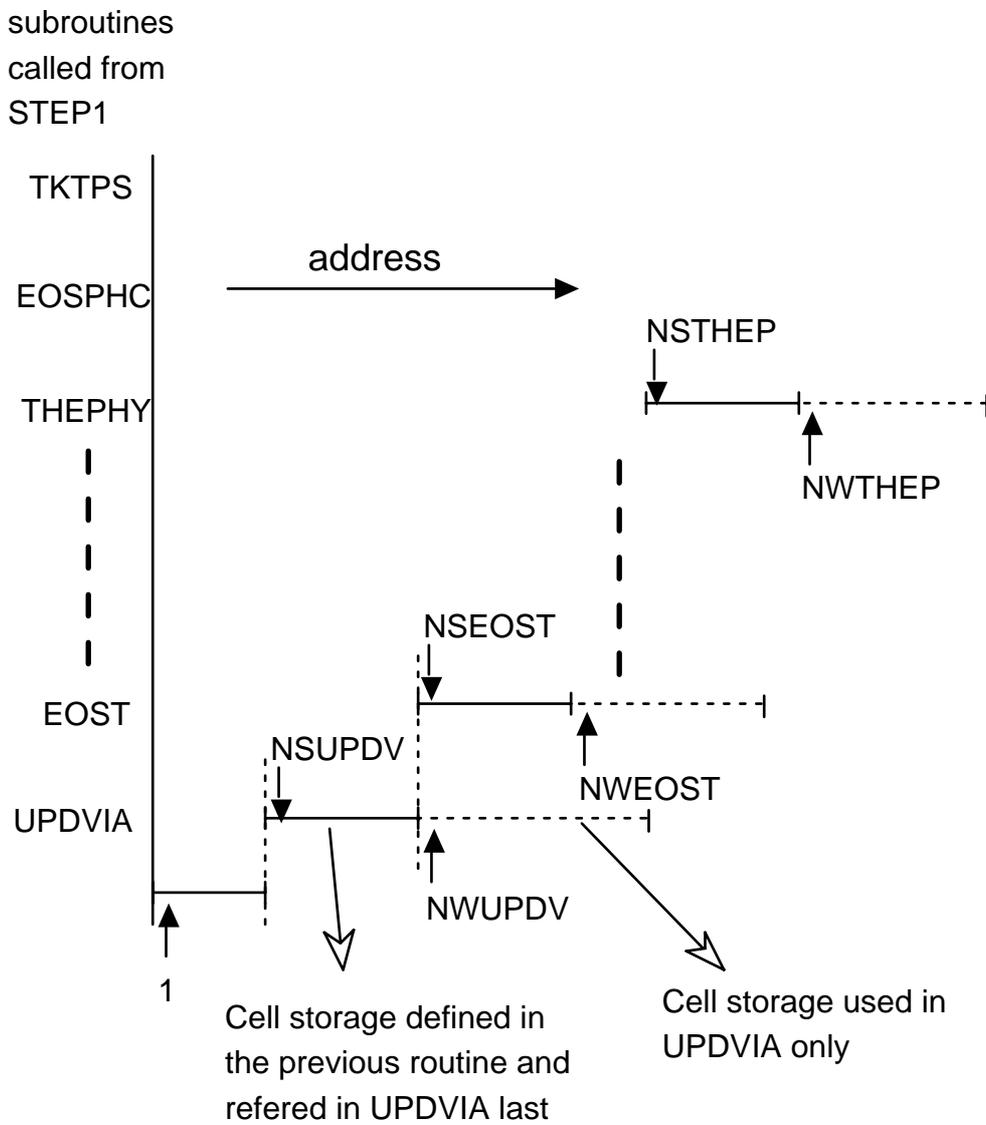


Fig. 3-5. Erasable Array Structure in Subroutine STEP1.

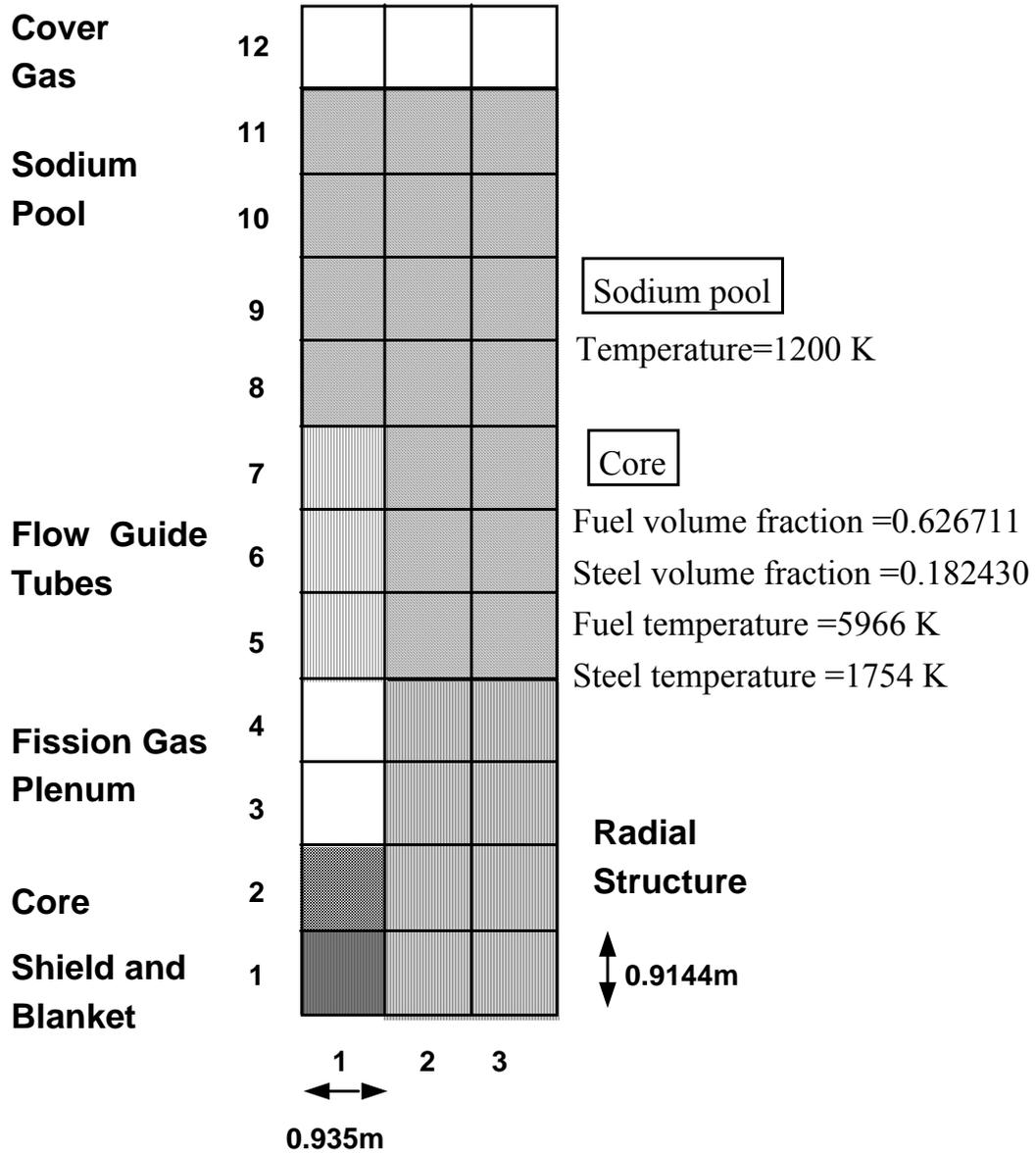


Fig. 3-6. Geometric Model and Initial Conditions for LWE Problem.

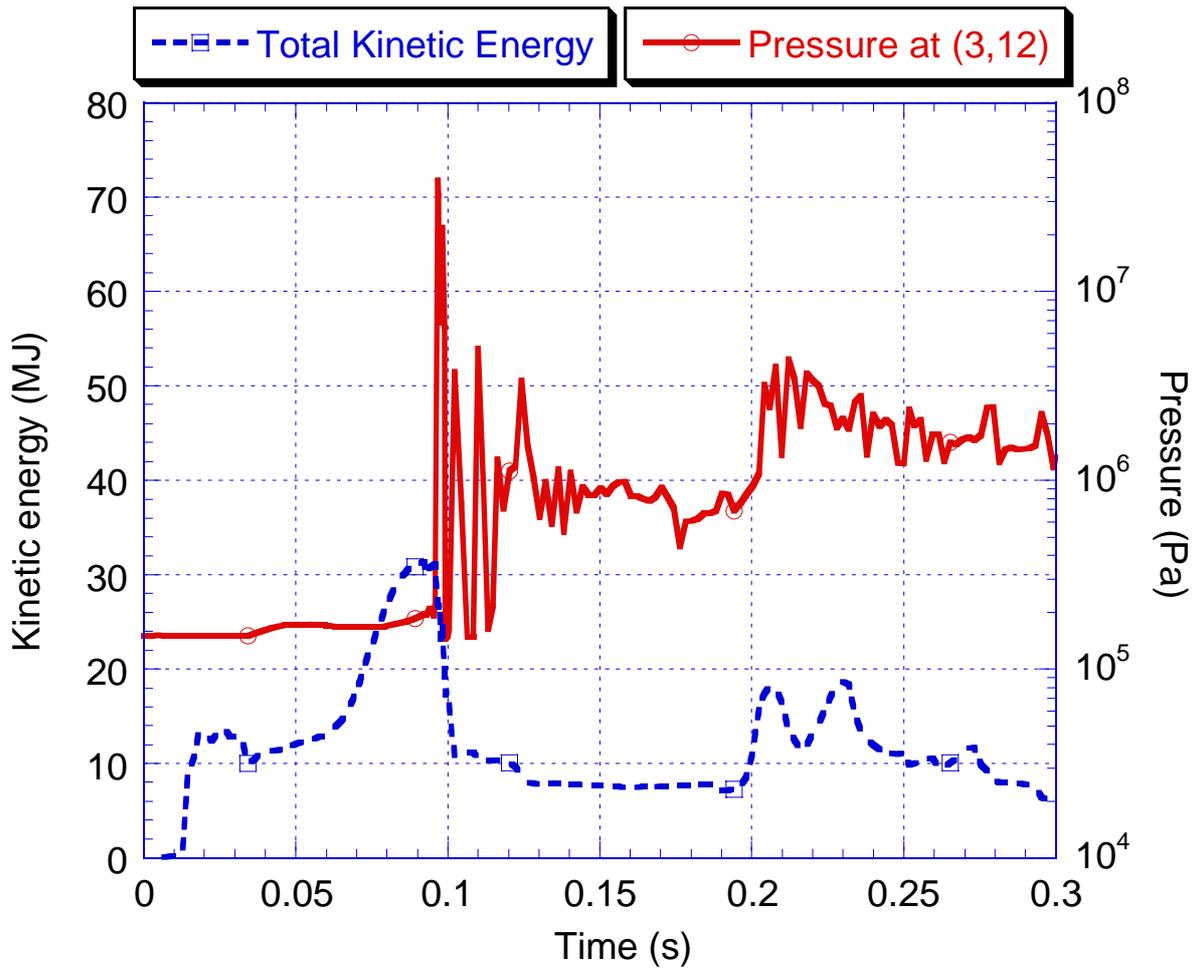


Fig. 3-7. Kinetic Energy and Pressure (EWS/RS6000).

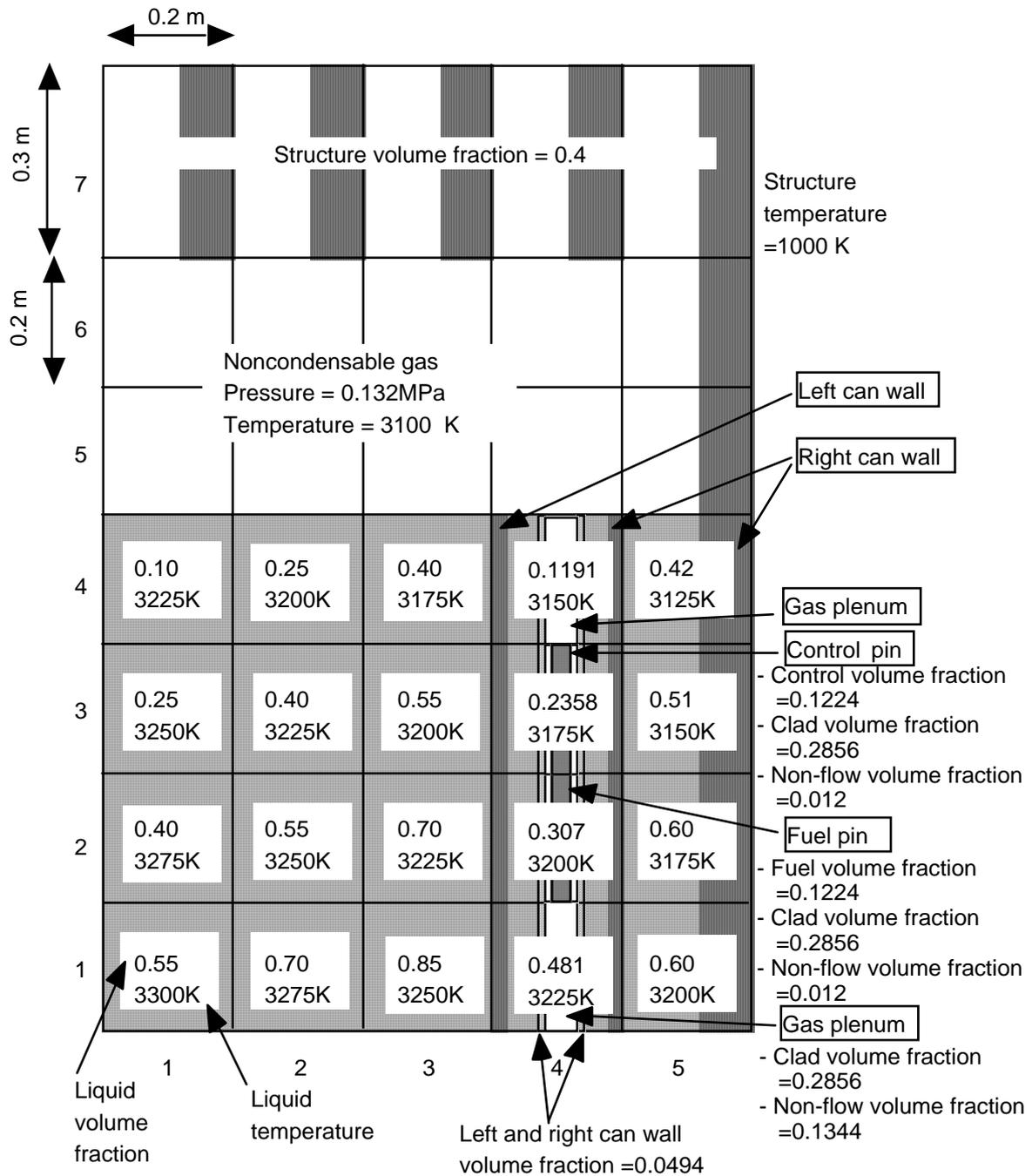


Fig. 3-8. Geometric Model and Initial Conditions for LBP Problem.

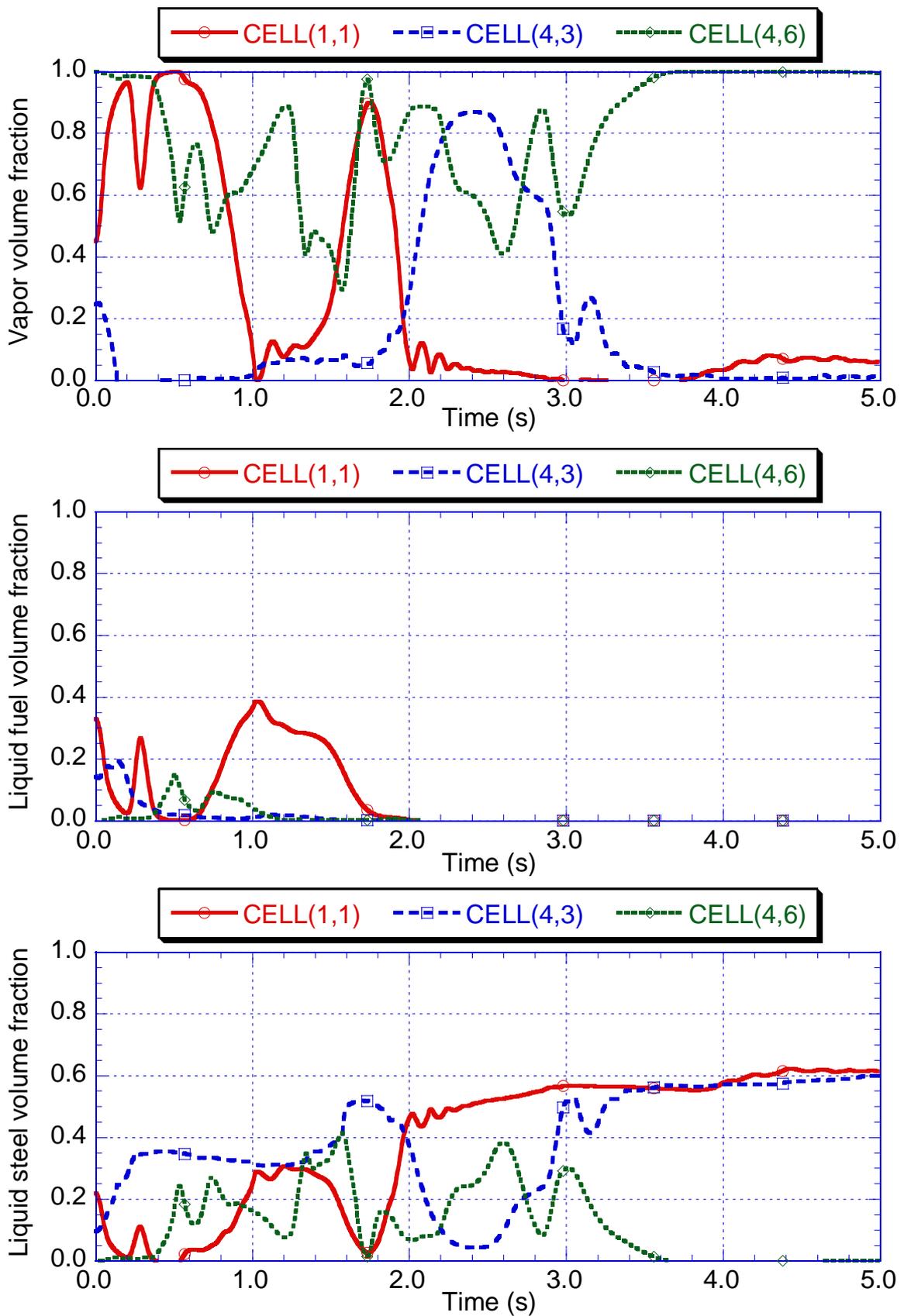


Fig. 3-9 (a). Volume Fractions of Vapor, Liquid Fuel and Liquid Steel in the LBP Problem (EWS/RS6000).

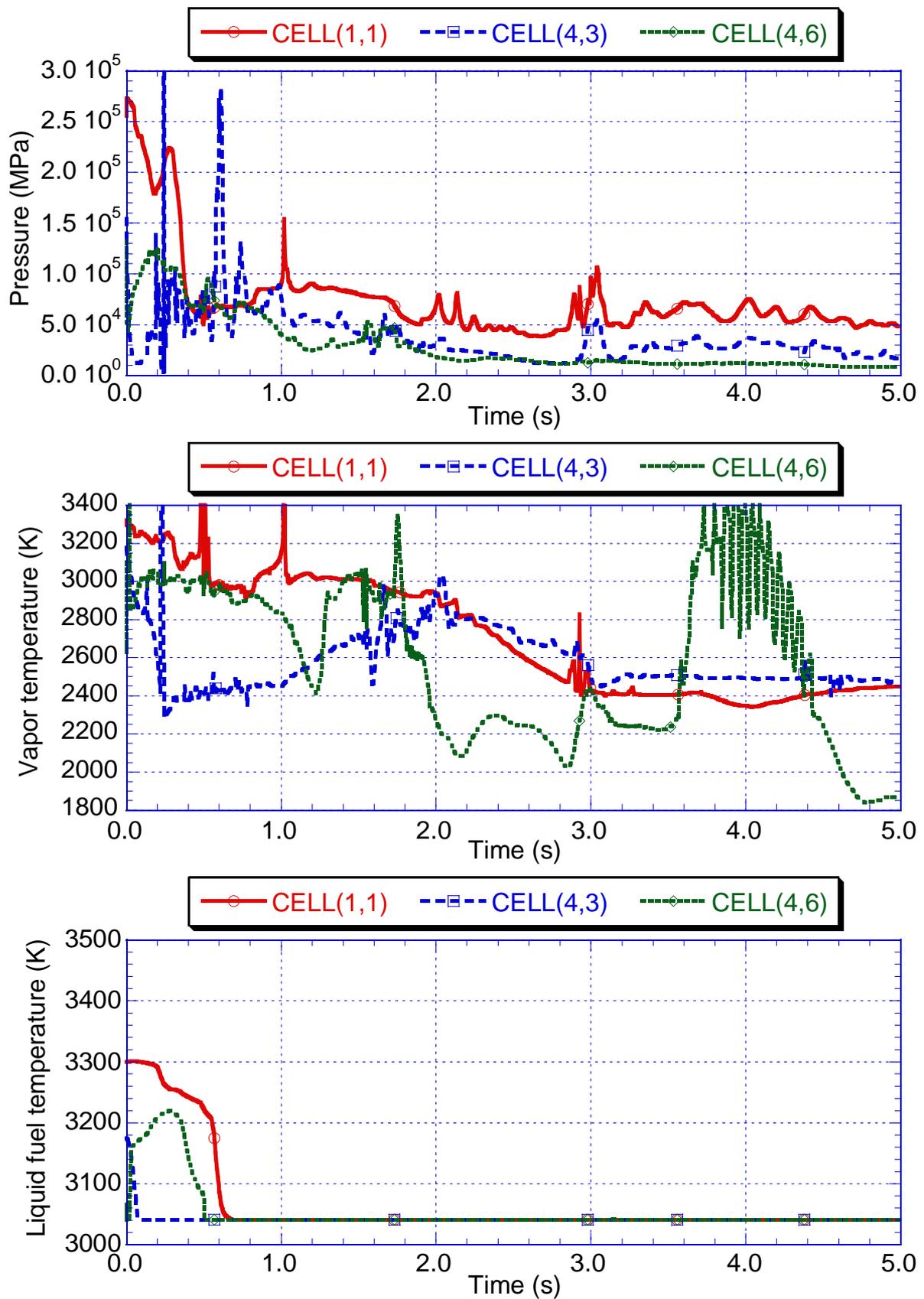


Fig. 3-9 (b). Pressure and Temperature of Vapor and Liquid Fuel in the LBP Problem (EWS/RS6000).

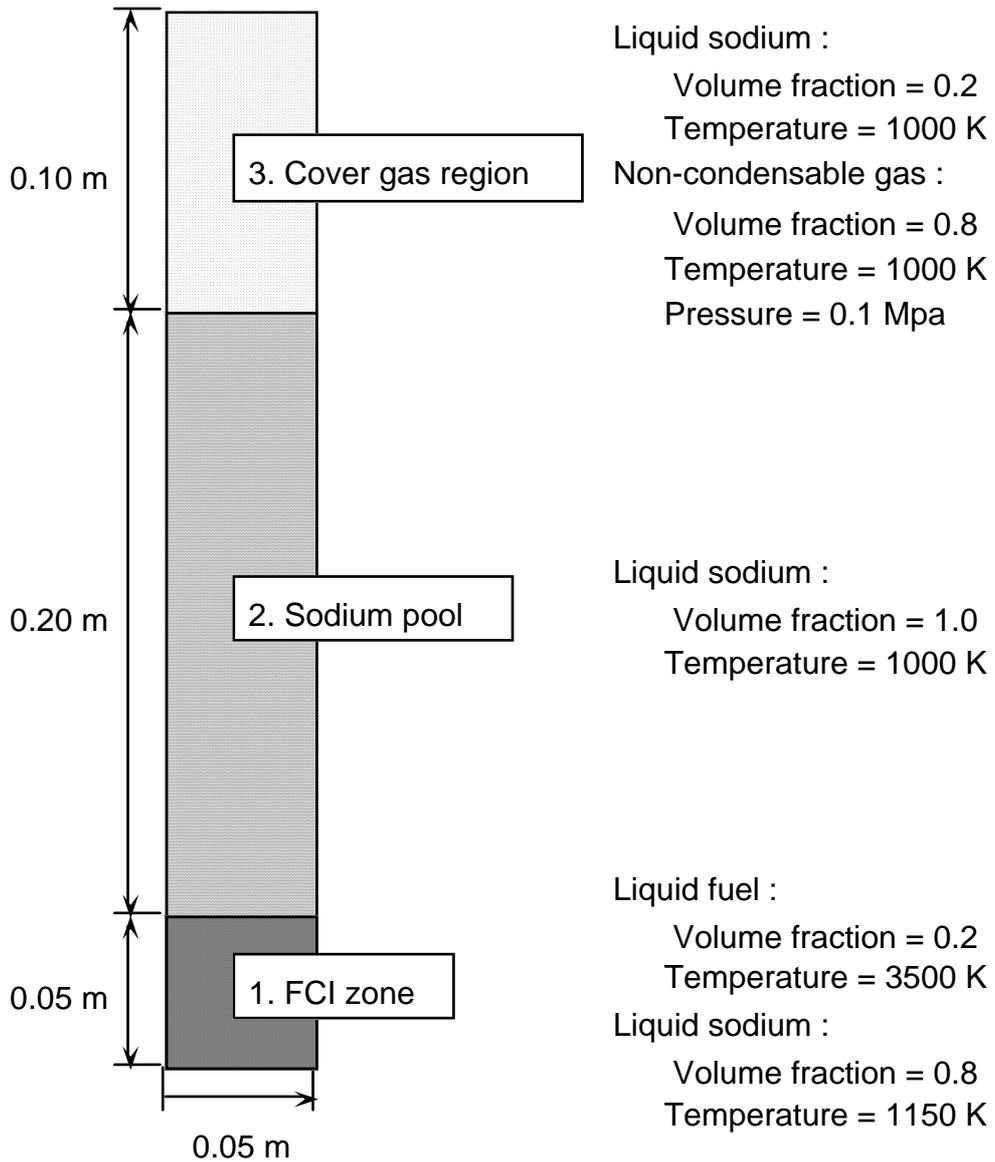


Fig. 3-10. Geometric Model and Initial Conditions for FCI Problem.

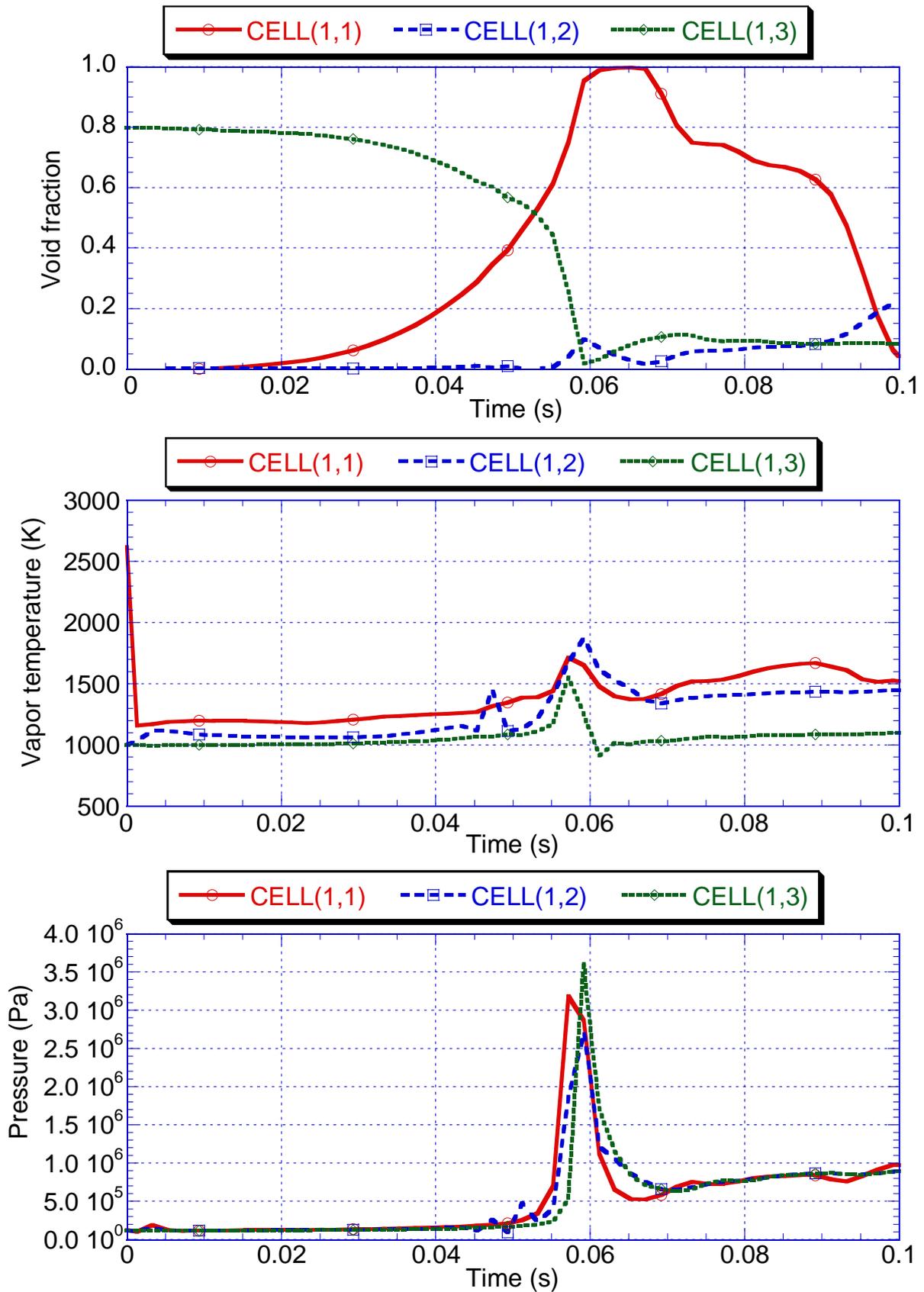


Fig. 3-11. Vapor Volume Fraction, Vapor Temperature and Pressure in the FCI Problem (EWS/RS6000).

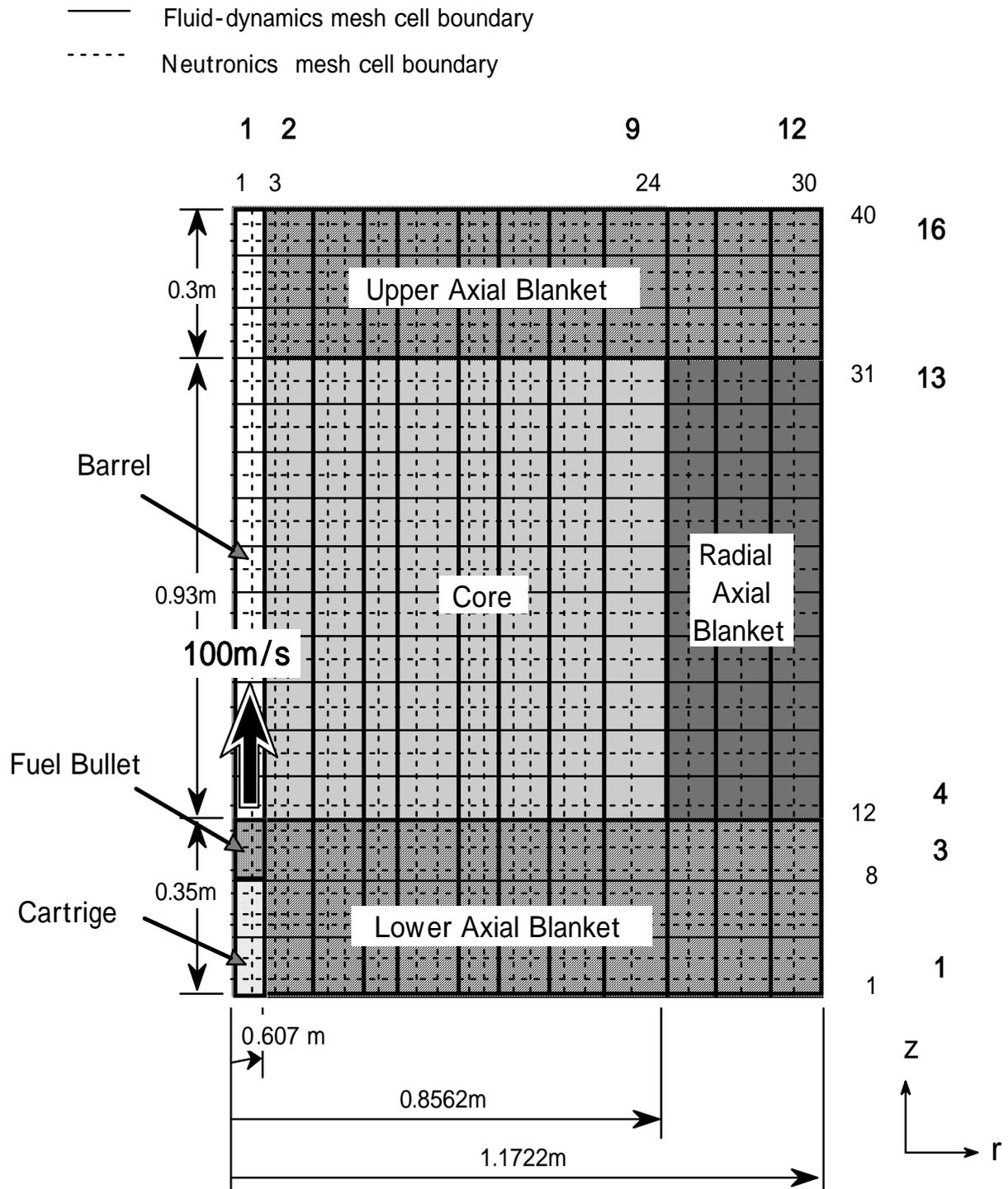


Fig. 3-12. Geometric Model and Initial Conditions for STN Problem.

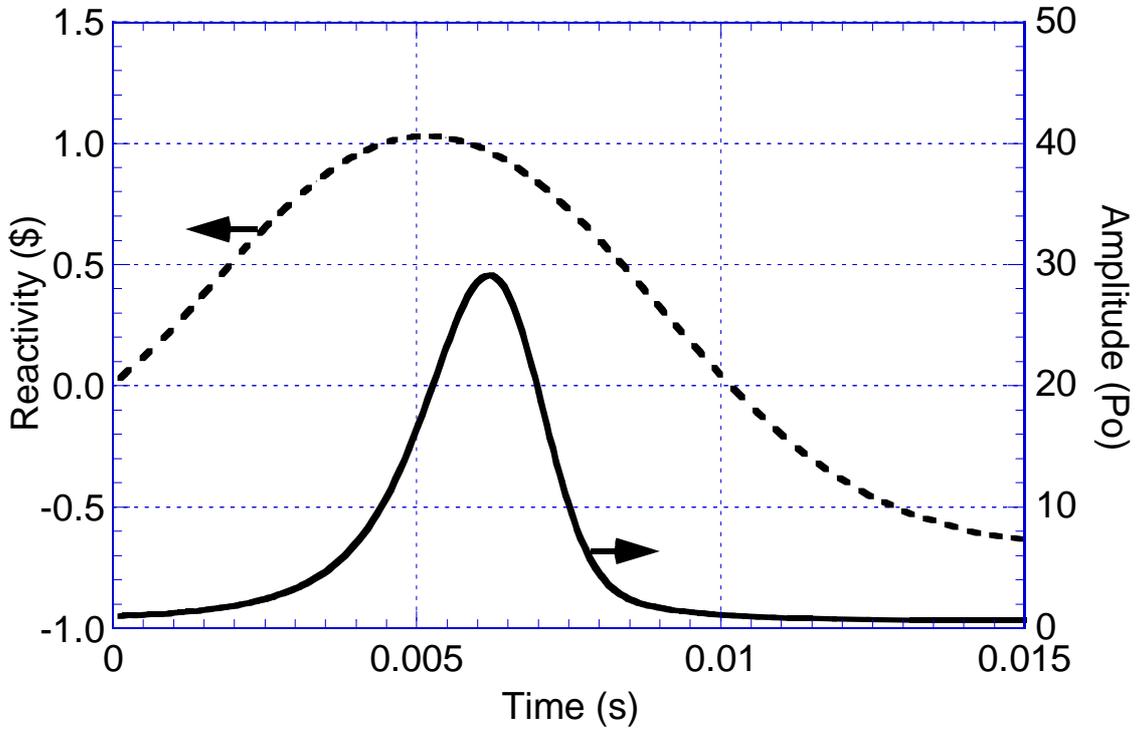


Fig. 3-13. Reactivity and Amplitude in the STN Problem (EWS/RS6000).

CHAPTER 4

CONCLUSIONS AND FUTURE WORK

The development and assessment of the SIMMER-III code has successfully reached the milestone integrated code application to reactor calculations is well feasible. The advanced features of the code can significantly improve the accuracy and reliability of safety assessment. The systematic code assessment program conducted in parallel to the code development has successfully demonstrated the broad applicability of the code and usefulness in not only LFMR analyses but many other nuclear and non-nuclear systems. It is noted that the models currently included in the latest version of SIMMER-III are much more advanced and detailed than the originally intended specifications for the SIMMER-III development project. This report briefly documents the models and methods of SIMMER-III Version 3.A and provides the detailed information for users of the code. Appendices to this report provide detailed programming and input/output information.

Based on the achievement in the SIMMER-III development and assessment programs, a fully three-dimensional version, SIMMER-IV Version 2, has been also made available. Modeling level of SIMMER-IV is completely compatible with SIMMER-III.

Concerning the future studies, even though the two-phase code assessment program has successfully completed, it is believed this should be a continuing effort to be conducted further under the JNC and FZK/CEA/IRSN agreement. The previous studies identified those areas which require future model improvement and refinement. There are on-going and future safety experimental programs that would provide valuable data for SIMMER-III model validation. Future applications of SIMMER-III are not restricted to sodium-cooled, mixed-oxide-fueled LMFR systems, but can cover all types of future advanced reactor concepts including an accelerator-driven subcritical system. The model refinement to broaden the future possibility should be considered accordingly.

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Recent achievement in the code development and assessment is only made under the successful collaboration with the European R&D organizations. Management support of German FZK and French CEA/IRSN are also acknowledged for supporting the project and delegating their specialists to take part in the project. The support from JNC's management both at O-arai Engineering Center and Head Office was one of the key elements to the success of this international program.

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NOMENCLATURE

Symbols

a	Binary-contact area per unit volume
A	Convectible interfacial area per unit volume
e	Specific internal energy
g	Gravitational acceleration
h	Heat-transfer coefficient
$H(x)$	Heaviside unit function
i	Enthalpy
k_c	Microscopic thermal conductivity.
k_T	Turbulent thermal conductivity.
K	Inter-field momentum exchange function
p	Pressure
q	Heat transfer rate
q_c	Intra-cell conductive heat flux
Q_{ic}	Energy source term by intra-cell heat transfer
Q_N	Nuclear heating rate
Q_{MF}	Rate of energy interchange due to melting/freezing
Q_{MF}	Rate of energy interchange due to vaporization/condensation
Q_{HT}	Rate of energy interchange due to heat transfer
S	Interfacial area source term
t	Time
T	Temperature
v	Velocity
VM	Virtual mass

Greek Symbols

α	Volume fraction
α_o	Maximum void fraction in a "single-phase" cell
α_B	Maximum void fraction for bubbly flow in a cell
α_D	Maximum void fraction for dispersed flow in a cell
$\bar{\rho}$	Macroscopic density
v	Specific volume
ΔT	Temperature difference between components
Γ	A mass-transfer rate per unit volume
Γ_m	Total mass-transfer rate per unit volume from component m

$\Gamma_{qq'}$	Mass-transfer rate from q to q'
Γ_{MF}	Melting or freezing rate for mass interchange
Γ_{VC}	Vaporization or condensation rate for mass interchange

Subscripts and superscripts

B	Bubbly flow regime
Crt	Critical point
D	Dispersed flow regime
G	Gas/vapor mixture
I	Interfacial quantity
GL	Terms existing at interfaces between vapor and an averaged liquid velocity
M	Energy component
m	Density component
q, q'	Velocity fields
qq'	Terms existing at interfaces between velocity field q and q'
qS	Terms existing at interfaces between velocity field q and structure
S	Structure
S	Structure-field energy component
s	Structure-field density component

APPENDIX A

SIMMER-III COMDECKS AND DECKS

All the Decks and Comdecks in the Historian code library have unique names. These are listed with their meanings in this appendix in the order appearing in the library. Comdecks represent groups of Common Blocks, Equivalences, Parameters and other Fortran declaration statements, and are called from Decks. The Comdecks are only expanded into calling Decks during Historian preprocessing to generate a compilable source file. Decks represent, on the other hand, individual Subroutines and Functions. In SIMMER-III, Deck names are made identical to Subroutine or Function names to avoid confusion occurring from having different names.

Lists of Comdecks and Decks in SIMMER-III are given in **Tables A-1** and **A-2**, respectively. The subprograms (subroutines and functions) are grouped into several categories, and the category numbers are assigned as shown in **Table A-2**.

Table A-1. List of SIMMER-III Comdecks

<u>Comdecks</u>	<u>Meaning</u>
IMPDBL	The implicit double-precision statement.
DIMEN	A set of parameter statements to define array dimensions.
LENGTH	The length of all common blocks written to a restart dump.
DUMPA	The common blocks containing the parameters for file dumps.
CONST	The constants used throughout the code. Defined in Subroutine INCNST.
UNITS	The input/output logical unit numbers.
TIME	Time and time-step control variables.
CPUTIM	The common blocks containing the CPU time.
OPTION	The flags to control the options available for individual models.
IFLAG	The flags indicating whether the current run is restart or not.
PARAM	The parameters necessary for SIMMER-III execution.
INPUT	The fluid-dynamics card input data.
EDIT	The editing output control variables.
VNAME	The common blocks containing the variable names required in the printing routine, PRTVAR.
MESHD	The common blocks containing the mesh sizes and dimensions.
CELLP	The common blocks containing the beginning-of-time-step cell variables.
CELLM	The common blocks containing the beginning of STEP2 cell variables.
CELLK	The common blocks containing the most up-to-date cell variables at each stage of calculation.
ERAS	The erasable arrays.
ST1ER	The dimension and equivalence statement for erasable array variables used in STEP1.
ITERCO	The common blocks for iteration counters.
BOUND	The common blocks containing the boundary condition data.
MBUND	The common blocks containing the boundary condition data.
CNSTBC	The common blocks keeping the initial condition of the boundary cells for constant boundary condition.
IFACD	Interfacial area model parameters.
IFAC	Interfacial area model parameters.
S1SP	The common blocks containing the void fractions and time steps in the previous 2 cycles to be used in parabolic extrapolation.
KQQC	Momentum exchange function model parameters.

INTURB	The common blocks containing the turbulent viscosity model parameters.
SWCOM	The common blocks containing the pressure drop model parameters for rod bundle, inner boundary model parameters and chemical reaction model parameters.
CHTC	Heat transfer coefficients model parameters.
FBC	Heat transfer coefficients model parameters for the film boiling.
HTCFBP	The arrays for the heat transfer coefficient model.
HEATSO	The heat source data (URANUS option only).
MEBA	The common block containing the mass and energy balance storage.
TPCOM	Non-equilibrium heat-and-mass transfer model (M/F and V/C) parameters.
CMFMOD	Non-equilibrium heat-and-mass transfer model parameters for the fuel caps freezing model.
IVCRG	The list vector arrays and vector length.
STRC	The arrays for the hydraulic diameters of mesh cells.
EOSPRU	EOS model parameters.
EOSREG	EOS region-related arrays.
EOSPAR	Fitting parameters for EOS functions.
THERPC	Thermophysical property variables.
S2TS3C	The common blocks containing the values to be transferred from STEP2 to STEP3.
S1TS4	The common blocks containing the values to be transferred from STEP1 to STEP4.
EPSILN	Convergence criteria data on the pressure iteration.
HODEGM	The common blocks containing the internal energy of each vapor component.
VISCO	The common block for momentum diffusion terms.
SOLCON	The common blocks containing the convergence criteria of the PCG-solver and the pressure iteration.
INPADD	The common blocks containing the calculational conditions related to algorithm.
FDINDEX	The common blocks containing the correspondence table of mass and energy components and velocity fields.
TIMECT	The common blocks containing the time-step control data for reduction of the source-term splitting error.
UVCSET	The common blocks containing the wall data.
METH1	The common blocks containing the variables related to remedies for improving source-term decoupling problem (methods 1 and 2).

CLOCAL	Work arrays for the inter-cell heat transfer model.
WPPFR	The common blocks containing the variables dumped to post-processor files.
WBSAV	The common blocks containing the variables dumped to base files for debug print of the cavity calculation.
PINC	Fuel pin to fluid coupling parameters.
PINK	The common blocks containing the most up-to-date fuel-pin heat-transfer variables at each stage of calculation.
PINP	The common blocks containing the beginning of time step fuel-pin heat-transfer variables.
PININ	Additional card input data for the fuel-pin heat-transfer model.
FPFL	The common blocks for FP gas blowout model (BLOW on).
CAVITY	The common blocks containing the fuel-pin cavity calculation for the detailed pin model (DPIN on).
NDIMEN	The parameters for the neutronics model (URANUS off).
NEUINP	The common block containing the neutronics integer input variables (URANUS off).
NMESH	The common block containing the neutronics mesh cell and geometry variables (URANUS off).
NEUFLG	The common block containing the neutronics calculation-control variables (URANUS off).
PSEEDIT	The common block containing the neutronics edit control variables (URANUS off).
RINCON	The common block containing the neutronics real-type input variables (URANUS off).
NFINT	The common blocks containing the interface variables between neutronics and fluid dynamics (URANUS off).
ISHILD	The common blocks containing the integer variables related to cross-section calculations (URANUS off).
SHLD	The common blocks containing the real-type variables related to cross-section calculations (URANUS off).
CELXS	The common block containing macroscopic cross sections (URANUS off).
FLUXC	The common block containing the real-type variables related to neutron flux shape calculations (URANUS off).
RVARI	The common block containing the neutronics real-type variables (URANUS off).
QUAS	The common block containing the variables related to neutron kinetics calculation (quasi-static method) (URANUS off).

NOPT	The common block containing the neutronics option flag input variables (URANUS off).
REACIN	The common block containing the neutronics real-type input variables for specifying external reactivity (URANUS off).
HETXS	The common blocks containing the real-type variables related to cross-section calculations with heterogeneous effect (URANUS off).
ALITLE	The common block containing the core memory array (URANUS off).
ANG	The common blocks containing the angular flux raflxm and the corresponding arrays (URANUS off).
C4S	The common blocks containing file open parameters (URANUS off).
C4TIME	The common block containing the data on the real-time clock and date (URANUS off).
CCHANG	The common blocks containing temporary variables for variable-type conversion (URANUS off).
CCHANGC	Temporary variable for variable-type conversion (URANUS off).
CM	The common block containing the variables related to random numbers (URANUS off).
CNFIX	The common block containing the neutronics input variables for the AWDD method (URANUS off).
CNSOU	The common block containing the neutronics input variables of the NAMELIST NSOU (URANUS off).
COMECS	The common block containing the maximum core memory length and number of print control variables (URANUS off).
COMEK	The common block containing the variables for Gamma iteration (URANUS off).
DIMENT	The common block containing the spatial dimension variables (URANUS off)."
ERRORS	The common block containing the error flag variable (URANUS off).
FLXDMP	The common block containing the information to be dumped on the RTFLUX file (URANUS off).
FUNMOD	The common block containing the real-type variables related to the quasi-static method (URANUS off).
GOMODS	The common block containing the control flag variables of the TWODANT-solver module calculation (URANUS off).
HED	The common block containing the title information variable (URANUS off).
HILITE	The common block containing the highlights arrays (URANUS off).

INSTAL	The common block containing the current core memory length variables (URANUS off).
ISENV	The common blocks containing the environmental variable indicators (URANUS off).
LNCONS	The common block containing the small and large value variables (URANUS off).
LNSTAL	The common blocks containing the core memory length and time parameters (URANUS off).
LOCAL	The common block containing the core memory parameters (URANUS off).
LONERR	The common blocks containing the error type indicators (URANUS off).
MISC	The common block containing the miscellaneous variables (URANUS off).
MISC1	The common block containing the adjustment factors of neutronics parameters for a transient-state start calculation (URANUS off).
MVLCK	The common blocks containing the mask arrays (URANUS off).
NCSIZE	Set parameter values (NCSIZE=8) (URANUS off).
NCSZCX	Set parameter values (NCSZFN=255) (URANUS off).
NCSZFN	Set parameter values (NCSZFN=255) (URANUS off).
NEWPARA	The common block containing the parameters used for increasing robustness of neutron flux calculation (URANUS off).
NWPASS	The common block containing the pass parameters of the TWODANT-solver module processing (URANUS off).
PARAMT	Set parameter values (NVEC=64, NVECP=65) (URANUS off).
PIDS	Set π value (URANUS off).
PRNTIDO	The common blocks containing the print setting parameters (URANUS off).
REACV	The common block containing the reactivity component variables (URANUS off).
REAIA	The common blocks containing the temporary storage arrays (URANUS off).
RMDM	The common block containing the parameters related to Monte Carlo calculation (URANUS off).
RUSS	The common blocks containing the Legendre order parameters (URANUS off).
SAD2SV	The common block containing the neutronics array element length parameters (URANUS off).
SEEKGEN	The common blocks containing the index of interface file names (URANUS off).

SEKBUG	The common block containing the maximum number of physical units required by SEEK and DOPC (URANUS off).
SHORTU	The common block containing the unit numbers for file I/O (URANUS off).
SHSTRY	The common block containing the variables used for printing storage history (URANUS off).
SOLIND	The common blocks containing temporary data arrays used for reading the SOLINP file (URANUS off).
SOLINR	The common blocks containing the temporary arrays for handling data on the core memory (URANUS off).
SPECXS	The common block containing the cross-section specific parameter variables (URANUS off).
STACK	The common block containing the stack variables (URANUS off).
STKFCK	The common block containing the parameters used for checking the dimensions of data arrays (URANUS off).
STKNER	The common block containing an error flag (URANUS off).
STKSTO	The common block containing the parameter used for interpreting characters in a text file (URANUS off).
SYSTEM	The common blocks containing some Hollerith variables (URANUS off).
THSTRY	The common blocks containing the variables used for printing timing history (URANUS off).
TIA	The common blocks containing data arrays used for neutron flux calculation (URANUS off).
TINY	Set constant value(TINY=1.0E-38) (URANUS off).
TRANSI	The common block containing the transfer indicator variables (URANUS off).
TRANST	The common blocks containing the parameters related to data transfer from / to binary files (URANUS off).
UNDIS	The common blocks containing the parameters for file handling (URANUS off).
UNDSKP	The common block containing the parameters for file handling (URANUS off).
UNTAP	The common blocks containing the parameters used for handling physical files (URANUS off).
VECT	The common blocks containing the parameters used for handling vector data (URANUS off).
VRDATE	The common blocks containing the information about TWODANT-solver modules (URANUS off).

VSCONS Set constant value (VSEM40=1.0E-40, VSEM50=1.0E-50) (URANUS off).

XTRAS The common block containing temporary data arrays (URANUS off).

Table A-2. List of SIMMER-III Decks

<u>Category</u>	<u>Decks</u>	<u>Meaning</u>
1.0 Main driver		
1.0 (1)	SIIPR	SIMMER-III main driver.
1.0 (2)	CPUSET	Initialize CPU time statistic information.
1.0 (3)	CPUGET	Calculate CPU time statistic information.
1.0 (4)	CPUPRT	Print the CPU time statistic information.
2.0 Input and initialization		
2.0 (1)	INITIL	Input and initialization driver.
2.0 (2)	RDCNTL	Set flags for the existing NAMELIST.
2.0 (3)	INCNST	Define constants used throughout the code.
2.0 (4)	VNAMEP	Date of the variable names required in the printing routine, PRTVAR.
2.0 (5)	INILEN	Obtain the length of common blocks.
2.0 (6)	RDINP	Read input data.
2.0 (7)	INIPAR	Initialize the parameters.
2.0 (8)	EOSUP	Initialize the EOS model parameters.
2.0 (9)	INICEL	Initialize the cell variables.
2.0 (10)	INIFPG	Initialize the FP gas blowout model parameters for the code option BLOW.
2.0 (11)	INIVAP	Initialize the EOS variables of vapor field.
2.0 (12)	INIPP	Output the first header record to the post-processor file.
2.0 (13)	INIBF	Output the first header record to the base files for post-processing.
2.0 (14)	EOSPRT	Print EOS functions and tabulated data as functions of temperature.
2.0 (15)	TPPPRT	Print functions and tabulated data of thermophysical properties as functions of temperature.
2.0 (16)	DEFAULT	Default the constants.
3.1 Fluid-dynamics driver and boundary conditions		
3.1 (1)	STPFLO	Fluid-dynamics driver.
3.1 (2)	TPTKS	Transfer CELLP variables to CELLK variables, to reset CELLK when the same cycle is re-calculated.

3.1 (3)	TPTKSP	Transfer PINP variables to PINK variables, to reset PINK when the same cycle is re-calculated.
3.1 (4)	SETBOU	Set the boundary conditions.
3.1 (5)	INIBOU	Initialize the boundary conditions.
3.1 (6)	SAVEIC	Save the initial value of cell variables in the boundary cell.
3.1 (7)	BCSET	Set the boundary condition at each cycle.
3.1 (8)	RESTIC	Restore the initial value of cell variables to the boundary cell.
3.1 (9)	RSTANV	Set the tangential boundary conditions.
3.1 (10)	INIPRT	Interpolate the input table of the boundary conditions linearly.
3.1 (11)	WALLST	Set the wall flag by considering the structure configuration in the surrounding cells.
3.1 (12)	SETWAL	Calculate the wall flag from four integers corresponding to left, right, bottom, and top boundaries.
3.1 (13)	SRCHUV	Set the virtual wall conditions.
3.1 (14)	WALLDG	Decompose the wall flag to four integers corresponding to left, right, bottom, and top boundaries.

3.2 Intra-cell transfers (Step 1)

3.2 (1)	STEP1	Perform the intra-cell heat and mass transfer without inter-cell fluid convection. Get momentum exchange functions.
3.2 (2)	TKTPS	Transfer CELLK variables to CELLP variables.
3.2 (3)	TKTPSP	Transfer PINK variables to PINP variables.
3.2 (4)	EOSPHC	Calculate the heat capacities of structure, liquid, and vapor components.
3.2 (5)	THEPHY	Calculate the thermophysical properties.
3.2 (6)	STRBRK	Calculate structure (fuel pin and can wall) breakup.
3.2 (7)	FPGFLW	Subroutine for FP gas blowout model for the code option BLOW.
3.2 (8)	PIPFLO	Calculate plenum fission gas flow rate for the code option BLOW.
3.2 (9)	EOSPBK	Adjust EOS variables after fuel-pin breakup.
3.2 (10)	PINMOT	A driver routine to calculate in-pin fuel motion for the code option DPIN.
3.2 (11)	INICAV	Initialize cavity after mechanical pin failure for the code option DPIN.
3.2 (12)	DEFCAV	Cavity definition after resizing for the code option DPIN.
3.2 (13)	PINMET	Calculate intra-pin molten fuel heat and mass transfer for the code option DPIN.

3.2 (14)	PCAVT2	Calculate the cavity pressure in the in-pin fuel motion model for the code option DPIN.
3.2 (15)	EJECT	Calculate fuel ejection model based on Bernoulli equation for the code option DPIN.
3.2 (16)	SASEJT	Calculate fuel ejection model based on equilibrium of pressure in cavity and channel for the code option DPIN.
3.2 (17)	PINEJT	Calculate the material ejection from the cavity in the in-pin fuel motion model for the code option DPIN (not used in this version).
3.2 (18)	EOSP	Update EOS variables in the in-pin fuel motion model for the code option DPIN (not used in this version).
3.2 (19)	PINMOM	Calculate in-pin fuel motion for the code option DPIN.
3.2 (20)	FALDSR	Predict fuel pin failure in the detailed fuel-pin calculation for the code option DPIN.
3.2 (21)	PINSTP	Control fluid dynamics time steps due to in the in-pin fuel motion model for the code option DPIN (not used in this version).
3.2 (22)	P RTPIN	Print calculated results of the in-pin fuel motion model for the code option DPIN.
3.2 (23)	UPDV	Update the velocities due to structure breakup.
3.2 (24)	STRCON	Define fuel-pin and can-wall structure configuration, and calculate structure-side and inter-structure-component heat-transfer coefficients.
3.2 (25)	CWCON0	Calculate the structure-fluid fields contact variables for a slab geometry
3.2 (26)	CWCON1	Calculate the structure-fluid fields contact variables for a cylindrical geometry
3.2 (27)	IFA	Calculate the binary contacts among the energy components.
3.2 (28)	IFARGM	Determine the flow regimes.
3.2 (29)	IFARGN	Determine the flow regimes.
3.2 (30)	EOSIFA	Calculate thermo-physical quantities for interfacial area model.
3.2 (31)	IFASRC	Update the convective interfacial areas with various IFA source terms.
3.2 (32)	DFDR	Calculate the radial gradient of cell variables using parabolic or linear fitting procedure.
3.2 (33)	DFDZ	Calculate the axial gradient of cell variables using parabolic or linear fitting procedure.
3.2 (34)	MXF	Calculate the momentum exchange functions.
3.2 (35)	PVSMF	Calculate the melt fraction for ALPMP2.

3.2 (36)	HTC	Calculate the heat-transfer coefficients for fluid energy components.
3.2 (37)	HTCFB	Calculate the heat-transfer coefficients for film boiling.
3.2 (38)	HTFRS	Interpolate logarithmically the heat-transfer coefficients for interpolated flow regimes.
3.2 (39)	NUCLHT	Update specific internal energies due to nuclear heating for all the fluid-dynamics energy components.
3.2 (40)	NUCSUM	Sum up nuclear heating in fuel-pin and fluid-dynamics components.
3.2 (41)	MASSPN	Calculate fission-gas release from the liquid-field fuel components.
3.2 (42)	EFDEN	Calculate the energy-field densities and the mass ratios of the fertile/fissile fuel.
3.2 (43)	SWCR	Calculate the chemical reaction between sodium and water for the code option SW.
3.2 (44)	CRSUB	Calculate the heat and mass transfer for the code option SW.
3.2 (45)	CALTR	Newton-Raphson iteration method for the code option SW.
3.2 (46)	MFHMT	Calculate the non-equilibrium melting/freezing (M/F) transfer.
3.2 (47)	MFHTCA	Adjust the heat-transfer coefficients for the non-equilibrium M/F calculation with the classical bulk freezing model.
3.2 (48)	MFHTFC	Adjust the heat-transfer coefficients for the non-equilibrium M/F calculation with the fuel caps freezing model.
3.2 (49)	MFGAFC	Calculate the mass-transfer rates for the non-equilibrium M/F transfer with the fuel caps freezing model.
3.2 (50)	MFGAM	Calculate the mass-transfer rates for the non-equilibrium M/F transfer with the classical bulk freezing model.
3.2 (51)	MFRBAJ	Calculate the mass transfer for the non-equilibrium M/F transfer.
3.2 (52)	MFARAJ	Adjust the interfacial areas for the non-equilibrium M/F calculation.
3.2 (53)	MFFGAS	Calculate the fission-gas mass transfer accompanied with the non-equilibrium M/F transfer.
3.2 (54)	MFL3ET	Update the coolant energy and temperature for the non-equilibrium M/F transfer.
3.2 (55)	MFSKFC	Update the structure energy for the non-equilibrium M/F transfer with the fuel caps freezing model.
3.2 (56)	MFSKIE	Update the structure energy for the non-equilibrium M/F transfer with the classical bulk freezing model.

3.2 (57)	MFLMFC	Update the liquid energy and temperature for the non-equilibrium M/F transfer with the fuel caps freezing except for coolant.
3.2 (58)	MFLME	Update the liquid energy and temperature for the non-equilibrium M/F transfer with the classical bulk freezing model except for coolant.
3.2 (59)	EOSLTV	Calculate the liquid temperature and specific volume from the internal energy.
3.2 (60)	EOSSTV	Calculate the temperature and specific volume of the fluid-contact structure from the internal energy.
3.2 (61)	VCHMT	Calculate the vaporization/condensation (V/C) transfer.
3.2 (62)	VCEINT	Initialize the cell components and adjust the EOS for the V/C calculation.
3.2 (63)	VCIEOS	Calculate the EOS variables and derivatives for the V/C iteration.
3.2 (64)	VCETG	Adjust the vapor and real-liquid temperature for the V/C calculation.
3.2 (65)	VCIGAM	Calculate the mass-transfer rate of the V/C transfer.
3.2 (66)	VCIDGM	Calculate the derivatives of the mass-transfer rates for the B matrix elements.
3.2 (67)	VCIRGL	Calculate the interface fractions and their derivatives for the V/C iteration.
3.2 (68)	VCERGL	Calculate the vapor densities for the diffusion-limited V/C model (not currently available).
3.2 (69)	VCMCD1	Calculate the multiplier of reduction factors for V/C binary contact area based on multi-component diffusion model (single condensable gas components).
3.2 (70)	VCMCD2	Calculate the multiplier of reduction factors for V/C binary contact area based on multi-component diffusion model (two condensable gas components).
3.2 (71)	VCMCD3	Calculate the multiplier of reduction factors for V/C binary contact area based on multi-component diffusion model (three condensable gas components).
3.2 (72)	VCFNC1	Calculate the boundary equation based on multi-component diffusion model (single condensable gas components).
3.2 (73)	VCFNC2	Calculate the boundary equation based on multi-component diffusion model (two condensable gas components).
3.2 (74)	VCFNC3	Calculate the boundary equation based on multi-component diffusion model (three condensable gas components).
3.2 (75)	VCIADJ	Adjust heat-transfer coefficients and binary contact areas in the case of non-convergence in the V/C iteration.

3.2 (76)	VCIMTR	Adjust the mass-transfer rates and interface temperatures for the V/C iteration.
3.2 (77)	VCICM	Calculate the column vector elements, C(m), for the V/C matrix calculation (m = 1 - 5).
3.2 (78)	VCIBML	Calculate the matrix elements, B(m, l), for the V/C matrix calculation (m = 1 - 3, l = 1 - 5).
3.2 (79)	VCIB4L	Calculate the matrix elements, B(4, l), for the V/C matrix calculation (l = 1 - 5).
3.2 (80)	VCIB5L	Calculate the matrix elements, B(5, l), for the V/C matrix calculation (l = 1 - 5).
3.2 (81)	VCIH TL	Calculate the value of \tilde{H}_l for the B matrix elements.
3.2 (82)	VCEMTR	Calculate the mass and energy transfers with the V/C phase change.
3.2 (83)	VCEENG	Update the liquid and structure energy after the V/C iteration except for coolant.
3.2 (84)	VCESUB	Calculate the condensation of unphysically existing subcooled vapor.
3.2 (85)	VCPRT1	Debug routine for the EOS variables in the V/C calculation.
3.2 (86)	VCPRT2	Debug routine for the V/C matrix calculation.
3.2 (87)	VCPRT3	Debug routine for the mass-transfer rates and the interface temperatures in the V/C calculation.
3.2 (88)	MXFCR	Calculate the momentum exchange functions for rod bundle.
3.2 (89)	MXFC	Calculate the drag coefficient for rod bundle.
3.2 (90)	ITCHTR	Calculate the inter-cell heat transfer between the same components.
3.2 (91)	UPDSTR	A driver for structure-related heat and mass transfer.
3.2 (92)	LCWCHT	Calculate left can wall heat transfer called by UPDSTR.
3.2 (93)	RCWCHT	Calculate right can wall heat transfer called by UPDSTR.
3.2 (94)	CWHT2	Calculate can wall heat transfer for two structure layers.
3.2 (95)	CWHT3	Calculate can wall heat transfer for three structure layers.
3.2 (96)	CWHT4	Calculate can wall heat transfer for four structure layers.
3.2 (97)	CWHT5	Calculate can wall heat transfer for five structure layers.
3.2 (98)	EQUIMF	Calculate equilibrium melting and freezing.
3.2 (99)	QHCHTP	Calculate heat and mass transfer rates summed over fluid-dynamics cycles to be transferred to SPIN/DPIN.
3.2 (100)	RBKDEN	Extract the density-field macroscopic densities from the energy-field macroscopic densities using the mass fractions.

3.2 (101) UPDVIA Update the velocities and interfacial areas by the mass transfer.

3.3 Fluid convection (Steps 2-4)

- 3.3 (1) STEP2 Solve the equations for the mass, energy, and momentum conservation without intra-cell source terms.
- 3.3 (2) STEP3 Get consistent values for end-of-time-step pressures and velocities.
- 3.3 (3) STEP4 Update all variable, particularly velocities for consistent convection.
- 3.3 (4) TKTMS Transfer CELLK variables to CELLM variables.
- 3.3 (5) CVECRB Solve the mass conservation equations without the intra-cell source terms.
- 3.3 (6) CVECE Solve the energy conservation equations without the intra-cell source terms.
- 3.3 (7) CVECMX Solve the momentum conservation equations without the intra-cell source terms.
- 3.3 (8) DISMX Calculate momentum diffusion terms to account for viscous drag.
- 3.3 (9) VITERP Calculate the velocity fields with drag iteration in STEP2.
- 3.3 (10) UVBOUP Set the boundaries for velocities and the derivatives of the velocity to the pressure.
- 3.3 (11) EOspd Calculate the EOS variables and derivatives for the pressure iteration.
- 3.3 (12) ADJUST Adjust the velocities, the partial derivative of the velocity with respect to the pressure, and the linear term of the momentum exchange function when the cell returns to single phase during the pressure iteration.
- 3.3 (13) AMATRIX Calculate the A-matrix for the pressure iteration.
- 3.3 (14) SVECT Calculate the S-vector of STEP3.
- 3.3 (15) BVECT Calculate the B-vector of STEP3.
- 3.3 (16) SBANDM Set up the banded matrix for BNDSOL.
- 3.3 (17) TRANSP Transpose a non-square matrix.
- 3.3 (18) BSAXS Complete the solution of the pressure matrix equation.
- 3.3 (19) STEFAC Accelerate the pressure iteration convergence by Steffensen's method.
- 3.3 (20) UPDITV Update the necessary pressure iteration variables.
- 3.3 (21) CEBWX Convect the energy convection by adding the X-term and subtracting the W-term.
- 3.3 (22) CVECAR Solve the interfacial area convection equation.

3.3 (23)	CNVECT	Calculate convection terms.
3.3 (24)	VCOUPL	Test for close coupling of the velocity fields and recalculate the velocities if necessary.
3.3 (25)	VITER	Calculate the velocity fields with drag iteration in STEP4.
3.3 (26)	UVBOU	Set the boundaries of the velocities.
3.3 (27)	EAJIHQ	Calculate the interfacial heating and update the internal energies.
3.3 (28)	WORK	Calculate the work being done by the system.
3.3 (29)	TSCSTE	Calculate the time step control to reduce source term splitting error.
3.3 (30)	JPMAS	Optionally adjust overfilling of single-phase cells.
3.3 (31)	AVARV	Calculate the average of a variable with respect to the axial velocity (HOD).
3.3 (32)	AVARRU	Calculate the average of a variable with respect to the radial velocity (HOD).
3.3 (33)	ASIEV	Calculate the average of the internal energy in the axial direction (HOD).
3.3 (34)	ASIERU	Calculate the average of the internal energy in the radial direction (HOD).
3.3 (35)	AFDCVR	Calculate the convection term in the radial direction (HOD).
3.3 (36)	AFDCVZ	Calculate the convection term in the axial direction (HOD).
3.3 (37)	FVARV	Calculate the donor cell flux with respect to the axial velocity.
3.3 (38)	FVARRU	Calculate the donor cell flux with respect to the radial velocity.
3.3 (39)	RSLOPE	Calculate the slope in the radial direction.
3.3 (40)	ASLOPE	Calculate the slope in the axial direction.

3.4 Other fluid dynamics routines

3.4 (1)	DIVRGV	Calculate the divergence of velocity or the divergence of (vDf) for the source-term decoupling error remedy Method-1 or -2 respectively (not used in standard calculations).
3.4 (2)	CVRBNC	Calculate the convection of the densities and the radial and axial components in non-conservative form for the nonlinearity reduction (not used in standard calculations).
3.4 (3)	CVRB	Calculate the mass convection term for the nonlinearity reduction (not used in standard calculations).
3.4 (4)	EBERLN	Get the eigenvalue of a matrix for the nonlinearity reduction (not used in standard calculations).
3.4 (5)	INVDET	Get the inverse of a matrix for the nonlinearity reduction (not used in standard calculations).

4.0 Fuel pin model

4.0 (1)	SPIN	A driver for the simplified fuel-pin heat-transfer calculations (standard simple model).
4.0 (2)	HTRCOF	Calculate heat-transfer coefficients for fuel-pin components.
4.0 (3)	PINHTR	Perform the fuel-pin heat-transfer calculation.
4.0 (4)	FGPHTR	Perform the fission-gas plenum heat-transfer calculation.
4.0 (5)	RSTHTR	Reset fluid-dynamics cell variables based on the fuel-pin heat-transfer calculation.
4.0 (6)	DMPHTR	Print fuel-pin heat-transfer results.
4.0 (7)	DPIN	A driver routine to calculate intra-pin radial temperature distribution for the code option DPIN.
4.0 (8)	INIFF	Output the first header record to the post-processing file for the code option DPIN.
4.0 (9)	CONHTR	Control material heat transfer for the code option DPIN.
4.0 (10)	WFF	A routine which outputs the post-processing file for the code option DPIN.
4.0 (11)	RSTRAD	Reset fluid-dynamics cell variables after the detailed fuel-pin calculation for the code option DPIN.
4.0 (12)	REZONE	Re-zone fuel pin radial cells after the detailed fuel-pin calculation for the code option DPIN (not used in this version).
4.0 (13)	REZON2	Re-zone fuel pin radial cells after the detailed fuel-pin calculation for the code option DPIN (not used in this version).
4.0 (14)	CAVSET	Calculate the fuel pin cavity boundary in the detailed fuel-pin calculation for the code option DPIN.
4.0 (15)	CAVHTR	Calculate the heat transfer between the fuel pin cavity and the inner pellet surface node in the detailed fuel-pin calculation for the code option DPIN.
4.0 (16)	PCAVTY	Calculate the fuel pin cavity pressure in the detailed fuel-pin calculation for the code option DPIN.
4.0 (17)	PCAVI	Calculate the fuel pin cavity pressure in the detailed fuel-pin calculation for the code option DPIN.
4.0 (18)	FALBST	Predict fuel pin failure in the detailed fuel-pin calculation for the code option DPIN.
4.0 (19)	FCTNEW	Newton method in order to calculate the choked flow for the code option DPIN.
4.0 (20)	FCTFX	Function calculating the ratio of the critical to cavity pressure with FCTNEW for the code option DPIN.
4.0 (21)	SASNEW	Newton method in order to calculate the ejected fuel fraction for the code option DPIN.

- 4.0 (22) SASFX Function calculating the relative difference between cavity and channel pressure with SASNEW for the code option DPIN.

5.0 EOS and TPP functions

- 5.0 (1) EOST Calculate the temperatures and specific volumes of cell components, consistent with the internal energies at the end of Step1 and Step4.
- 5.0 (2) EOSSTR Calculate the temperature, specific volume of structure component from the internal energy.
- 5.0 (3) XESM Calculate the internal energy of structure or sublimate particles (EOS function).
- 5.0 (4) XTSM Calculate the temperature of structure or sublimate particles (EOS function).
- 5.0 (5) XTSMDE Calculate the derivative of solid temperature with respect to internal energy (EOS function).
- 5.0 (6) XVSM Calculate the specific volume of solid (EOS function).
- 5.0 (7) XTPM Calculate the particles temperature (EOS function).
- 5.0 (8) XVPM Calculate the specific volume of particles (EOS function).
- 5.0 (9) XELM Calculate the internal energy of saturated liquid (EOS function).
- 5.0 (10) XTLM Calculate the liquid temperature (EOS function).
- 5.0 (11) XTLMZ Calculate the temperature of saturated liquid (EOS function).
- 5.0 (12) XTLMDE Calculate the derivative of liquid temperature with respect to internal energy (EOS function).
- 5.0 (13) XDTDPE Calculate the derivative of liquid temperature with respect to pressure (EOS function).
- 5.0 (14) XDTDPD Calculate the derivative of XDTDEP with respect to internal energy (EOS function).
- 5.0 (15) XPLMZ Calculate the liquid vapor pressure (EOS function).
- 5.0 (16) XPLMDZ Calculate the derivative of vapor pressure of saturated liquid (EOS function).
- 5.0 (17) XVVAPD Calculate the derivative of saturation vapor volume (EOS function).
- 5.0 (18) XVCOND Calculate the derivative of condensate volume (EOS function).
- 5.0 (19) XVLM Calculate the specific volume of liquid (EOS function).
- 5.0 (20) XVLMZ Calculate the specific volume of saturated liquid (EOS function).
- 5.0 (21) XVLMDE Calculate the derivative of specific volume of saturated liquid (EOS function).
- 5.0 (22) XVGM Calculate the vapor specific volume (EOS function).

5.0 (23)	XDVDPZ	Calculate the derivative of liquid specific volume with respect to pressure (EOS function).
5.0 (24)	XDVDPE	Calculate the derivative of liquid specific volume with respect to pressure (EOS function).
5.0 (25)	XPGM	Calculate the vapor pressure (EOS function).
5.0 (26)	XPGMDR	Calculate the derivative of vapor pressure with respect to density (EOS function).
5.0 (27)	XPGMDT	Calculate the derivative of vapor pressure with respect to temperature (EOS function).
5.0 (28)	XPSAT	Calculate the saturation pressure (EOS function).
5.0 (29)	XPSATD	Calculate the derivative of saturation pressure (EOS function).
5.0 (30)	XPSTD2	Calculate the second derivative of saturation pressure (EOS function).
5.0 (31)	XEGM	Calculate the internal energy of vapor (EOS function).
5.0 (32)	XEGMDR	Calculate the derivative of vapor internal energy with respect to density (EOS function).
5.0 (33)	XEGMDT	Calculate the derivative of vapor internal energy with respect to temperature (EOS function).
5.0 (34)	XTSAT	Calculate the saturation temperature (EOS function).
5.0 (35)	XTSATD	Calculate the derivative of saturation temperature with respect to pressure (EOS function).
5.0 (36)	XTMZ	Calculate temperature on sublimation or saturation curve (EOS function).
5.0 (37)	XTMDE	Calculate the liquid-temperature derivative on saturation curve (EOS function).
5.0 (38)	XVMZ	Calculate specific volume on sublimation or saturation curve (EOS function).
5.0 (39)	XVMDE	Calculate liquid-specific-volume derivative on saturation curve (EOS function).
5.0 (40)	XVCON	Calculate the condensate specific volume (EOS function).
5.0 (41)	XECON	Calculate the condensate energy (EOS function).
5.0 (42)	XECOND	Calculate the derivative of condensate energy (EOS function).
5.0 (43)	XVVAP	Calculate the saturation vapor volume (EOS function).
5.0 (44)	XEVAP	Calculate the saturation vapor energy (EOS function).
5.0 (45)	XEVAPD	Calculate the derivative of saturation vapor energy (EOS function).
5.0 (46)	XVSPN	Calculate the spinodal volume of vapor (EOS function).
5.0 (47)	XEOSLM	Calculate the liquid temperature and specific volume.

5.0 (48)	XEOSPD	Calculate the liquid temperature, specific volume and its derivative with respect to the pressure.
5.0 (49)	XSATT	Calculate the saturation properties.
5.0 (50)	XSATE	Calculate the saturation properties (Fitting-Free EOS model).
5.0 (51)	XKPSM	Calculate the thermal conductivity of solid (TPP function).
5.0 (52)	XKPLM	Calculate the thermal conductivity of liquid (TPP function).
5.0 (53)	XKPGM	Calculate the thermal conductivity of vapor (TPP function).
5.0 (54)	XKPG	Calculate the thermal conductivity of vapor mixture (TPP function).
5.0 (55)	XDIFG	Calculate the binary diffusion coefficient of 1-2 gas mixture system for the diffusion-limited V/C model (not currently available) (TPP function).
5.0 (56)	XMULM	Calculate the viscosity of liquid (TPP function).
5.0 (57)	XMUPM	Calculate the viscosity of particles (TPP function).
5.0 (58)	XMUGM	Calculate the viscosity of vapor (TPP function).
5.0 (59)	XMUG	Calculate the viscosity of vapor mixture (TPP function).
5.0 (60)	XSGML	Calculate the surface tension of liquid (TPP function).
5.0 (61)	XCPLM	Calculate the heat capacity of saturated liquid at constant pressure (TPP function).
5.0 (62)	XCPGM	Calculate the heat capacity of vapor at constant pressure (TPP function).
5.0 (63)	XVSLM	Calculate the velocity of sound in saturated liquid (TPP function).
5.0 (64)	XAPPLM	Calculate the volumetric thermal expansion coefficient of saturated liquid (TPP function).

6.0 Matrix solvers

6.0 (1)	TD3AXY	The tridiagonal matrix solver for a (3,3)-matrix.
6.0 (2)	TD4AXY	The tridiagonal matrix solver for a (4,4)-matrix.
6.0 (3)	TD5AXY	The tridiagonal matrix solver for a (5,5)-matrix.
6.0 (4)	TRDSOL	The tridiagonal matrix solver for a (n, n)-matrix.
6.0 (5)	S5X5	The direct-inversion full matrix solver for a (5,5)-matrix.
6.0 (6)	BNDSOL	The direct banded matrix solver used in pressure iteration. It calls BNDSL1 or BNDSL2.
6.0 (7)	BNDSL1	The direct banded matrix solver for the case that jc is not 0.
6.0 (8)	BNDSL2	The direct banded matrix solver for the case that jc is 0.
6.0 (9)	PCGSOL	The driver of the pre-conditioned conjugate gradient (PCG) matrix solver called from STEP3.

6.0 (10)	ILUBCG	The PCG (ILUBCG) banded matrix solver. Recommended for a standard use.
6.0 (11)	ILUCR	The PCG (ILUCR) banded matrix solver.
6.0 (12)	INDEX	Set up the list vector for the PCG solver.
6.0 (13)	NDECOMP	This is called by the PCG solver.
6.0 (14)	NAXSUB	This is called by the PCG solver.
6.0 (15)	NLU	This is called by the PCG solver.
6.0 (16)	NATSUB	This is called by the PCG solver.
6.0 (17)	NUTLT	This is called by the PCG solver.
6.0 (18)	CPMDD	Pack cell variables into contiguous storage. For machines requiring double precision, double to double precision.
6.0 (19)	CPMDS	Pack cell variables into contiguous storage. For machines requiring double precision, double to single precision.
6.0 (20)	CPMDSI	Pack cell variables into contiguous storage. Integer to single.
6.0 (21)	CPMDSV	Pack velocities into contiguous storage.

7.0 Printing (mainly for fluid dynamics)

7.0 (1)	NETMAS	Calculate the net mass overflow over the time step for printing.
7.0 (2)	DEOFS	Start the calculation of the energy overflow for printing.
7.0 (3)	DEOVFL	Complete the energy overflow calculation for printing.
7.0 (4)	MECALC	Print the mass and energy balance data.
7.0 (5)	RGMAS	Print region-wise summation of mass and energy.
7.0 (6)	PRTCEL	Provide cell status edits.
7.0 (7)	PRTVAR	Print the real cell variable value in the whole calculational region.
7.0 (8)	PRTBT	Print cell-wise input variables.
7.0 (9)	INIPTC	Print cell-wise input variables.
7.0 (10)	XCWDC	Print cell-wise input variables.
7.0 (11)	PRTVRI	Print the integer cell variable value in the whole calculational region.
7.0 (12)	PRTINT	Print mass and energy summation data.
7.0 (13)	MCLCPT	Print mass and energy deviation data.
7.0 (14)	MCLCHK	Print mass and energy deviation data.
7.0 (15)	ISITTM	Determine print and dump timings.
7.0 (16)	ERROR	Print the error message (neutronics).
7.0 (17)	ERRMSG	Print the error message (fluid dynamics).

7.0 (18)	COVERP	Print the cover page for the listing output.
7.0 (19)	ZTABLE	Print the array values in table format.
7.0 (20)	ZTITLE	Print the title for the listing output.
7.0 (21)	ZWRITE	Print the messages.
7.0 (22)	CREAD	Internal I/O routine.
7.0 (23)	ZWRITI	Print the integer scalar value, variable name, and its description.
7.0 (24)	ZWRITR	Print the real scalar value, variable name, and its description.
7.0 (25)	ZWRITC	Print the character string.

8.1 Neutronics input and initialization (URANUS off)

8.1 (1)	NEUDEF	Set default data for the neutronics.
8.1 (2)	NTINP	Read input data for the neutronics.
8.1 (3)	CLRDIM	Initialize input data arrays.
8.1 (4)	CHKPAR	Check input data against the code parameters.
8.1 (5)	CHGISO	Convert data format for the input names for isotopes and materials.
8.1 (6)	NEIPRT	Print input data for the neutronics.
8.1 (7)	NEINIT	Initialize the neutronics variables.
8.1 (8)	FILINP	A driver routine to read the binary cross-section files.
8.1 (9)	INFF	Read the binary cross-section file BRKCOXS.
8.1 (10)	INXS	Read the binary cross-section file ISOTXS.
8.1 (11)	IFINSN	Read the Sn constants from the file ISNCON if optionally specified by input.
8.1 (12)	SNCON	Set internally the Sn constants (standard procedure).
8.1 (13)	INFLX	Read the initial neutron flux shape from the file ATFLUX (or RTFLUX) if optionally specified by input.
8.1 (14)	NEUSTP	Control the time steps (reactivity and shape steps) for the neutronics.

8.2 Neutronics driver and cross-section handling (URANUS off)

8.2 (1)	GRIND	A driver routine for the neutronics.
8.2 (2)	NEUINT	Transfer macroscopic densities and temperatures from the fluid dynamics into material-wise averaged data used in the neutronics.
8.2 (3)	FLDINT	Convert specific energy generation rates calculated by the neutronics into the fluid-dynamics cell variables.
8.2 (4)	SHLDXS	A driver to calculate self-shielding factors and effective macroscopic cross sections.

8.2 (5)	BKGINT	Interpolate self-shielding factors for each background cross sections (ISOTOPE off).
8.2 (6)	BINT4	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (7)	BSPVD	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (8)	BSPVN	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (9)	BNFAC	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (10)	BNSLV	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (11)	BVALU	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (12)	INTRV	A routine related to B-spline interpolation of shielding factors (ISOTOPE off).
8.2 (13)	CALCXS	Calculate the macroscopic cross sections .

8.3 Quasi-static kinetics (URANUS off)

8.3 (1)	PKDRIV	A driver routine for transient kinetics with an improved quasi-static method.
8.3 (2)	EXTRAP	A general routine for linear data interpolation.
8.3 (3)	POWCAL	Calculate reactor power and material-wise heat sources (specific energy generation rates).
8.3 (4)	INPROD	Calculate kinetics parameters including reactivities.
8.3 (5)	AMPSOU	Calculate the effective source for amplitude function.
8.3 (6)	TSPK	Calculate the amplitude function for each reactivity step.
8.3 (7)	PCALC	Calculate the delayed-neutron precursor concentrations for each reactivity step.
8.3 (8)	TIMSTP	Determine the next time steps (reactivity and shape steps) for the neutronics.
8.3 (9)	FITZ	A general routine for parabolic data interpolation.
8.3 (10)	WNP	A routine which outputs the post-processing file SIMNP.
8.3 (11)	PCINT	Adjust the cell-wise delayed-neutron precursor concentrations.
8.3 (12)	TRINIT	A routine to adjust kinetics parameters for transient-state neutronics initialization.
8.3 (13)	EPSILON	The epsilon value for the computer accuracy.
8.3 (14)	AMPFM	Compute the amplitude of the fundamental mode fraction of the current source shape.

8.4 Flux shape calculation with TWODANT (URANUS off)

8.4.1 Main driver

8.4.1 (1)	LINKM	Linking-Module for data exchange between the TWODANT-solver module and other neutronics modules.
8.4.1 (2)	CMEMRY	Set SCM (the small core memory) length used for a flux shape calculation.
8.4.1 (3)	TWODANT	A driver routine for TWODANT-solver module.
8.4.1 (4)	VRSION	Set TWODANT-solver module comment card.
8.4.1 (5)	LOEHR	Compute a normalization factor to be used for accelerating convergence for an inhomogeneous source case at steady-state.

8.4.2 Flux shape solver modules

8.4.2.1 Driver

8.4.2.1 (1)	TIGF20	A driver routine for the TWODANT-solver module.
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8.4.2.2 Solver input

8.4.2.2 (1)	TINP21	Controls solver module initializations.
8.4.2.2 (2)	RDSOL	Read portions of the SOLINP file.
8.4.2.2 (3)	SORTMC	Sort the input variables for the Monte Carlo calculation into the IA and RIA arrays.
8.4.2.2 (4)	SORTIA	Sort the input IA array into the IA array used by solver.
8.4.2.2 (5)	SORTRI	Sort the input RIA array into the RIA array used by solver.
8.4.2.2 (6)	PRINTMC	Prints the Monte Carlo input parameters.
8.4.2.2 (7)	SCMADD	Calculates the small core memory storage pointers.
8.4.2.2 (8)	LCMADD	Calculates the large core memory storage pointers.
8.4.2.2 (9)	PRNTIA	Prints the input integer and floating parameters.

8.4.2.3 Transport calculation

8.4.2.3 (1)	TGND25	Calculates initially required functions and grid structure.
8.4.2.3 (2)	TINITA	Generate coarse mesh numbers on the fine mesh.
8.4.2.3 (3)	TINITQ	Normalize sources.
8.4.2.3 (4)	SCATTG	Computes scatter to group.
8.4.2.3 (5)	SCATTH	Computes full source.
8.4.2.3 (6)	TRANSO	Controls the inner iteration.
8.4.2.3 (7)	TOUTER	Transport outer iteration calculation and gets diffusion parameters.
8.4.2.3 (8)	SINNER	Transport inner iteration calculation.

8.4.2.3 (9)	SNSRCMC	Computes the boundary flux for a white boundary condition.
8.4.2.3 (10)	MASWEP	Sweeps along diagonals normal to the direction of particle flow to enhance vectorization of the solution algorithm.
8.4.2.3 (11)	MASWEPD	This routine is DD in angle, AWDD in space.
8.4.2.3 (12)	MASWEPW	The adaptive weighted diamond differencing method is used in this routine to compute the angular flux.
8.4.2.3 (13)	MASWMC	Sweeps along diagonal normal to the direction of particle flow to enhance vectorization of the solution algorithm.
8.4.2.3 (14)	TGSUMS	Calculates leakages and a few other quantities and does group sum all for the system balance table.
8.4.2.3 (15)	TESTGO	Tests for global outer convergence.
8.4.2.3 (16)	TNEWPA	Computes new parameters for implicit eigenvalue search.

8.4.2.4 Diffusion synthetic acceleration (DSA)

8.4.2.4 (1)	CONDIF	Calculates ordinary diffusion matrix from cross section.
8.4.2.4 (2)	RDFCOF	Diffusion equation with unknowns on mesh vertices.
8.4.2.4 (3)	TSYNDI	Calculates synthetic diffusion matrix from transport fluxes.
8.4.2.4 (4)	ZEROF	Computes the vertex centered transport scalar flux and the vertex removal rate to be used in the DSA equation.
8.4.2.4 (5)	DIFFO	Controls the outer iteration.
8.4.2.4 (6)	DOUTER	Run diffusion or sub-outers to convergence.
8.4.2.4 (7)	CHEBY	Chebyshev acceleration of the fission source.
8.4.2.4 (8)	SCASTG	Computes scatter to neutron energy group.
8.4.2.4 (9)	SCASTH	Computes isotopic source.
8.4.2.4 (10)	SRCCAL	Partitions the centered source to the corners.
8.4.2.4 (11)	TLNLBC	Takes a mesh cell centered quantity.
8.4.2.4 (12)	GREYACC	Controls the multigrid solution of then grey accelerator for up-scatter problems.
8.4.2.4 (13)	ONEGRP	diffusion equation parameters for use in the one-group grey accelerator for DSA up-scatter problem.

8.4.2.5 Fission source

8.4.2.5 (1)	TFISCA	Does all the fission source calculations during initialization.
8.4.2.5 (2)	PTFISS	Calculates the point-wise fission source.
8.4.2.5 (3)	GSUMFS	Control code to compute fission sum for each neutron energy.
8.4.2.5 (4)	AQFLUX	Compute the neutron energy group flux pointer for a one level machine.
8.4.2.5 (5)	ASUMFS	Compute fission sum for a neutron energy group.

8.4.2.5 (6) FS Integrates the point-wise fission source.

8.4.2.6 Scattering source

8.4.2.6 (1) ISITFC Checks the scattering source input and sets the indicator.
 8.4.2.6 (2) CHKIFC Checks scattering source input.
 8.4.2.6 (3) UCFLUX Computes the uncollided flux for an isotropic point.
 8.4.2.6 (4) SIGRAY Computes the optical distance from a source.
 8.4.2.6 (5) RTHST1 A driver routine for scattering source Monte Carlo calculation.
 8.4.2.6 (6) RTGET Storage of the stack word assignments.
 8.4.2.6 (7) MVZTOX Move stack word.
 8.4.2.6 (8) MVBTOX Move stack word.
 8.4.2.6 (9) MVBTOZ Move stack word.
 8.4.2.6 (10) RTTRCK Calculates distance to boundary and flight path length for scattering source.
 8.4.2.6 (11) RTHST2 Score angular moments.
 8.4.2.6 (12) RTFLUX Performs ray tracing on fixed source to get uncollided flux.
 8.4.2.6 (13) RTSRC Samples fixed source for ray tracing.
 8.4.2.6 (14) FCSRCE Computes the scattering source from the uncollided flux just obtained.

8.4.2.7 Multigrid

8.4.2.7 (1) GRIDS Sets up some pointers for the two dimensional multigrid solver.
 8.4.2.7 (2) GRDFN Calculate grid structures for the multigrid solver.
 8.4.2.7 (3) KEY Set key.
 8.4.2.7 (4) MFSFC Do the nine point condensation.
 8.4.2.7 (5) MULTIG Controls the two dimensional multigrid cycling.
 8.4.2.7 (6) RELAXZ Relaxation in vector mode using every other point in the X-Y plane.
 8.4.2.7 (7) RELAXR Does line relaxation in the X direction assuming a two dimensional mesh.
 8.4.2.7 (8) PUTC Loop over grids to compute each coarse grid diffusion equation coefficients for use in multigrid acceleration.
 8.4.2.7 (9) FIXIT Revised a value smaller than 0.
 8.4.2.7 (10) INTADD Interpolate coarse grid correction and add to fine grid solution.

8.4.2.8 Set up the Monte Carlo calculation

8.4.2.8 (1) MCXSPT Calculates the cross-section table position.

- 8.4.2.8 (2) MCXS Sets up the cross-section for the adjoint calculation.
- 8.4.2.8 (3) SRCDEF Set up source in Monte Carlo region.
- 8.4.2.8 (4) SETUP Defines angular weight matrix.
- 8.4.2.8 (5) ADJBNK Adjusts bank size.
- 8.4.2.8 (6) ADVIJK Advance source random number.
- 8.4.2.8 (7) BINS Sets up the angle bins around the Sn discrete angles.

8.4.2.9 Stacks for the Monte Carlo calculation

- 8.4.2.9 (1) RMHST1 Driver routine for response matrix and down-scatter source Monte Carlo calculations.
- 8.4.2.9 (2) SWFIX Stores integer words from a stack.
- 8.4.2.9 (3) RMGET Stack of parameters.
- 8.4.2.9 (4) RMHST2 Empty out collision and random walk stacks.
- 8.4.2.9 (5) COLL Collision routine, down-scattering allowed.
- 8.4.2.9 (6) XYRW Track particle across internal boundary.
- 8.4.2.9 (7) RW Transfers particles from STACK3.
- 8.4.2.9 (8) TRCK Determines destination of STACK1.
- 8.4.2.9 (9) CALC Calculates distance to boundaries and flight path length.
- 8.4.2.9 (10) XYSCORE Scores particles in directly into vector.
- 8.4.2.9 (11) MCTOSN Transfers particles from Monte Carlo region to Sn region when in-scattering, scores angular moments.
- 8.4.2.9 (12) SNTOMC Sample Sn cell sources in Monte Carlo region.
- 8.4.2.9 (13) RESSRC Sample the residual incoming boundary flux.
- 8.4.2.9 (14) FIXSRC Samples fixed source inside Monte Carlo region.
- 8.4.2.9 (15) RAN Gets random number vector.
- 8.4.2.9 (16) GETMSK Not used.

8.4.2.10 Calculates the source matrix and leakage currents for the Monte Carlo region

- 8.4.2.10 (1) SRCMC Determines source matrix and leakage currents for the Monte Carlo region.
- 8.4.2.10 (2) VARACC Accumulates leakage from Monte Carlo region for variable calculation leakage are accumulated on coarse mesh.
- 8.4.2.10 (3) LINKO Controls the Sn/Monte Carlo iterations.
- 8.4.2.10 (4) LINKMC Check for Monte Carlo problem.
- 8.4.2.10 (5) SNMOM Get current group's Sn point-wise source moments.
- 8.4.2.10 (6) RESFIT Fit incoming flux.

- 8.4.2.10 (7) RESPJ Projected fit coefficients.
- 8.4.2.10 (8) DWNSRC Get variance for coarse mesh leakages from Monte Carlo region.
- 8.4.2.10 (9) CONVCK Calculate Monte Carlo to Sn sources.
- 8.4.2.10 (10) SFTFIX Conserve particles locally.
- 8.4.2.10 (11) SRCVAR Determines variable for ray tracing calculation.

8.4.2.11 Miscellaneous

- 8.4.2.11 (1) RDGEOD Reads the GEODST file.
- 8.4.2.11 (2) RDGEO2 Reads the GEODST file for two dimensional input.
- 8.4.2.11 (3) RDMACR Read parts of the MACRXS file for storage information only.
- 8.4.2.11 (4) TLOCNW Determines the scattering table lengths and the scattering source group also calculates the length of the cross section records.
- 8.4.2.11 (5) RDASGM Reads the ASGMAT file.
- 8.4.2.11 (6) TSMIXC Checks the MACRXS file input and material to zone assignment data.
- 8.4.2.11 (7) RDFIXS Reads the FIXSRC file.
- 8.4.2.11 (8) TLCMBL Computes large core memory cross section blocking.
- 8.4.2.11 (9) TINP22 Controls flux guess and inhomogeneous source processing.
- 8.4.2.11 (10) TFINFM Reads standard interface file for flux moments.
- 8.4.2.11 (11) TFINQF Reads standard interface file for source or flux.
- 8.4.2.11 (12) TREADQ Process sources from SOLINP file and FIXSRC file.
- 8.4.2.11 (13) RDQS Process Q-source.
- 8.4.2.11 (14) PTQ1D Prints one dimensional Q array for component.
- 8.4.2.11 (15) BSREAD Reads 1 groups worth of boundary source for one face from file SOLINP into small core memory.
- 8.4.2.11 (16) TINP23 Controls quadrature selection.
- 8.4.2.11 (17) TFINSN Reads Sn constants from standard interface file.
- 8.4.2.11 (18) TSNCON Transfer to the Cheby Legendre product quadrature set.
- 8.4.2.11 (19) TPNGEN Copied mostly from DTF-IV.
- 8.4.2.11 (20) TINP24 Checks spatial mesh input for consistency.
- 8.4.2.11 (21) TMAPPE Generates a material map on the fine mesh.
- 8.4.2.11 (22) MACMIX Prepare active cross sections in large core memory.
- 8.4.2.11 (23) SUMF2C Sums as to coarse mesh.
- 8.4.2.11 (24) RDFLUX Process neutron flux.
- 8.4.2.11 (25) EPXS2D Expands a cross section set given as a zone into a fine mesh.

8.4.2.11 (26) EXPXS2D	Obtain the cross section including density factor.
8.4.2.11 (27) EXPCHI2D	Calculate fission source.
8.4.2.11 (28) TMONIT	Prints monitor line.
8.4.2.11 (29) CIFLSM	Maps fine mesh currents on to the coarse mesh.
8.4.2.11 (30) SMOM	Gets scattering source moments for Sn.
8.4.2.11 (31) DXITE	Performs large core memory write operations.
8.4.2.11 (32) DXEED	Performs large core memory read operations.
8.4.2.11 (33) TOT28	Controls final TWODANT-solver module printing.
8.4.2.11 (34) TFINAL	Prints TWODANT-solver module final.
8.4.2.11 (35) TFINP6	Prints six vectors with scaling of second vector sums division of neutron gamma will be done.
8.4.2.11 (36) TFINP3	Prints three vectors sums division of neutron gamma will be done.
8.4.2.11 (37) PCMBAL	Prints coarse mesh balance tables.
8.4.2.11 (38) TOT29	Controls binary file preparation.
8.4.2.11 (39) DMPFLX	Writes interface output scalar flux.
8.4.2.11 (40) REWASH	Code re-writes ASGMAT file for concentration searches.
8.4.2.11 (41) TFRITE	Write a CCCC standard interface file.
8.4.2.11 (42) CHIMOD	Modifies for adjoint calculations the fission spectrum.
8.4.2.11 (43) SRCBAL	Performs balance calculations for coarse mesh balances.
8.4.2.11 (44) EXPANQ	Expands total source into neutron flux dimensioned source.
8.4.2.11 (45) MCBFADJ	Adjusts the Monte Carlo coarse mesh boundary fluxes if the Monte Carlo region boundary does not on a coarse mesh boundary.
8.4.2.11 (46) SUMNEG	Sums the negative flux fixup counts over the coarse mesh cell.
8.4.2.11 (47) QRSGET	Converts residual flux to leakage.
8.4.2.11 (48) QBSGET	Calculates total absolute residual source from moments.
8.4.2.11 (49) GAUELM	Divide pivot row by pivot element.
8.4.2.11 (50) QGET	Gets sources from Monte Carlo region.
8.4.2.11 (51) LGET	Gets leakages from Monte Carlo region.
8.4.2.11 (52) PT23D	Print arrays.
8.4.2.11 (53) PRTNFX	Prints the negative flux fixup monitor for each group and each coarse mesh cell.
8.4.2.11 (54) SNFLUX	Calculated coarse mesh scalar fluxes from Monte Carlo track lengths, insert average into Sn fine mesh array.

8.4.3 Miscellaneous modules

8.4.3 (1)	ONETBD	Set TWODANT-solver module seek names and labels.
8.4.3 (2)	SEEKBD	Set unit number of file.
8.4.3 (3)	C4S77D	Set file open parameters.
8.4.3 (4)	DOPCBD	Set unit number and name of physical random files.
8.4.3 (5)	FHLPRL	False routine to contain large letter information.
8.4.3 (6)	ENVSET	Set the environmental variable name.
8.4.3 (7)	LCMSET	Set core memory length of SCM (Small Core Memory) and CM (Large Core Memory).
8.4.3 (8)	STACKV	Place holder for stack based locals.
8.4.3 (9)	UGONOW	A driver routine for general initialization of TWODANT-solver module.
8.4.3 (10)	SEEK4C	Set unit control code of hollerith names and unit numbers.
8.4.3 (11)	ANLVER	Convert a hollerith name.
8.4.3 (12)	A4CRGT	Determine the access of a file name.
8.4.3 (13)	CLOSEQ	Close a logical file unit.
8.4.3 (14)	RUT4C	Routine checks for existence of a interface file.
8.4.3 (15)	AUN4C	Associate a unit number and hollerith name for interface files.
8.4.3 (16)	AB4CRD	Associate a unit number and interface file name.
8.4.3 (17)	DST4C	Destroys a interface file.
8.4.3 (18)	DOPOFF	Resets offset of a interface file.
8.4.3 (19)	SECONI	Initializes time functions (CPU/charge/remaining/date). Obtains current CPU and charge times.
8.4.3 (20)	TIMER	Prepares system times (CPU/charge) and date.
8.4.3 (21)	SECNDS	Returns time since start of execution.
8.4.3 (22)	NAFIX	Used with a fixed-point vector found in the floating-point vector to give correct value.
8.4.3 (23)	TIMDAT	Obtains date and time in Hollerith A6 form from master clock.
8.4.3 (24)	PRTLAG	Prints large character heading.
8.4.3 (25)	FHLPR	Code prints in large characters one integer 8-byte format word.
8.4.3 (26)	ELAPSE	Calculates elapsed CPU and I/O times for each executed module.
8.4.3 (27)	STOP	Stops a execution for implementation errors.
8.4.3 (28)	OFFUGO	Check transfer output indicator.
8.4.3 (29)	MDOPC	Converts 8 byte word to 4 byte word.
8.4.3 (30)	DOPC	Assigns physical random files from maximum number of records and maximum length.

8.4.3 (31)	WATRMD	Obtain physical unit number.
8.4.3 (32)	TRNSUM	Sums transfer counts for MCRED/MCRIT routines by index.
8.4.3 (33)	FILECK	Check dimension variables from input files (TWOANT-solver module BLOCK-I card data).
8.4.3 (34)	EXCEED	Checks for a core memory storage.
8.4.3 (35)	ERRORT	Prints error message.
8.4.3 (36)	NXTSGE	Searches real array X for XCOMP variable.
8.4.3 (37)	MESSAG	Remembers messages to print on highlights board at end of run.
8.4.3 (38)	SUNASG	Requests new storage block for core memory and sets current amount.
8.4.3 (39)	morec	A C-routine which requests 8 byte words but returns the address as a byte address and this will be converted into a 4 byte address prior to storage.
8.4.3 (40)	lessc	A C-routine which frees the allocated kernel virtual memory (ALPHA off).
8.4.3 (41)	iaccess	A C-routine which check a file present.
8.4.3 (42)	SUNOFF	computes core memory offsets address.
8.4.3 (43)	NOWERR	Sets the error counts.
8.4.3 (44)	EFBYTE	Converts real 8 byte array to 4 byte array.
8.4.3 (45)	REGCMV	Computes the neutronics mesh cell volume for GEODST file.
8.4.3 (46)	ISMIN	Finds the first index of the smallest value of a vector.
8.4.3 (47)	R8THOL	Moves real 8 variable to horrerith.
8.4.3 (48)	R8XHOL	Converts character and real 8 data through common.
8.4.3 (49)	IBM8R8	Determines the equality of two real 8 values.
8.4.3 (50)	STOPIT	Sets exit value.
8.4.3 (51)	FEBYTE	Converts 4 byte floating to 8 byte floating.
8.4.3 (52)	OPENWR	Opens a sequential file for writing.
8.4.3 (53)	CLEAR4	Fill an array with a real unique value.
8.4.3 (54)	OPENRD	Opens a sequential file for reading.
8.4.3 (55)	SREED	Controls of record for reading or writing.
8.4.3 (56)	REED	Transfers information between the small core memory and sequential disk.
8.4.3 (57)	SUBRD	Process physical binary read.
8.4.3 (58)	SUBWR	Process physical binary write.
8.4.3 (59)	IKR8R8	Searches of table for entry and returns index.
8.4.3 (60)	MCRED	Controls of core memory transfers.

8.4.3 (61)	LCMCHK	Checks the assigned large core memory length against the requested for the transfer routines.
8.4.3 (62)	MDRED	Controls the core memory transfers.
8.4.3 (63)	DRED8	Transfers record from random disk to the large core memory.
8.4.3 (64)	DRIT8	Transfers record from the large core memory to random disk.
8.4.3 (65)	SKOPRD	Reads the identification record given the index.
8.4.3 (66)	MACIN	Process the compressed input and form working output.
8.4.3 (67)	MACCOR	Corrects the principal and scatter cross sections.
8.4.3 (68)	MACSCG	Obtain from the compact scatter the desired value.
8.4.3 (69)	MACOUT	Processes the compressed output.
8.4.3 (70)	IGPRNT	Finds the mini print setting.
8.4.3 (71)	PRTRRN	Prints transfer counts and zeros.
8.4.3 (72)	ERADDP	Test if additional error print required.
8.4.3 (73)	USERDA	To place user data on file.
8.4.3 (74)	MACTRC	Code transport corrects a cross section set and prepares the correct temporary read file name.
8.4.3 (75)	FCNG	Used by FZERO routine to evaluate the probability.
8.4.3 (76)	RANYGT	Compares values.
8.4.3 (77)	ISORT	Sorts the input vector.
8.4.3 (78)	NEWPAS	Produces a file with new core memory requirements.
8.4.3 (79)	CLRLCM	Clears large core memory using small core memory.
8.4.3 (80)	FILLU	Enters logical file information.
8.4.3 (81)	LGNDRX	Gets the Cheby Legendre product quadrature set.
8.4.3 (82)	MPLY	Multiplies a floating point SCM (small core memory) block by a constant.
8.4.3 (83)	SSUM	Sums the elements of a real vector.
8.4.3 (84)	RANYLT	Compares values.
8.4.3 (85)	SCOPY	Moves the array in small core memory.
8.4.3 (86)	SSCAL	Initialize needed parameters.
8.4.3 (87)	RANYEQ	Set indicator and check count.
8.4.3 (88)	ISMAX	Set index and return.
8.4.3 (89)	ACOSH	Support of the Chebychev acceleration.
8.4.3 (90)	SDOT	Check count.
8.4.3 (91)	ISAMAX	Initialize parameter.

8.4.3 (92)	SPBFA	Factors a real symmetric positive definite matrix stored in band form.
8.4.3 (93)	SGECO	Factors a real matrix by Gaussian elimination and estimates the condition number of the matrix.
8.4.3 (94)	SGEFA	Factors a real matrix by Gaussian elimination and estimates the condition number of the matrix.
8.4.3 (95)	SASUM	Routine forms the sum of the absolute value of the entries.
8.4.3 (96)	SAXPY	Initialize needed parameters.
8.4.3 (97)	RANYLE	Compares values.
8.4.3 (98)	SPBSL	Direct three dimensional solver on grid.
8.4.3 (99)	SGESL	Direct three dimensional solver on grid.
8.4.3 (100)	PRTNGS	Prints the integral sums.
8.4.3 (101)	EDTBAI	Initializes the group balance special output file EDGBAL.
8.4.3 (102)	MGEODF	Prepares a new GEODST file.
8.4.3 (103)	SIDRD	Obtains the information in the mixed identification.
8.4.3 (104)	SEKPHL	Translates logical unit number to physical file number or closes physical file.
8.4.3 (105)	NSGBOX	Prints a message in a box regardless of local terminal setting.
8.4.3 (106)	ASCOPW	Code opens the file for ASCII writing given the index.
8.4.3 (107)	STNAA	Stores fixed point value in floating point array.
8.4.3 (108)	HYLITE	Prints highlights of the run.
8.4.3 (109)	KEYWRD	Prints keyword block.
8.4.3 (110)	HISTORY	Prints storage and timing history.
8.4.3 (111)	ADJLCM	Checks a core memory length requests after fixed adjustment.
8.4.3 (112)	MSGBOX	Prints a message in a box only if terminal is set locally.
8.4.3 (113)	NUMIGT	Searches integer array.
8.4.3 (114)	XREP	Generates an exponential representation of the scattering function which attempts to conserve the moments.
8.4.3 (115)	GAUS8	Integrate a real function of one variable over finite intervals.
8.4.3 (116)	FUN8	Used by GAUS8 routine to provide the value of the integrand at m.
8.4.3 (117)	IIMACH	Return integer machine dependent constants.
8.4.3 (118)	RIMACH	Return floating point machine dependent constants.
8.4.3 (119)	CONSIST	Checks to see if a positive solution is possible, given the set of moments.

8.4.3 (120)	SSPEV	Compute the eigenvalues and , optionally, the eigenvectors.
8.4.3 (121)	TRED3	Reduce a real symmetric matrix stored in packed form to.
8.4.3 (122)	TQLRAT	Compute the eigenvalues of symmetric tridiagonal matrix.
8.4.3 (123)	PYTHAG	Compute the complex square root of a complex number without.
8.4.3 (124)	IMTQL2	Compute the eigenvalues and eigenvectors of a symmetric.
8.4.3 (125)	TRBAK3	Form the eigenvectors of a real symmetric matrix.
8.4.3 (126)	MOMCOR	Corrects polynomial moments for negative eigenvalue case.
8.4.3 (127)	SSPFA	Factor a real symmetric matrix stored in packed form by elimination with symmetric pivoting.
8.4.3 (128)	SSWAP	Interchange two vectors.
8.4.3 (129)	SSPDI	Compute the determinant, inertia, inverse of a real.
8.4.3 (130)	SNSQ	Find a zero of a system.
8.4.3 (131)	FCN	Used by SNSQE routine to evaluate the functions.
8.4.3 (132)	ENORM	Calculates the euclidean normalization of X.
8.4.3 (133)	FDJAC1	Subsidiary to SNSQ routine.
8.4.3 (134)	QRFAC	Subsidiary to SNSQ routine.
8.4.3 (135)	QFORM	Subsidiary to SNSQ routine.
8.4.3 (136)	DOGLEG	Subsidiary to SNSQ routine.
8.4.3 (137)	R1UPDT	Subsidiary to SNSQ routine.
8.4.3 (138)	R1MPYQ	Subsidiary to SNSQ routine.
8.4.3 (139)	GENBIN	Generates equiprobable bins from the exponential representation.
8.4.3 (140)	FZERO	Search for a zero of a array in a given interval.
8.4.3 (141)	FUN	Used by GAUS8 routine to provide the value of the integrand at m.
8.4.3 (142)	IANYGT	Computes values of vector.
8.4.3 (143)	FUN8D	Used by GAUS8 routine to provide the value of at m.

9.0 Miscellaneous operations

9.0 (1)	WRDMP	Output restart dump.
9.0 (2)	WRUNF	Write unformatted file.
9.0 (3)	RDDMP	Read restart dump.
9.0 (4)	RDUNF	Read unformatted data.
9.0 (5)	WPPF	Write post-processing file.
9.0 (6)	WTSTR	Calculate structure-component volume fractions for printing and post-processing.

9.0 (7)	WBF	Write base files.
9.0 (8)	ISITTR	Determine a restart time for each output files.
9.0 (9)	SKIPRC	Skip n records.
9.0 (10)	LENG	Get the length of a common using the function LOC.
9.0 (11)	SETR	Fill an array with a real unique value.
9.0 (12)	SETI	Fill an array with a integer unique value.
9.0 (13)	COPYR	Transfer array data.
9.0 (14)	SETRAL	Convert a two-dimensional array into a one-dimensional array.
9.0 (15)	SEPER	Separate a message into fields.
9.0 (16)	NWCELL	A function to calculate the internal IJ cell number from the external IJ number (real cells only without boundary cells).
9.0 (17)	ICELL	A function to calculate I from IJ.
9.0 (18)	JCELL	A function to calculate J from IJ.
9.0 (19)	IFLGC	A function to generate a list vector.
9.0 (20)	INTIRP	Linearly interpolate a one-dimensional array.
9.0 (21)	ISAMAXT	Find a pointer to the first occurrence of the maximum in an array.
9.0 (22)	LSAMAX	Find a pointer to the first occurrence of the maximum in an array. This routine does not search boundary cells.
9.0 (23)	CVMGT	A conditional vector merge function for real variables. Merges on the condition of logical truth.
9.0 (24)	ICVMGT	A conditional vector merge function for integer variables. Merges on the condition of logical truth.
9.0 (25)	SIGTRP	A special routine for IBM RS6000 workstation.
9.0 (26)	AIXSIG	A special routine for IBM RS6000 workstation.

10.0 System-dependent routines

10.0 (1)	CDATE	Get the current date as YY/MM/DD.
10.0 (2)	CCLOCK	Get the current time as HH.MM.SS.
10.0 (3)	SECOND	Obtain the CPU elapsed time in second.
10.0 (4)	TLEFT	A function to obtain the remaining CPU time in 1/100 s.

APPENDIX B

SYSTEM DEPENDENT ROUTINES AND FUNCTIONS

In SIMMER-III, use of installation-dependent system routines is minimized to facilitate code transfer. The system dependent routines only used account for monitoring job time limit, extracting memory address, etc. These are described in this Appendix. The subroutines and functions are shown in **Tables B-1** and **B-2**, respectively.

Table B-1. List of SIMMER-III System Dependent Subroutines.

CDATE(CD)	A routine to obtain the current date as YY/MM/DD. CD Character*8 : the current date
CCLOCK(CT)	A routine to obtain the wall clock time as HH.MM.SS. CT Character*8 : the current time
SECOND(ET)	A routine to obtain the elapsed time in second. ET Real*8 : the current time
SECONI(ET,CHT)	A routine to obtains current CPU and charge times (URANUS off). ET Real*8 : the current CPU time CHT Real*8 : the charge time

Table B-2. List of SIMMER-III System Dependent Functions.

TLEFT(DUM)	A function to obtain the remaining CPU time in 1/100s. DUM any : dummy argument
SECNDS(DUM)	A function to obtain the current time (URANUS off). DUM Real*4 : dummy argument

APPENDIX C

EQUATION-OF-STATE FUNCTIONS

In SIMMER-II [1] or AFDM [2], the equation-of-state model was programmed in relatively large subroutines having multiple purposes. This tends to introduce many maintenance problems. Therefore in SIMMER-III, all the EOS relationships are separated into individual function subprograms, each of which has a single function. In this appendix, the basic functions are described first. Then EOS functions are listed (in **Table C-1**), followed by the tables of reference EOS parameters for UO₂, mixed-oxide fuel, steel, sodium and fission gas (in **Tables C-2** through **C-6**, respectively). The parameters used in the FFEOS model are also shown in **Tables C-7** through **C-9**, for mixed-oxide fuel, steel and sodium, respectively.

1. EOS functions for solid properties

The EOS relationships are given for the structure components and solid particles in the liquid fields. Structure components, such as can wall, cladding, pin fuel and crust fuel, are assumed to be incompressible with polynomial fits for temperature, T_{Sm} , and specific volume, v_{Sm} , as a function of specific internal energy, e_{Sm} . The function for the structure temperature is given by

$$T_{Sm} = T_{Sol,M} [1 - a_{S1,M}(1 - u_{Sm}) - a_{S2,M}(1 - u_{Sm})^2 - a_{S3,M}(1 - u_{Sm})^3],$$

$$e_{Sm} < e_{Sol,M}, \text{ and} \tag{C-1a}$$

$$T_{Sm} = T_{Sol,M} + \frac{T_{Liq,M} - T_{Sol,M}}{h_{f,M}} (e_{Sm} - e_{Sol,M}),$$

$$e_{Sol,M} \leq e_{Sm} < e_{Liq,M}, \tag{C-1b}$$

where $a_{S1,M}$, $a_{S2,M}$ and $a_{S3,M}$ are the fitting constants, $u_{Sm} = \frac{e_{Sm}}{e_{Sol,M}}$ and $h_{f,M} = e_{Liq,M} - e_{Sol,M}$.

For the structure specific volume,

$$v_{Sm} = v_{Sol,M} [1 + b_{S1,M}(1 - u_{Sm}) + b_{S2,M}(1 - u_{Sm})^2 + b_{S3,M}(1 - u_{Sm})^3],$$

$$e_{Sm} < e_{Sol,M}, \text{ and} \tag{C-2a}$$

$$u_{Sm} = u_{Sol,M} + \frac{u_{Liq,M} - u_{Sol,M}}{h_{f,M}} (e_{Sm} - e_{Sol,M}),$$

$$e_{Sol,M} \leq e_{Sm} < e_{Liq,M}, \quad (C-2b)$$

where $b_{S1,M}$, $b_{S2,M}$ and $b_{S3,M}$ are the fitting constants. Equations (C-1b) and (C-2b) are used for extrapolation to the metastable state above the liquidus temperature.

For particles, such as fuel, steel and control, compression resulting from higher cell pressure, P , is assumed such that they can be treated similar to liquid, but otherwise obey structure functional relationships. The expressions for the particle temperature, T_{Lm} , and specific volume, v_{Lm} , are

$$T_{Lm} = T_{Lm}^+ + \left(\frac{\partial T_{Lm}}{\partial p} \right)_M^{\circ} p, \text{ and} \quad (C-3)$$

$$v_{Lm} = v_{Lm}^+ + \left(\frac{\partial v_{Lm}}{\partial p} \right)_M^{\circ} p, \quad (C-4)$$

where a subscript Lm applies to particles this case. The terms with a “+” superscript in Eqs. (C-3) and (C-4) lack pressure dependence and apply to the sublimation curve of a solid state. The actual sublimation pressure is considered to be low enough to be ignored. The terms, T_{Lm}^+ and v_{Lm}^+ , have the same energy-dependent curves as those for structure. The pressure derivatives, $\left(\frac{\partial T_{Lm}}{\partial p} \right)_M^{\circ}$ and $\left(\frac{\partial v_{Lm}}{\partial p} \right)_M^{\circ}$, are assumed to be constant independent of specific internal energy.

2. EOS functions for vapor properties

2.1. Vapor-pressure curve

The saturated liquid vapor pressure, p_{Lm}^+ , is defined as a function of liquid temperature, T_{Lm}^+ :

$$p_{Lm}^+ = \exp \left[b_{L1,M} + b_{L2,M} T_{Lm}^+ + \frac{b_{L3,M}}{T_{Lm}^+} + b_{L4,M} \ln \left(\frac{T_{Lm}^+}{T_{Cr,M}} \right) \right]. \quad (C-5)$$

The constants, $b_{L1,M}$, $b_{L2,M}$, $b_{L3,M}$ and $b_{L4,M}$ in Eq. (C-5) can be fit or taken directly from

the available data. The inverted saturated-vapor pressure curve is also used to calculate the saturation temperature, $T_{\text{Sat,Gm}}$, as a function of vapor pressure, p_{Gm} . The expression is

$$T_{\text{Sat,Gm}} = \frac{1}{a_{\text{Sat1,M}} + a_{\text{Sat2,M}} \ln p_{\text{Gm}} + a_{\text{Sat3,M}} (\ln p_{\text{Gm}})^2 + a_{\text{Sat4,M}} (\ln p_{\text{Gm}})^3}, \quad (\text{C-6})$$

where $a_{\text{Sat1,Gm}}$, $a_{\text{Sat2,Gm}}$, $a_{\text{Sat3,Gm}}$ and $a_{\text{Sat4,Gm}}$ are the fitting constants.

2.2. Modified Redlich-Kwong equations

A modified Redlich-Kwong (MRK) equation [3] is used for the vapor phase. The function form of the MRK equation is

$$p_{\text{Gm}} = \frac{R_{\text{M}} T_{\text{G}}}{v_{\text{Gm}} - a_{\text{G1,M}}} - \frac{a(T_{\text{G}})}{v_{\text{Gm}} (v_{\text{Gm}} + a_{\text{G3,M}})}, \quad (\text{C-7})$$

where

$$a(T_{\text{G}}) = a_{\text{G2,M}} \left(\frac{T_{\text{G}}}{T_{\text{Cr,M}}} \right)^{a_{\text{G4,M}}}, \quad T_{\text{G}} < T_{\text{Cr,M}}, \text{ and} \quad (\text{C-8a})$$

$$a(T_{\text{G}}) = a_{\text{G2,M}} \left[1 + a_{\text{G4,M}} \left(\frac{T_{\text{G}}}{T_{\text{Cr,M}}} - 1 \right) \right], \quad T_{\text{G}} \geq T_{\text{Cr,M}}, \quad (\text{C-8b})$$

and $a_{\text{G1,M}}$, $a_{\text{G2,M}}$, $a_{\text{G3,M}}$ are the EOS parameters.

The MRK equation is practically simple similar to the well-known van der Waals equation, but it can be made reasonably accurate especially at high temperatures and reproduces the evaluated oxide fuel vapor data rather well [3]. It was found, however, that the MRK equation poorly reproduces the evaluated data of the internal energy and the heat capacity of sodium vapor. To solve this problem, it was proposed to extend the MRK equation to a reacting system [4], which describe the dimerization of sodium vapor, and thereby satisfactory agreement was obtained. The proposed function form is

$$p_{\text{Gm}} = \frac{R_{\text{M}} T_{\text{G}}}{(1 + y_{\text{B,Gm}})(v_{\text{Gm}} - a_{\text{G1,M}})} - \frac{a(T_{\text{G}})}{v_{\text{Gm}} (v_{\text{Gm}} + a_{\text{G3,M}})}. \quad (\text{C-9})$$

In Eq. (C-9), $y_{\text{B,Gm}}$ is the dimer fraction expressed by

$$y_{\text{B,Gm}} = \frac{1 + 2x_{\text{Gm}} - \sqrt{1 + 8x_{\text{Gm}}}}{2(x_{\text{Gm}} - 1)}, \quad (\text{C-10})$$

where

$$x_{Gm} = \frac{k_{2,Gm} R_M T_G}{v_{Gm} - a_{G1,M}}, \quad (C-11)$$

and $k_{2,Gm}$ is the equilibrium constant given by

$$k_{2,Gm} = \exp\left(d_{G1,M} + \frac{d_{G2,M}}{T_G}\right), \quad (C-12)$$

where $d_{G1,M}$ and $d_{G2,M}$ are the fitting constants.

The location where $\left(\frac{\partial p_{Gm}}{\partial v_{Gm}}\right)_{T_G}$ changes from negative to positive is called the limit of intrinsic stability or the spinodal limit [5]. The spinodal curve is the locus of spinodal limit points in the vapor dome and satisfies the following condition:

$$\left(\frac{\partial p_{Gm}}{\partial v_{Gm}}\right)_{T_G} = 0. \quad (C-13)$$

Here, the vapor specific volume on the spinodal curve, or spinodal volume, $v_{Spn,Gm}$, is defined as a function of vapor temperature. The proposed function form is

$$v_{Spn,Gm} = v_{Cr,M} \left[1 + f_{G1,M}(1 - \eta_{G1,M})^{1/3} + f_{G2,M}(1 - \eta_{G2,M}) + f_{G3,M}(1 - \eta_{G3,M})^2 + f_{G4,M}(1 - \eta_{G4,M})^5 \right], \quad (C-14)$$

where $f_{G1,M}$, $f_{G2,M}$, $f_{G3,M}$ and $f_{G4,M}$ are the fitting constants and $\eta_{Gm} = \frac{T_G}{T_{Cr,M}}$.

The equation for the specific internal energy of vapor, e_{Gm} , is derived from the MRK equation for pressure to satisfy the following thermodynamic relation:

$$\left(\frac{\partial e_{Gm}}{\partial v_{Gm}}\right)_{T_G} = T_G \left(\frac{\partial p_{Gm}}{\partial T_G}\right)_{v_{Gm}} - p_{Gm}. \quad (C-15)$$

This gives

$$e_{Gm} = e_{Gm}^+ + \frac{a(T_G) - T_G \frac{da}{dT_G}}{a_{G3,M}} \ln \left(\frac{1 + \frac{a_{G3,M}}{v_{Gm}^+}}{1 + \frac{a_{G3,M}}{v_{Gm}}} \right), \quad (C-16)$$

where e_{Gm}^+ and v_{Gm}^+ are reference values. The specific internal energy of vapor mixture is given by a mass-weighted average of the vapor material internal energies as

$$e_G = \frac{\sum_m \rho_{Gm} e_{Gm}}{\sum_m \rho_{Gm}}. \quad (C-17)$$

Using the specific volume and specific internal energy of infinitely dilute vapor as the reference values, the specific internal energy of vapor is given as a function of T_G and v_{Gm} :

$$e_{Gm} = c_{vG,M}(T_G - T_{Liq,M}) + e_{LiqG,M}^D - \frac{a_{G2,M}(1 - a_{G4,M})\psi}{a_{G3,M}} \ln\left(1 + \frac{a_{G3,M}}{v_{Gm}}\right), \quad (C-18)$$

with

$$\psi = \left(\frac{T_G}{T_{Cr,M}}\right)^{a_{G4,M}}, \quad T_G < T_{Cr,M}, \text{ and} \quad (C-19a)$$

$$\psi = 1, \quad T_G \geq T_{Cr,M}. \quad (C-19b)$$

where $e_{LiqG,M}^D$ is the specific internal energy of infinitely dilute vapor at the liquidus temperature and $c_{vG,M}$ is the heat capacity at constant volume. For a reacting system, we apply the following equation derived from Eqs. (C-9) and (C-15):

$$e_{Gm} = c_{vG,M}(T_G - T_{Liq,M}) + e_{LiqG,M}^D + \frac{y_{B,Gm} R_M T_G}{1 + y_{B,Gm}} \left(1 - \frac{d_{G2,M}}{T_G}\right) - \frac{a_{G2,M}(1 - a_{G4,M})\psi}{a_{G3,M}} \ln\left(1 + \frac{a_{G3,M}}{v_{Gm}}\right). \quad (C-20)$$

The vapor heat capacity at constant volume, $c_{vG,M}$, is calculated from Eq. (C-18):

$$c_{v,Gm} = \left(\frac{\partial e_{Gm}}{\partial T_G}\right)_{v_{Gm}} = c_{vG,M} - \frac{a_{G2,M}(1 - a_{G4,M})\psi^*}{a_{G3,M}} \ln\left(1 + \frac{a_{G3,M}}{v_{Gm}}\right), \quad (C-21)$$

where

$$\psi^* = \frac{a_{G4,M}}{T_{Cr,M}} \left(\frac{T_G}{T_{Cr,M}}\right)^{a_{G4,M}-1}, \quad T_G < T_{Cr,M}, \text{ and} \quad (C-22a)$$

$$\psi^* = 0, \quad T_G \geq T_{\text{Cr},M}. \quad (\text{C-22b})$$

For a reacting system, we obtain the following equation from Eq. (C-20):

$$c_{v,Gm} = c_{vG,M} - \frac{a_{G2,M}(1-a_{G4,M})\psi^*}{a_{G3,M}} \ln \left(1 + \frac{a_{G3,M}}{v_{Gm}} \right) + \frac{y_{B,Gm} R_M}{1+y_{B,Gm}} \left\{ 1 + \frac{1-y_{B,Gm}}{1+3y_{B,Gm}} \left(1 - \frac{d_{G2,M}}{T_G} \right)^2 \right\}. \quad (\text{C-23})$$

2. 3. Saturated vapor

For the specific volume of saturated vapor, or vaporization volume, $v_{\text{vap},Gm}$, we select the following polynomial functional form originally used for water [6]:

$$v_{\text{vap},Gm} = v_{\text{Cr},M} \exp [b_{G1,M}(1-\eta_{\text{Sat},Gm})^{1/3} + b_{G2,M}(1-\eta_{\text{Sat},Gm})^{2/3} + b_{G3,M}(1-\eta_{\text{Sat},Gm})^{4/3} + b_{G4,M}(1-\eta_{\text{Sat},Gm})^3 + b_{G5,M}(1-\eta_{\text{Sat},Gm})^{37/6} + b_{G6,M}(1-\eta_{\text{Sat},Gm})^{71/6}],$$

$$T_{\text{Sat},Gm} \leq T_{\text{Cr},M}, \quad (\text{C-24})$$

where $b_{G1,M}$, $b_{G2,M}$, $b_{G3,M}$, $b_{G4,M}$, $b_{G5,M}$ and $b_{G6,M}$ are the fitting constants and $\eta_{\text{Sat},Gm} = \frac{T_{\text{Sat},Gm}}{T_{\text{Cr},M}}$.

The specific internal energy of saturated vapor, or the vaporization energy, $e_{\text{vap},Gm}$, is defined by the function:

$$e_{\text{vap},Gm} = e_{\text{Liq},Gm} + c_{G1,M}(T_{\text{Sat},Gm} - T_{\text{Liq},M}) + c_{G2,M}(T_{\text{Sat},Gm} - T_{\text{Liq},M})^2 + c_{G3,M}(T_{\text{Sat},Gm} - T_{\text{Liq},M})^3,$$

$$T_{\text{Liq},M} < T_{\text{Sat},Gm} \leq c_{G4,M} T_{\text{Cr},M}, \text{ and} \quad (\text{C-25a})$$

$$e_{\text{vap},Gm} = e_{\text{Cr},M} [1 + c_{G5,M} (T_{\text{Cr},M} - T_{\text{Sat},Gm})^{1/2} + c_{G6,M} (T_{\text{Cr},M} - T_{\text{Sat},Gm})^2],$$

$$c_{G4,M} T_{\text{Cr},M} < T_{\text{Sat},Gm} \leq T_{\text{Cr},M}, \quad (\text{C-25b})$$

where $c_{G1,M}$, $c_{G2,M}$, $c_{G3,M}$, $c_{G4,M}$, $c_{G5,M}$ and $c_{G6,M}$ are the fitting constants.

3. EOS functions for liquid properties

3.1. Saturated liquid

The function for the specific volume of saturated liquid, or condensate volume, $v_{\text{Con,Gm}}$, is given by

$$v_{\text{Con,Gm}} = v_{\text{Liq,M}} [1 + b_{\text{Sat1,M}}(T_{\text{Sat,Gm}} - T_{\text{Liq,M}}) + b_{\text{Sat2,M}}(T_{\text{Sat,Gm}} - T_{\text{Liq,M}})^2 + b_{\text{Sat3,M}}(T_{\text{Sat,Gm}} - T_{\text{Liq,M}})^3]^{-1},$$

$$T_{\text{Liq,M}} < T_{\text{Sat,Gm}} \leq b_{\text{Sat4,M}} T_{\text{Cr,M}}, \text{ and} \quad (\text{C-26a})$$

$$v_{\text{Con,Gm}} = v_{\text{Cr,M}} [1 + b_{\text{Sat5,M}}(T_{\text{Cr,M}} - T_{\text{Sat,Gm}})^{1/2} + b_{\text{Sat6,M}}(T_{\text{Cr,M}} - T_{\text{Sat,Gm}})^2]^{-1},$$

$$b_{\text{Sat4,M}} T_{\text{Cr,M}} < T_{\text{Liq,M}} \leq T_{\text{Cr,M}}, \quad (\text{C-26b})$$

where $b_{\text{Sat1,M}}$, $b_{\text{Sat2,M}}$, $b_{\text{Sat3,M}}$, $b_{\text{Sat4,M}}$, $b_{\text{Sat5,M}}$ and $b_{\text{Sat6,M}}$ are the fitting constants.

The expressions of the condensate energy, $e_{\text{Con,Gm}}$, defined as the specific internal energy of saturated liquid, are

$$e_{\text{Con,Gm}} = e_{\text{Liq,M}} + c_{\text{Sat1,M}}(T_{\text{Sat,Gm}} - T_{\text{Liq,M}}) + c_{\text{Sat2,M}}(T_{\text{Sat,Gm}} - T_{\text{Liq,M}})^2 + c_{\text{Sat3,M}}(T_{\text{Sat,Gm}} - T_{\text{Liq,M}})^3,$$

$$T_{\text{Liq,M}} < T_{\text{Sat,Gm}} \leq c_{\text{Sat4,M}} T_{\text{Cr,M}}, \text{ and} \quad (\text{C-27a})$$

$$e_{\text{Con,Gm}} = e_{\text{Cr,M}} [1 - c_{\text{Sat5,M}}(T_{\text{Cr,M}} - T_{\text{Sat,Gm}})^{1/2} - c_{\text{Sat6,M}}(T_{\text{Cr,M}} - T_{\text{Sat,Gm}})^2],$$

$$c_{\text{Sat4,M}} T_{\text{Cr,M}} < T_{\text{Sat,Gm}} \leq T_{\text{Cr,M}}, \quad (\text{C-27b})$$

where $c_{\text{Sat1,M}}$, $c_{\text{Sat2,M}}$, $c_{\text{Sat3,M}}$, $c_{\text{Sat4,M}}$, $c_{\text{Sat5,M}}$ and $c_{\text{Sat6,M}}$ are the fitting constants.

2.3.2. Compressed liquid

To assist in compressing each liquid to the cell pressure and to optimize the numerical algorithm for the pressure iteration, the independent EOS variables selected for the real liquid are pressure, p , and the component specific internal energy, e_{Lm} . We assume that temperature, T_{Lm} , and specific volume, v_{Lm} , can be defined by adding deviations from the saturation properties. The expressions for the liquid temperature and specific volume are

$$T_{\text{Lm}} = T_{\text{Lm}}^+ + \left(\frac{\partial T_{\text{Lm}}}{\partial p} \right)_{e_{\text{Lm}}} (p - p_{\text{Lm}}^+), \text{ and} \quad (\text{C-28})$$

$$v_{Lm} = v_{Lm}^+ + \left(\frac{\partial v_{Lm}}{\partial p} \right)_{e_{Lm}} (p - p_{Lm}^+), \quad (C-29)$$

where p_{Lm}^+ is the saturation pressure corresponding to the liquid temperature, T_{Lm}^+ , and is given by Eq. (C-5). For liquid specific volume a more general equation is used:

$$v_{Lm} = v_{Lm}^+ \left\{ 1 - \frac{1}{\beta_M v_{Lm}^+} \left(\frac{\partial v_{Lm}}{\partial p} \right)_{e_{Lm}} (p - p_{Lm}^+) \right\}^{-\beta_M}, \quad (C-30)$$

where β_M is an EOS parameter and $\beta_M = -1$ leads to Eq. (C-29).

The saturated liquid temperature, T_{Lm}^+ , and specific volume, v_{Lm}^+ , are defined as a function of specific internal energy, e_{Lm} . The function for the saturated liquid temperature is expressed by

$$T_{Lm}^+ = T_{Liq,M} [1 + a_{L1,M}(u_{Lm} - 1) + a_{L2,M}(u_{Lm} - 1)^2 + a_{L3,M}(u_{Lm} - 1)^3],$$

$$e_{Liq,M} < e_{Lm} \leq a_{L4,M} e_{Liq,M}, \text{ and} \quad (C-31a)$$

$$T_{Lm}^+ = T_{Cr,M} [1 - a_{L5,M}(1 - \xi_{Lm})^2 - a_{L6,M}(1 - \xi_{Lm})^3],$$

$$a_{L4,M} e_{Liq,M} < e_{Lm} \leq e_{Cr,M}, \quad (C-31b)$$

where $a_{L1,M}$, $a_{L2,M}$, $a_{L3,M}$, $a_{L4,M}$, $a_{L5,M}$ and $a_{L6,M}$ are the fitting constants, and

$$u_{Lm} = \frac{e_{Lm}}{e_{Liq,M}} \text{ and } \xi_{Lm} = \frac{e_{Lm}}{e_{Cr,M}}. \text{ For the liquid specific volume,}$$

$$v_{Lm}^+ = v_{Liq,M} [1 + d_{L1,M}(u_{Lm} - 1) + d_{L2,M}(u_{Lm} - 1)^2 + d_{L3,M}(u_{Lm} - 1)^3],$$

$$e_{Liq,M} < e_{Lm} \leq d_{L4,M} e_{Liq,M}, \text{ and} \quad (C-32a)$$

$$v_{Lm}^+ = v_{Cr,M} [1 + d_{L5,M}(1 - \xi_{Lm})^{1/2} + d_{L6,M}(1 - \xi_{Lm})^2],$$

$$d_{L4,M} e_{Liq,M} < e_{Lm} \leq e_{Cr,M}, \quad (C-32b)$$

where $d_{L1,M}$, $d_{L2,M}$, $d_{L3,M}$, $d_{L4,M}$, $d_{L5,M}$ and $d_{L6,M}$ are the fitting constants.

3.3. Pressure derivatives

The pressure derivative of liquid temperature, $\left(\frac{\partial T_{Lm}}{\partial p} \right)_{e_{Lm}}$, in Eq. (C-28) is expressed by

$$\left(\frac{\partial T_{Lm}}{\partial p}\right)_{e_{Lm}} = \max\left\{\left(\frac{\partial T_{Lm}}{\partial p}\right)_M^0, f(\xi_{Lm})\right\}, \quad e_{Lm} < e_{Cr,M}, \quad (C-33)$$

where

$$f(\xi_{Lm}) = \left(\frac{\partial T_{Lm}}{\partial p}\right)_{e_{Cr,M}}^0 \exp[c_{L1,M}(1-\xi_{Lm}) + c_{L2,M}(1-\xi_{Lm})^{3/2} + c_{L3,M}(1-\xi_{Lm})^2 + c_{L4,M}(1-\xi_{Lm})^3], \quad (C-34)$$

and $c_{L1,M}$, $c_{L2,M}$, $c_{L3,M}$ and $c_{L4,M}$ are the fitting constants. In Eq. (C-33), the constant lower limit, $\left(\frac{\partial T_{Lm}}{\partial p}\right)_M^0$, is used to be consistent with a pressure derivative for solid.

The pressure derivative of liquid specific volume, $\left(\frac{\partial v_{Lm}}{\partial p}\right)_{e_{Lm}}$, in Eq. (C-29) is expressed

by

$$\left(\frac{\partial v_{Lm}}{\partial p}\right)_{e_{Lm}} = \min\left\{\left(\frac{\partial v_{Lm}}{\partial p}\right)_M^0, \max[g(\xi_{Lm}), f_{L6,M}]\right\}, \quad e_{Lm} < e_{Cr,M}, \quad (C-35)$$

where

$$g(\xi_{Lm}) = f_{L1,M} \exp[f_{L2,M}(1-\xi_{Lm})^{-1/2} + f_{L3,M}(1-\xi_{Lm}) + f_{L4,M}(1-\xi_{Lm})^3 + f_{L5,M}(1-\xi_{Lm})^4], \quad (C-36)$$

and $f_{L1,M}$, $f_{L2,M}$, $f_{L3,M}$, $f_{L4,M}$ and $f_{L5,M}$ are the fitting constants. In Eq. (C-35), the constant higher limit, $\left(\frac{\partial v_{Lm}}{\partial p}\right)_M^0$, is also used to be consistent with the solid value.

Nomenclature

c_{Sat}	heat capacity along a saturation curve ($J\ kg^{-1}\ K^{-1}$)
c_p, c_v	heat capacities at constant pressure, constant volume ($J\ kg^{-1}\ K^{-1}$)
e	specific internal energy ($J\ kg^{-1}$)
h_f	heat of fusion ($J\ kg^{-1}$)
k_2	equilibrium constant (Pa^{-1})
p	pressure (Pa)
T	temperature (K)
y_B	dimer fraction

Greek letters

$\bar{\rho}$	macroscopic density (kg m^{-3}) specific volume ($\text{m}^3 \text{kg}^{-1}$)
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Subscripts

Con	saturated liquid
Crt	critical point
G	vapor mixture
Gm	material component m in vapor field
Liq	liquidus point
LiqG	vapor at liquidus point
Lm	energy component m in liquid field
M	material number
Sat	saturation
Sm	energy component m in structure field
Sol	solidus point
Vap	saturated vapor

Superscripts

D	dilute vapor
+	lack of pressure dependence

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Table C-1. List of EOS Functions.**Arguments**

M : Material number
 P : Pressure (Pa)
 E : Internal energy (J/kg)
 T : Temperature (K)
 V : Specific volume (m^3/kg)
 V1 : Specific volume of vapor material component 1 (m^3/kg)
 V2 : Specific volume of vapor material component 2 (m^3/kg)
 V3 : Specific volume of vapor material component 3 (m^3/kg)
 V4 : Specific volume of vapor material component 4 (m^3/kg)
 T : Temperature (K)
 EPF : Porosity of solid fuel

Functions*Solid*

XTSM (M,E) : Temperature of structure or sublimate particles
 XVSM (M,E,EPF) : Solid specific volume
 XTPM (M,E,P) : Particles temperature
 XVPM (M,E,P,EPF) : Specific volume of particles
 XTSMDE (M,E) : Derivative of solid temperature
 XESM (M,T) : Internal energy of structure or sublimate particles*

Liquid

XTLM (M,E,P) : Liquid temperature
 XTLMZ (M,E) : Saturated liquid temperature
 XTLMDE (M,E) : Derivative of saturated liquid temperature
 XDTDPE (M,E) : Derivative of liquid temperature with respect to pressure
 XDTDEP (M,E,P) : Derivative of liquid temperature with respect to energy
 XPLMZ (M,T) : Liquid vapor pressure
 XPLMDZ (M,T) : Derivative of liquid vapor pressure
 XVLM (M,E,P) : Liquid specific volume
 XVLMZ (M,E) : Specific volume of saturated liquid
 XVLMDE (M,E) : Derivative of specific volume of saturated liquid
 XDVPZ (M,E) : Derivative of liquid specific volume with respect to pressure along saturation curve
 XDVDPE (M,E,P) : Derivative of liquid specific volume with respect to pressure
 XELM (M,E) : Internal energy of saturated liquid*

Vapor

XPGM	(M,T,V)	: Vapor pressure
XPGMDR	(M,T,V)	: Derivative of vapor pressure with respect to density
XPGMDT	(M,T,V)	: Derivative of vapor pressure with respect to temperature
XEGM	(M,T,V)	: Vapor internal energy
XEGMDR	(M,T,V)	: Derivative of vapor internal energy with respect to density
XEGMDT	(M,T,V)	: Derivative of vapor internal energy with respect to temperature
XVSPN	(M,T)	: Spinodal volume of vapor**

Saturation properties

XTSAT	(M,P)	: Saturation temperature
XTSATD	(M,P)	: Derivative of saturation temperature
XVCON	(M,T)	: Condensate volume
XVCOND	(M,T)	: Derivative of condensate volume
XECON	(M,T)	: Condensate energy
XECOND	(M,T)	: Derivative of condensate energy
XVVAP	(M,T)	: Vaporization volume
XVVAPD	(M,T)	: Derivative of vaporization volume
XEVAP	(M,T)	: Vaporization energy
XEVAPD	(M,T)	: Derivative of vaporization energy

* The Newton-Raphson method is used to obtain the solution.

** Either Newton-Raphson method or analytical fit is used.

Table C-2. EOS parameters for UO₂.

(IFREE=0, IMRK=0)

ESOL = 1.12157E+06	TSOL = 3.12000E+03	VSOL = 1.04656E-04
ELIQ = 1.39871E+06	TLIQ = 3.12000E+03	VLIQ = 1.12867E-04
ECRIT= 4.99290E+06	TCRIT= 1.06000E+04	RHOC = 1.56000E+03
PCRT = 1.57873E+08	ELIQG= 3.04328E+06	ELQGD= 3.04329E+06
CVG = 3.01247E+02	RUG = 3.07945E+01	W = 2.70000E+02
PTS = 0.10000D+00		
AS1 = 4.44390E-01	AS2 = 4.89576E-01	AS3 = -2.83438E-02
BS1 = -1.44971E-01	BS2 = -7.36914E-03	BS3 = 2.60596E-02
AL1 = 8.81083E-01	AL2 = -2.04486E-02	AL3 = 1.86174E-02
AL4 = 3.47820E+00	AL5 = 2.95237E+01	AL6 = -1.69116E+02
BL1 = 2.17296E+01	BL2 = 4.42327E-04	BL3 = -7.99342E+04
BL4 = -8.88130E+00		
CL1 = -3.51500E+01	CL2 = 6.72600E+01	CL3 = -4.70436E+01
CL4 = 8.08263E+00		
DL1 = 3.93703E-01	DL2 = -1.81812E-01	DL3 = 1.74487E-01
DL4 = 2.89613E+00	DL5 = -1.54733E+00	DL6 = 2.07800E+00
FL1 = -3.61402E-12	FL2 = -4.22202E-02	FL3 = -1.68215E+01
FL4 = 3.17194E+01	FL5 = -2.92392E+01	FL6 = -1.42655E-11
DTDPS= 5.52486E-08	DVDPS=-5.46331E-16	DTDPC= 1.91288E-05
BETA = -1.00000D+00		
AG1 = 1.41301E-04	AG2 = 2.94299E+02	AG3 = 2.85846E-04
AG4 = 2.00000E-01		
BG1 = 3.90118E-01	BG2 = 2.64047E+00	BG3 = 1.79946E+00
BG4 = 9.17799E+00	BG5 = 2.31365E+01	BG6 = 6.07538E+01
CG1 = 2.97266E+02	CG2 = 2.35586E-03	CG3 = -8.26332E-07
CG4 = 9.69434E-01	CG5 = 4.22861E-04	CG6 = -8.11911E-08
DG1 = -----	DG2 = -----	
FG1 = 5.57168E-01	FG2 = 2.78675E+00	FG3 = 1.85168E+00
FG4 = 1.07188E+01		
ASAT1= 4.50854E-04	ASAT2=-1.57919E-05	ASAT3= 1.69876E-07
ASAT4=-1.76528E-08	PSMIN= 2.19149E-05	
BSAT1=-1.03384E-04	BSAT2=-1.48030E-10	BSAT3=-3.78342E-16
BSAT4= 8.01887E-01	BSAT5= 2.53025E-02	BSAT6= 7.62684E-08
CSAT1= 5.14152E+02	CSAT2= 5.84459E-04	CSAT3=-8.30648E-07
CSAT4= 9.81132E-01	CSAT5= 1.91882E-03	CSAT6= 2.59729E-08

Table C-3. EOS parameters for MOX.

(IFREE=0, IMRK=0)

ESOL = 1.05162E+06	TSOL = 3.00200E+03	VSOL = 1.00230E-04
ELIQ = 1.31829E+06	TLIQ = 3.04100E+03	VLIQ = 1.08814E-04
ECRIT= 4.99290E+06	TCRIT= 1.06000E+04	RHOC = 1.56000E+03
PCRT = 1.57873E+08	ELIQG= 2.98033E+06	ELQGD= 2.98034E+06
CVG = 3.06427E+02	RUG = 3.07945E+01	W = 2.70000E+02
PTS = 0.10000D+00		
AS1 = 4.68166E-01	AS2 = 5.24030E-01	AS3 = -9.59833E-02
BS1 = -6.48590E-03	BS2 = -1.62062E-01	BS3 = 7.27906E-02
AL1 = 8.41923E-01	AL2 = -1.69174E-02	AL3 = 1.47156E-02
AL4 = 3.68955E+00	AL5 = 2.89670E+01	AL6 = -1.66741E+02
BL1 = 2.17296E+01	BL2 = 4.42327E-04	BL3 = -7.99342E+04
BL4 = -8.88130E+00		
CL1 = -4.16525E+01	CL2 = 9.47848E+01	CL3 = -7.88238E+01
CL4 = 1.97832E+01		
DL1 = 3.72680E-01	DL2 = -1.67343E-01	DL3 = 1.44446E-01
DL4 = 3.06379E+00	DL5 = -1.55974E+00	DL6 = 2.09893E+00
FL1 = -1.32899E-12	FL2 = 1.90472E-01	FL3 = -1.42352E+01
FL4 = 2.15440E+01	FL5 = -1.93115E+01	FL6 = -1.42655E-11
DTDPS= 5.85547E-08	DVDPS=-5.46331E-16	DTDPC= 1.91288E-05
BETA = -1.00000D+00		
AG1 = 1.41301E-04	AG2 = 2.94299E+02	AG3 = 2.85846E-04
AG4 = 2.00000E-01		
BG1 = 3.90118E-01	BG2 = 2.64047E+00	BG3 = 1.79946E+00
BG4 = 9.17799E+00	BG5 = 2.31365E+01	BG6 = 6.07538E+01
CG1 = 3.02512E+02	CG2 = 2.41081E-03	CG3 = -8.14218E-07
CG4 = 9.69623E-01	CG5 = 4.17946E-04	CG6 = -8.32298E-08
DG1 = -----	DG2 = -----	
FG1 = 5.57168E-01	FG2 = 2.78675E+00	FG3 = 1.85168E+00
FG4 = 1.07188E+01		
ASAT1= 4.50854E-04	ASAT2=-1.57919E-05	ASAT3= 1.69876E-07
ASAT4=-1.76528E-08	PSMIN= 2.19149E-05	
BSAT1=-1.03373E-04	BSAT2=-1.47509E-10	BSAT3=-4.25199E-16
BSAT4= 9.43396E-01	BSAT5= 2.30701E-02	BSAT6= 1.25429E-07
CSAT1= 5.20115E+02	CSAT2= 4.38079E-04	CSAT3=-7.99968E-07
CSAT4= 9.81132E-01	CSAT5= 1.93566E-03	CSAT6= 2.74910E-08

Table C-4. EOS parameters for stainless steel.

(IFREE=0, IMRK=0)

ESOL = 9.12379E+05	TSOL = 1.71300E+03	VSOL = 1.36168E-04
ELIQ = 1.25158E+06	TLIQ = 1.75300E+03	VLIQ = 1.41420E-04
ECRIT= 8.20580E+06	TCRIT= 9.60000E+03	RHOC = 1.14300E+03
PCRT = 4.56760E+08	ELIQG= 7.73961E+06	ELQGD= 7.73961E+06
CVG = 2.22969E+02	RUG = 1.48646E+02	W = 5.59354E+01
PTS = 0.18000D+00		
AS1 = 8.56796E-01	AS2 = -3.28896E-01	AS3 = 2.92311E-01
BS1 = -9.08374E-02	BS2 = 4.23217E-02	BS3 = -1.96932E-02
AL1 = 1.02425E+00	AL2 = -6.82077E-02	AL3 = 6.60477E-03
AL4 = 6.00388E+00	AL5 = 5.95140E+00	AL6 = 0.00000E+00
BL1 = 2.37361E+01	BL2 = 1.54890E-04	BL3 = -5.07204E+04
BL4 = -3.30628E+00		
CL1 = -9.23249E+00	CL2 = -1.74176E+01	CL3 = 3.84477E+01
CL4 = -1.89791E+01		
DL1 = 1.81594E-01	DL2 = -6.22683E-03	DL3 = 8.98282E-03
DL4 = 5.17704E+00	DL5 = -1.62972E+00	DL6 = 2.71165E+00
FL1 = -2.58082E-013	FL2 = 1.01637E+00	FL3 = -1.55026E+01
FL4 = 4.54114E+01	FL5 = -4.07002E+01	FL6 = -1.01686E-12
DTDPS= 1.92381E-08	DVDPS=-6.58746E-16	DTDPC= 6.06817E-06
BETA = -1.00000D+00		
AG1 = 1.51243E-04	AG2 = 2.02244E+03	AG3 = 6.50753E-04
AG4 = 2.57346E-01		
BG1 = -1.19877E-01	BG2 = 4.83281E+00	BG3 = -1.04117E+00
BG4 = 1.28107E+01	BG5 = 9.77240E+00	BG6 = 6.14938E+01
CG1 = 2.15388E+02	CG2 = 9.04415E-03	CG3 = -2.83239E-06
CG4 = 8.33333E-01	CG5 = 2.19035E-03	CG6 = -8.43355E-09
DG1 = -----	DG2 = -----	
FG1 = 3.48245E-01	FG2 = 4.39524E+00	FG3 = -7.32274E-01
FG4 = 1.43431E+01		
ASAT1= 5.77921E-04	ASAT2=-2.08089E-05	ASAT3=-1.61242E-08
ASAT4=-6.56103E-09	PSMIN= 1.96268E-11	
BSAT1=-9.11919E-05	BSAT2= 0.00000E+00	BSAT3= 0.00000E+00
BSAT4= 8.33333E-01	BSAT5= 4.03621E-02	BSAT6= 1.86344E-08
CSAT1= 6.80662E+02	CSAT2= 3.91671E-02	CSAT3=-2.32314E-06
CSAT4= 8.33333E-01	CSAT5= 4.14974E-03	CSAT6= 1.79897E-08

Table C-5. EOS parameters for sodium.

(IFREE=0, IMRK=1)

ESOL = -----	TSOL = -----	VSOL = -----
ELIQ = 2.06717E+05	TLIQ = 3.71000E+02	VLIQ = 1.08029E-03
ECRIT= 4.17692E+06	TCRIT= 2.50370E+03	RHOC = 2.19000E+02
PCRT = 2.56406E+07	ELIQG= 4.57699E+06	ELQGD= 4.57844E+06
CVG = 4.60613E+02	RUG = 3.61661E+02	W = 2.29898E-02
PTS = 5.00000E-01		
AS1 = -----	AS2 = -----	AS3 = -----
BS1 = -----	BS2 = -----	BS3 = -----
AL1 = 5.76094E-01	AL2 = -2.33486E-02	AL3 = 4.72888E-04
AL4 = 1.99989E+01	AL5 = -1.08409E+02	AL6 = 8.96169E+03
BL1 = 2.21057E+01	BL2 = 0.00000E+00	BL3 = -1.26337E+04
BL4 = -4.67200E-01		
CL1 = -2.42195E+01	CL2 = 2.99496E+01	CL3 = -3.39662E+00
CL4 = -8.16499E+00		
DL1 = 6.27665E-02	DL2 = -2.21705E-03	DL3 = 2.27740E-04
DL4 = 1.70725E+01	DL5 = -1.26722E+00	DL6 = 2.59838E+00
FL1 = -3.09510E-12	FL2 = 5.59746E-01	FL3 = -4.64421E+00
FL4 = 4.33770E+00	FL5 = -3.36198E+00	FL6 = -1.46413E-10
DTDPS= 9.51892E-08	DVDPS=-1.85485E-13	DTDPC= 2.11232E-05
BETA = 1.50000D-01		
AG1 = 2.93447E-04	AG2 = 1.23634E+04	AG3 = 1.96134E-02
AG4 = 4.92937E-01		
BG1 = 2.42590E-01	BG2 = 7.33754E+00	BG3 = -3.20191E+00
BG4 = 1.88331E+01	BG5 = 3.94583E+00	BG6 = 7.19859E+01
CG1 = 3.35053E+02	CG2 = -4.36960E-01	CG3 = 1.83657E-04
CG4 = 6.98966E-01	CG5 = 6.74084E-03	CG6 = -1.09662E-07
DG1 = -2.14845E+01	DG2 = 9.21571E+03	
FG1 = 9.50847E-01	FG2 = 6.26498E+00	FG3 = 9.88924E+00
FG4 = 2.19575E+01		
ASAT1= 1.80128E-03	ASAT2=-8.05016E-05	ASAT3= 4.82697E-08
ASAT4=-8.53040E-09	PSMIN= 3.27460E-09	
BSAT1=-2.57567E-04	BSAT2= 3.02115E-08	BSAT3=-2.75445E-11
BSAT4= 9.18640E-01	BSAT5= 5.35439E-02	BSAT6= 4.88971E-08
CSAT1= 9.98522E+02	CSAT2= 1.14342E-01	CSAT3= 1.40119E-04
CSAT4= 9.98522E-01	CSAT5= 2.76460E-03	CSAT6= 1.18490E-05

Table C-6. EOS parameters for xenon.

TLIQ = 1.61250E+02 TCRIT= 2.89730E+02 ELQGD=-1.30152E+04
 CVG = 9.50710E+01 RUG = 6.33293E+01 W = 1.31290E+02

Table C-7. FFEOS parameters for MOX.

(IFREE=2, IMRK=0)

ELIQ = 1.31829E+06 TLIQ = 3.04100E+03 VLIQ = 1.08814E-04
 TCRIT= 1.06000E+04 RHOC = 1.56000E+03 CVG = 3.06427E+02
 W = 2.70000E+02

 BL1 = 2.17296E+01 BL2 = 4.42327E-04 BL3 = -7.99342E+04
 BL4 = -8.88130E+00

 BSAT1=-1.03373E-04 BSAT2=-1.47509E-10 BSAT3=-4.25199E-16
 TLBND= 1.00000E+04

 AG4 = 2.00000E-01

 BSL1 = 3.19439E-11 BSL2 = 2.05900E-01
 BETA = -1.00000E+00

Table C-8. FFEOS parameters for stainless steel.

(IFREE=1, IMRK=0)

ELIQ = 1.25158E+06 TLIQ = 1.75300E+03 VLIQ = 1.41420E-04
 TCRIT= 9.60000E+04 RHOC = 1.14300E+03 CVG = 2.22969E+02
 W = 5.59354E+01

 BL1 = 2.37361E+01 BL2 = 1.54890E-04 BL3 = -5.07204E+04
 BL4 = -3.30628E+00

 BSAT1=-9.11919E-05 BSAT2= 0.00000E+00 BSAT3= 0.00000E+00
 TLBND= 8.00000E+03

 BSL1 = 8.62126E-12 BSL2 = 2.48538E-01
 BETA = -1.00000E+00

Table C-9. FFEOS parameters for sodium.

(IFREE=1, IMRK=1)

ELIQ = 2.06717E+05 TLIQ = 3.71000E+02 VLIQ = 1.08029E-03
 TCRIT= 2.50370E+03 RHOC = 2.19000E+02 CVG = 4.60613E+02
 W = 2.29898E+01 PTS = 5.00000E-01

 BL1 = 2.21057E+01 BL2 = 0.00000E+00 BL3 = -1.26337E+04
 BL4 = -4.67200E-01

 BSAT1=-2.57567E-04 BSAT2= 3.02115E-08 BSAT3=-2.75445E-11
 TLBND= 2.30000E+03

 BSL1 = 1.71700E-10 BSL2 = 3.26820E+00
 BETA = 1.50000E-01

APPENDIX D

THERMOPHYSICAL-PROPERTY FUNCTIONS

Thermophysical properties (TPP) used in SIMMER-III include: thermal conductivity of solid, liquid and vapor materials; viscosity of liquid and vapor materials; surface tension and heat capacity of liquid materials; and vapor diffusion coefficient for binary system. The functional forms of each thermophysical properties are described in this appendix. Sets of parameters used to fit the thermophysical properties are specified by inputs in NAMELISTs /XEOS/ and /XTPP/. The TPP functions are listed in **Table D-1**, followed by the tables of reference TPP parameters for fuel, steel, sodium, control, fission gas, water and air in **Tables D-2~8**.

1. Solid thermal conductivity

The thermal conductivity is given for the structure components and solid particles in the liquid fields. The function for the structure thermal conductivity is expressed as a function of temperature:

$$\kappa_{Sm} = a_{KS1,M} + \frac{a_{KS2,M}}{T_{Sm}} + \frac{a_{KS3,M}}{T_{Sm}^2} + a_{KS4,M}T_{Sm} + a_{KS5,M}T_{Sm}^2, \quad (D-1)$$

where $a_{KS1,M}$, $a_{KS2,M}$, $a_{KS3,M}$, $a_{KS4,M}$, and $a_{KS5,M}$ are fitting constants. This function is applied over the whole solid temperature range. The same function as the structure is used for a solid particle component as well.

The thermal conductivity of solid fuel decreases with increasing porosity. Harding et al. [1] proposed that the following formula be used to correct for this porosity effect over a range of porosity of practical interest:

$$\kappa_{Sm}^p = \kappa_{Sm}(1 - \varepsilon_{Sm})^{2.5}, \quad (D-2)$$

where ε_{Sm} is the fractional porosity of solid fuel and κ_{Sm}^p is the corresponding thermal conductivity. Equation (D-2) is employed to take into account the porosity effect on the thermal conductivity of solid fuel.

2. Thermal conductivity and viscosity of liquid and vapor phases

2.1. Simple function model

The simple function model to calculate liquid properties uses a quadratic equation for the thermal conductivity, and the Andrade equation for the viscosity. The expression for the thermal conductivity is

$$\kappa_{Lm} = a_{KL1,M} + a_{KL2,M}T_{Lm} + a_{KL3,M}T_{Lm}^2, \quad (D-3)$$

where $a_{KL1,M}$, $a_{KL2,M}$, and $a_{KL3,M}$ are fitting constants. For the viscosity,

$$\mu_{Lm} = b_{ML1,M} \exp\left(\frac{b_{ML2,M}}{T_{Lm}}\right), \quad (D-4)$$

where $b_{ML1,M}$ and $b_{ML2,M}$ can be fit or taken directly from the available database. An upper limit of the liquid temperature range allowed in Eqs. (D-3) and (D-4) is specified by an input maximum liquid temperature, $T_{Lmax,M}$, which determines limit values of the properties.

If properties of a vapor component are known by experimental data or other reliable sources, simple functions can be used as a function of temperature. The formula for the thermal conductivity is taken from the empirical equation of fuel thermal conductivity [2], and a quadratic equation is used for the viscosity. The expression for the thermal conductivity is

$$\kappa_{Gm} = \exp\left(a_{KG1,M} + \frac{a_{KG2,M}}{T_G} + a_{KG3,M}T_G + a_{KG4,M}T_G^2 + a_{KG5,M}T_G^3\right), \quad (D-5)$$

where $a_{KG1,M}$, $a_{KG2,M}$, $a_{KG3,M}$, $a_{KG4,M}$, and $a_{KG5,M}$ are fitting constants. For the viscosity,

$$\mu_{Gm} = b_{MG1,M} + b_{MG2,M}T_G + b_{MG3,M}T_G^2, \quad (D-6)$$

where $b_{MG1,M}$, $b_{MG2,M}$, and $b_{MG3,M}$ are fitting constants. An upper limit of the vapor temperature range allowed in Eqs. (D-5) and (D-6) is specified by an input maximum vapor temperature, $T_{Gmax,M}$, which determines limit values of the properties.

2.2. Extended function model

The extended function model for the calculation of liquid and vapor properties uses formulas consistent in the vicinity of the critical point and treats dependence of vapor

properties on density and temperature [3]. The formulas give the correct behavior of the properties, that is, the increase of the vapor viscosity and thermal conductivity due to increased density near the critical point. For the liquid properties, the simple analytical functions are replaced near the critical point with an additional equation so as to represent an infinite slope and a value consistent with the vapor phase at the critical point. The proposed formula for the liquid thermal conductivity is

$$\kappa_{Lm} = a_{KL1,M} + a_{KL2,M}T_{Lm} + a_{KL3,M}T_{Lm}^2, \quad T_{Lm} \leq a_{SL4,M}T_{Cr,M}, \quad (D-7a)$$

$$\kappa_{Lm} = \kappa_{Cr,M} + a_{KL5,M}(T_{Cr,M} - T_{Lm})^{1/2} + a_{KL6,M}(T_{Cr,M} - T_{Lm})^2, \quad (D-7b)$$

$$a_{SL4,M}T_{Cr,M} < T_{Lm} \leq T_{Cr,M}, \text{ and}$$

$$\kappa_{Lm} = \kappa_{Cr,M}, \quad T_{Lm} > T_{Cr,M}, \quad (D-7c)$$

where $a_{KL1,M}$, $a_{KL2,M}$, $a_{KL3,M}$, $a_{KL4,M}$, $a_{KL5,M}$, and $a_{KL6,M}$ are fitting constants. For the liquid viscosity,

$$\mu_{Lm} = b_{ML1,M} \exp\left(\frac{b_{ML2,M}}{T_{Lm}}\right), \quad T_{Lm} \leq b_{ML3,M}T_{Cr,M}, \quad (D-8a)$$

$$\mu_{Lm} = \mu_{Cr,M} + b_{ML4,M}(T_{Cr,M} - T_{Lm})^{1/2} + b_{ML5,M}(T_{Cr,M} - T_{Lm})^2, \quad (D-8b)$$

$$b_{ML3,M}T_{Cr,M} < T_{Lm} \leq T_{Cr,M}, \text{ and}$$

$$\mu_{Lm} = \mu_{Cr,M}, \quad T_{Lm} > T_{Cr,M}, \quad (D-8c)$$

where $b_{ML1,M}$, $b_{ML2,M}$, $b_{ML3,M}$, $b_{ML4,M}$, and $b_{ML5,M}$ are fitting constants.

For the vapor phase, the properties are assumed to depend on the density and the temperature and are calculated by a simple power function up to the critical temperature and a constant value beyond it. The value above the critical temperature is made consistent with the liquid-side equations at the critical point. The formula for the vapor thermal conductivity is

$$\kappa_{Gm} = \kappa_{Gm}^D + [\kappa_{Cr,M} - \kappa_{Gm}^D(T_{Cr,M})] \left(\frac{T_G}{T_{Cr,M}}\right)^{n_{f,M}} \frac{\nu_{Cr,M}}{\nu_{Gm}}, \quad (D-9a)$$

$$T_G \leq T_{Cr,M}, \text{ and}$$

$$\kappa_{Gm} = \kappa_{Cr,M}, \quad T_G > T_{Cr,M}, \quad (D-9b)$$

where $n_{f,M}$ is a fitting constant, and κ_{Gm}^D refers to the thermal conductivity of the dilute gas and is expressed by a linear equation as a function of temperature:

$$\kappa_{Gm}^D = a_{KG1,M} + a_{KG2,M}T_G, \quad (D-10)$$

where $a_{KG1,M}$ and $a_{KG2,M}$ are fitting constants. For the viscosity,

$$\mu_{Gm} = \mu_{Gm}^D + [\mu_{Cr1,M} - \mu_{Gm}^D(T_{Cr1,M})] \left(\frac{T_G}{T_{Cr1,M}} \right)^{n_{f,M}} \frac{\nu_{Cr1,M}}{\nu_{Gm}}, \quad (D-11a)$$

$$T_G \leq T_{Cr1,M}, \text{ and}$$

$$\mu_{Gm} = \mu_{Cr1,M}, \quad T_G > T_{Cr1,M}, \quad (D-11b)$$

where μ_{Gm}^D refers to the viscosity of the dilute gas and is also expressed by a linear equation as a function of temperature:

$$\mu_{Gm}^D = b_{MG1,M} + b_{MG2,M}T_G, \quad (D-12)$$

where $b_{MG1,M}$ and $b_{MG2,M}$ are fitting constants.

2.3. Theoretical model

In the theoretical model, the vapor properties can be calculated using the Chapman-Enskog kinetic theory of gases and the Lennard-Jones model for the potential energy of interaction [4,5,6]. The viscosity is given by

$$\mu_{Gm} = 2.6993 \times 10^{-6} \frac{\sqrt{W_M T_G}}{\sigma_M^2 \Omega_{k,m}}, \quad (D-13)$$

where σ_M is the Lennard-Jones collision diameter in angstrom units and the parameter, $\Omega_{k,m}$, is called collision integral as a function of the vapor temperature. An empirical equation for $\Omega_{k,m}$ was proposed by Neufeld et al. [7]:

$$\Omega_{k,m} = [A(T^*)^{-B}] + C[\exp(-DT^*)] + E[\exp(-FT^*)], \quad (D-14)$$

where $T^* = k_B T_G / \varepsilon_M$, $A = 1.16145$, $B = 0.14874$, $C = 0.52487$, $D = 0.77320$, $E = 2.16178$, and $F = 2.43787$, and k_B is Boltzmann's constant. Equation (D-14) is applicable from $0.3 \leq T^* \leq 100$ with an average deviation of only 0.064 %. In SIMMER-III, the Lennard-Jones parameters, σ_M and ε_M / k_B , are treated as input constants of material M.

For monatomic gases, the thermal conductivity is given by

$$\kappa_{Gm} = \frac{5}{2} c_{v,Gm} \mu_{Gm}, \quad (D-15)$$

where $c_{v,Gm}$, is the vapor heat capacity at constant volume, and is calculated by the EOS function. For polyatomic gases, with the use of a modified Eucken correction, the thermal conductivity is given by

$$\kappa_{Gm} = (1.32 c_{v,Gm} + 1.77 R_m) \mu_{Gm}. \quad (D-16)$$

where R_m is the gas constant.

2.4. Vapor mixture properties

To calculate the exchange functions involving the vapor field, the average thermal conductivity and viscosity of the vapor mixture are required. Chawla et al. [4] used the following semi-empirical formulas of Wilke [8] for the properties of a vapor mixture:

$$\mu_G = \sum_{i=1}^{MCGM1} \frac{x_i \mu_{Gi}}{\sum_{j=1}^{MCGM1} x_j \phi_{ij}}, \text{ and} \quad (D-17)$$

$$\kappa_G = \sum_{i=1}^{MCGM1} \frac{x_i \kappa_{Gi}}{\sum_{j=1}^{MCGM1} x_j \phi_{ij}}, \quad (D-18)$$

where MCGM1 is the number of vapor components in the mixture,

$$\phi_{ij} = \frac{\left[1 + \left(\frac{\mu_{Gi}}{\mu_{Gj}} \right)^{1/2} \left(\frac{W_{M(Gj)}}{W_{M(Gi)}} \right)^{1/4} \right]}{2\sqrt{2} \left(1 + \frac{W_{M(Gj)}}{W_{M(Gi)}} \right)^{1/2}}, \quad (D-19)$$

x_i is the mole fraction of a component i in the mixture, and is related to the specific volume, v_{Gi} , through the relation

$$x_i = \frac{\frac{1}{v_{Gi} W_{M(Gi)}}}{\sum_{j=1}^{MCGM1} \frac{1}{v_{Gj} W_{M(Gj)}}}. \quad (D-20)$$

3. Binary diffusion coefficient

The diffusion coefficient for a binary system is calculated from the Chapman-Enskog theory assuming the potential between the molecules is represented by the Lennard-Jones type [6]. The binary diffusion coefficient for species i and j is expressed as

$$D_{ij} = \frac{3}{16} \frac{\sqrt{4\pi k_B \frac{1}{2} \left(\frac{1}{W_{M(Gi)}} + \frac{1}{W_{M(Gj)}} \right)}}{n\pi\sigma_{ij}^2 \Omega_D} f_D, \quad (D-21)$$

where n is the number density of molecules in the mixture, σ_{ij} is the Lennard-Jones collision diameter for diffusion in angstrom units, f_D is a correction factor close to unity, and Ω_D is the collision integral for diffusion as a function of the vapor temperature. An empirical equation for Ω_D was proposed by Neufeld et al. [7]:

$$\Omega_D = [A(T^*)^{-B}] + C[\exp(-DT^*)] + E[\exp(-FT^*)] + G[\exp(-HT^*)], \quad (D-22)$$

where $T^* = k_B T_G / \varepsilon_{ij}$, $A = 1.06036$, $B = 0.15610$, $C = 0.19300$, $D = 0.47635$, $E = 1.03587$, $F = 1.52996$, $G = 1.76474$, and $H = 3.89411$. The values of ε_{ij} and σ_{ij} are obtained by combining the Lennard-Jones parameters of species i and j empirically:

$$\sigma_{ij} = \frac{1}{2}(\sigma_{M(Gi)} + \sigma_{M(Gj)}), \text{ and} \quad (D-23)$$

$$\varepsilon_{ij} = (\varepsilon_{M(Gi)}\varepsilon_{M(Gj)})^{1/2}. \quad (D-24)$$

We use the following simplified expression of Eq. (D-21) assuming that f_D is chosen as unity and n is expressed by the ideal gas law:

$$D_{ij} = 2.66 \times 10^{-2} \frac{T_G^{3/2} \sqrt{\frac{1}{2} \left(\frac{1}{W_{M(Gi)}} + \frac{1}{W_{M(Gj)}} \right)}}{(P_{Gi} + P_{Gj})\sigma_{ij}^2 \Omega_D}. \quad (D-25)$$

The diffusion coefficient in multicomponent gas systems is simply defined by an effective binary diffusivity D_{im} for the diffusion of i in a mixture [5]. We use the following formula for D_{im} expressed as the effective diffusion coefficient of i with respect to a multicomponent mixture of stagnant gases [8]:

$$D_{im} = (1 - x_i) \left(\sum_{\substack{j=1 \\ j \neq i}}^n \frac{x_j}{D_{ij}} \right)^{-1}. \quad (\text{D-26})$$

4. Specific heat at constant pressure

The liquid heat capacity at constant pressure can be evaluated using EOS functions based on thermodynamic relationships. However, it was found that this poorly reproduces the sodium heat capacity in the temperature range where the experimental data are well developed. This is due to simplification assumed in the modified Redlich-Kwong (MRK) equation extended to a reacting system by Morita and Fischer (1998), although this equation provides an improved description of thermodynamic states of sodium vapor, which cannot be obtained by the MRK equation for a single component. The liquid heat capacity at constant pressure is used to calculate Prandtl number in Nusselt number correlations and hence it is not necessary for a TPP function to consistently satisfy thermodynamic relationships among state variables. We use the following polynomial function form to fit liquid heat capacity data:

$$c_{p,Lm} = f(\eta_{Lm})^{-1}, \quad (\text{D-27})$$

where

$$f(\eta_{Lm}) = d_{CL1,M}(1 - \eta_{Lm}) + d_{CL2,M}(1 - \eta_{Lm})^{3/2} + d_{CL3,M}(1 - \eta_{Lm})^2 + d_{CL4,M}(1 - \eta_{Lm})^3 + d_{CL5,M}(1 - \eta_{Lm})^4 + d_{CL6,M}(1 - \eta_{Lm})^5, \quad (\text{D-28})$$

and $\eta_{Lm} = \frac{T_{Lm}}{T_{Cr,M}}$. An upper limit of liquid heat capacity is specified by an input parameter

$c_{pLmax, M}$.

The vapor heat capacity at constant pressure is evaluated using the thermodynamic relationship:

$$c_{p,Gm} = c_{v,Gm} - \frac{T_G \left(\frac{\partial p_{Gm}}{\partial T_G} \right)^2}{\left(\frac{\partial p_{Gm}}{\partial v_{Gm}} \right)_{T_G} v_{Gm}}. \quad (\text{D-29})$$

An upper limit of vapor heat capacity is specified by an input parameter $c_{pGmax, M}$. The

values of $\left(\frac{\hat{a}_{Gm}}{\partial T_G}\right)_{v_{Gm}}$, $\left(\frac{\hat{\phi}_{Gm}}{\partial T_G}\right)_{v_{Gm}}$, and $\left(\frac{\hat{\phi}_{Gm}}{\partial v_{Gm}}\right)_{T_G}$ are obtained from the EOS functions.

The heat capacity of the vapor mixture is defined by the derivative of the specific internal energy of the vapor mixture with respect to the vapor temperature:

$$c_{p,G} = \frac{\sum_{m=1}^{MCGM1} v_{Gm} c_{p,Gm}}{\sum_{m=1}^{MCGM1} v_{Gm}}. \quad (D-30)$$

5. Surface tension

Since the interface between liquid and gas phase disappears at the critical temperature, the surface tension of liquid is reduced to zero at the critical temperature and decreases with increasing temperature. The general form of the surface tension is given by the van der Waals equation:

$$\sigma_{Lm} = c_{SL1,M} \left(1 - \frac{T_{Lm}}{T_{Cr,M}}\right)^{c_{SL2,M}}, \quad (D-31)$$

where $c_{SL1,M}$ and $c_{SL2,M}$ are fitting constants. The minimum value of the surface tension can be specified by an input parameter $c_{SL3,M}$ to avoid numerical difficulties. Equation (D-31) is fit to the data of surface tension when in contact with a third gas or vapor phase. The surface tension of between two immiscible liquid phases Lm and Lm' is calculated by

$$\sigma_{Lm,Lm'} = \sigma_{Lm} + \sigma_{Lm'} - 2(\sigma_{Lm}\sigma_{Lm'})^{1/2}. \quad (D-32)$$

Although this relation is strictly appropriate to nonpolar materials, Eq. (D-32) is usually a good approximation for the case where either Lm and Lm' is nonpolar [9].

6. Mechanical and adiabatic properties

The coefficients of volumetric thermal expansion, $\alpha_{p,Lm}$, and of isothermal compressibility, $\beta_{T,Lm}$, are called the mechanical properties of a liquid. They are defined as follows:

$$\alpha_{p,Lm} = \frac{1}{v_{Lm}} \left(\frac{\partial v_{Lm}}{\partial T_{Lm}}\right)_p, \text{ and} \quad (D-33)$$

$$\beta_{T,Lm} = -\frac{1}{\nu_{Lm}} \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{T_{Lm}}. \quad (D-34)$$

Using known thermodynamic relationships, we obtain the following equations:

$$\alpha_{p,Lm} = \frac{1}{\nu_{Lm} T_{Lm}} \left[c_{p,Lm} \left(\frac{\partial T_{Lm}}{\partial p} \right)_{e_{Lm}} - p \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \right], \text{ and} \quad (D-35)$$

$$\beta_{T,Lm} = \frac{1}{\nu_{Lm}} \left\{ \frac{1}{T_{Lm}} \left(\frac{\partial T_{Lm}}{\partial p} \right)_{e_{Lm}} \left[c_{p,Lm} \left(\frac{\partial T_{Lm}}{\partial p} \right)_{e_{Lm}} - p \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \right] - \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \right\}. \quad (D-36)$$

The adiabatic properties of a liquid, that is, the adiabatic compressibility, $\beta_{S,Lm}$, and the speed of sound, $\nu_{S,Lm}$, are defined by the following equations:

$$\beta_{S,Lm} = -\frac{1}{\nu_{Lm}} \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{S_{Lm}}, \quad (D-37)$$

$$\beta_{S,Lm} = \frac{\nu_{Lm}}{\nu_{S,Lm}^2}, \quad (D-38)$$

Using known thermodynamic relationships, we obtain the following equations:

$$\beta_{S,Lm} = \frac{1}{\nu_{Lm}} \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \left\{ \frac{p}{T_{Lm}} \left[\left(\frac{\partial T_{Lm}}{\partial p} \right)_{e_{Lm}} - \frac{p}{c_{p,Lm}} \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \right] - 1 \right\}, \text{ and} \quad (D-39)$$

$$\nu_{S,Lm} = \nu_{Lm} \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \left\{ \frac{p}{T_{Lm}} \left[\left(\frac{\partial T_{Lm}}{\partial p} \right)_{e_{Lm}} - \frac{p}{c_{p,Lm}} \left(\frac{\partial \nu_{Lm}}{\partial p} \right)_{e_{Lm}} \right] - 1 \right\}^{-1/2}. \quad (D-40)$$

For these liquid properties along the saturation curve, Eqs. (D-35), (D-36), (D-39), and (D-40) can be calculated using the EOS and TPP functions.

For vapor phase, the volumetric thermal expansion coefficient $\alpha_{p,Gm}$, the isothermal compressibility $\beta_{T,Gm}$, and the adiabatic compressibility $\beta_{S,Gm}$ are expressed by

$$\alpha_{p,Gm} = -\frac{1}{\nu_{Gm}} \frac{\left(\frac{\partial p_{Gm}}{\partial T_G} \right) p}{\left(\frac{\partial p_{Gm}}{\partial \nu_{Gm}} \right)_{T_G}}, \quad (D-41)$$

$$\beta_{T,Gm} = -\frac{1}{\nu_{Gm}} \left(\frac{\partial p_{Gm}}{\partial \nu_{Gm}} \right)_{T_G}^{-1}, \text{ and} \quad (\text{D-42})$$

$$\beta_{S,Gm} = \beta_{T,Gm} \frac{c_{v,Gm}}{c_{p,Gm}}. \quad (\text{D-43})$$

These are also calculated using the EOS functions with the MRK equations for vapor phase.

7. Code options and TPP functions

The analytic TPP model used for the calculation of liquid and vapor properties for a material with the material number M is controlled by the input option, KPOPT(N, M) for thermal conductivities and MUOPT(N, M) for viscosities, in the NAMELIST class, XTPP. Here N refers to the sub-material number. If KPOPT(N, M) = 1 or MUOPT(N, M) = 1, the properties of a material M with the sub-material number N are calculated using the simple analytical functions. If KPOPT(N, M) = 2 or MUOPT(N, M) = 2, the properties are calculated using the extended function model. Otherwise, the liquid properties are calculated using the simple function model alone and the vapor properties are theoretically evaluated. Sets of parameters used to calculate the thermophysical properties are specified by inputs in the NAMELIST classes, XTPP and XEOS. The TPP functions prepared for SIMMER-III are listed in **Table D-1**. A complete set of parameters in the proposed TPP functions is presented in **Tables D-2~5** for the basic reactor-core materials: uranium dioxide, mixed-oxide fuel, stainless steel, and sodium.

Nomenclature

c_p, c_v	heat capacities at constant pressure, constant volume ($\text{J kg}^{-1} \text{K}^{-1}$)
D_{ij}	binary diffusion coefficient for species i and j ($\text{m}^2 \text{s}^{-1}$)
D_{im}	effective binary diffusivity for the diffusion of i in a mixture ($\text{m}^2 \text{s}^{-1}$)
e	specific internal energy (J kg^{-1})
f_D	correction factor close to unity in Eq. (D-21)
k_B	Boltzmann's constant (J K^{-1})
N	Avogadro's number
n	number density of molecules in a mixture
p	pressure (Pa)
R_m	gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
T	temperature (K)
W	molecular weight (kg mol^{-1})
x_i	mole fraction of a component i in the mixture

Greek letters

α_p	volumetric thermal expansion coefficient (K^{-1})
β_S	adiabatic compressibility (Pa^{-1})
β_T	isothermal compressibility (Pa^{-1})
ϵ_{ij}	maximum attractive energy between two molecules (J)
ϵ_M	fractional porosity of solid fuel
	thermal conductivity ($W m^{-1} K^{-1}$)
μ	viscosity (Pa s)
ν_s	speed of sound ($m s^{-1}$)
	density ($kg m^{-3}$)
	surface tension ($N m^{-1}$)
σ_{ij}, σ_M	collision diameter (\AA)
$\Omega_D, \Omega_{k,m}$	collision integral
	specific volume ($m^3 kg^{-1}$)

Subscripts

Crt	critical point
G	vapor mixture
Gm	material component m in vapor field
Liq	liquidus point
Lm, Lm'	energy component m in liquid field
M	material number
m	melting point
N	sub-material number
Sat	saturation
Sm	energy component m in structure field
Vap	saturated vapor

Superscripts

D	dilute vapor
---	--------------

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Table D-1. TPP functions for SIMMER-III.

Arguments

- EPF : Fractional porosity of solid fuel
- M : Material number
- M1 : Material number of component 1
- M2 : Material number of component 2
- N : Sub-material number
- N1 : Sub-material number of component 1
- N2 : Sub-material number of component 2
- P1 : Partial pressure of vapor component 1 (Pa)
- P2 : Partial pressure of vapor component 2 (Pa)
- T : Temperature (K)
- V : Specific volume (m³/kg)
- V1 : Specific volume of vapor material component 1 (m³/kg)
- V2 : Specific volume of vapor material component 2 (m³/kg)
- V3 : Specific volume of vapor material component 3 (m³/kg)
- V4 : Specific volume of vapor material component 4 (m³/kg)

Functions

- XAPPLM (M,N,T) : Liquid heat capacity at constant pressure
- XCPLM (M,N,T) : Vapor heat capacity at constant pressure
- XDIFG (N1,M1,P1,N2,M2,P2,T) : Gas diffusion coefficient for binary system
- XKPSM (M,N,T,EPF) : Solid thermal conductivity
- XKPLM (M,N,T) : Liquid thermal conductivity
- XKPGM (M,N,T,V) : Vapor thermal conductivity
- XKPG (N,T,V1,V2,V3,V4) : Thermal conductivity of vapor mixture
- XMULM (M,N,T) : Liquid viscosity
- XMUGM (M,N,T,V) : Vapor viscosity
- XMUG (N,T,V1,V2,V3,V4) : Viscosity of vapor mixture
- XSGML (M,N,T) : Surface tension of liquid

Table D-2. TPP parameters for UO₂.

(M=1, N=2)

(D-KPOPT(2,1)=1, MUOPT(2,1)=0)

AKPS1= 2.02070E+00	AKPS2= 4.68440E+03	AKPS3=-1.04430E+06
AKPS4=-2.60310E-03	AKPS5= 8.93780E-07	
AKPL1= 3.15000E+00	AKPL2= 0.00000E+00	AKPL3= 0.00000E+00
AKPG1= 2.74937E+02	AKPG2=-3.19190E+05	AKPG3=-8.96730E-02
AKPG4= 1.28610E-05	AKPG5=-6.79170E-10	
TGMAX= 6.00000E+03	TLMAX= 1.06000E+04	
BMUL1= 9.88000E-04	BMUL2= 4.62000E+03	
CSSL1= 1.34800E+00	CSSL2= 2.77000E+00	CSSL3= 2.56608E-02
DCPL1= 1.12590E-01	DCPL2=-5.35780E-01	DCPL3= 8.45640E-01
DCPL4=-9.71270E-01	DCPL5= 9.60050E-01	DCPL6=-4.42520E-01
CPMAX= 1.00000E+04		
EPSM = 5.69400E+03	SIGM = 4.03000E+00	NATOM= 3

Table D-3. TPP parameters for fuel MOX.

(M=1, N=1)

(D-KPOPT(1,1)=1, MUOPT(1,1)=0)

AKPS1= 3.69720E+00	AKPS2= 5.17160E+02	AKPS3= 8.35470E+03
AKPS4=-2.29210E-03	AKPS5= 7.17150E-07	
AKPL1= 3.15000E+00	AKPL2= 0.00000E+00	AKPL3= 0.00000E+00
AKPG1= 2.74937E+02	AKPG2=-3.19190E+05	AKPG3=-8.96730E-02
AKPG4= 1.28610E-05	AKPG5=-6.79170E-10	
TGMAX= 6.00000E+03	TLMAX= 1.06000E+04	
BMUL1= 9.88000E-04	BMUL2= 4.62000E+03	
CSSL1= 1.34800E+00	CSSL2= 2.77000E+00	CSSL3= 2.64185E-02
DCPL1= 1.12590E-01	DCPL2=-5.35780E-01	DCPL3= 8.45640E-01
DCPL4=-9.71270E-01	DCPL5= 9.60050E-01	DCPL6=-4.42520E-01
CPMAX= 1.00000E+04		
EPSM = 5.69400E+03	SIGM = 4.03000E+00	NATOM= 3

Table D-4. TPP parameters for stainless steel.

(M=2, N=1)

(D-KPOPT(1,2)=1, MUOPT(1,2)=0)

AKPS1= 9.73500E+00	AKPS2= 0.00000E+00	AKPS3= 0.00000E+00
AKPS4= 1.43400E-02	AKPS5= 0.00000E+00	
AKPL1= 1.09810E+01	AKPL2= 3.21400E-03	AKPL3= 0.00000E+00
AKPG1=-1.93570E+00	AKPG2=-2.38340E+03	AKPG3=-8.71460E-05
AKPG4= 8.71000E-08	AKPG5=-7.10690E-12	
TGMAX= 6.00000E+03	TLMAX= 9.60000E+03	
BMUL1= 2.93000E-05	BMUL2= 9.71500E+03	
CSSL1= 1.70400E+00	CSSL2= 1.47700E+00	CSSL3= 6.32561E-02
DCPL1= 1.19300E-02	DCPL2= 1.43520E-02	DCPL3=-9.72070E-02
DCPL4= 1.94770E-01	DCPL5=-1.94480E-01	DCPL6= 7.20490E-02
CPMAX= 1.00000E+04		
EPSM = 3.26400E+03	SIGM = 2.41400E+00	NATOM= 1

Table D-5. TPP parameters for sodium.

(M=3, N=1)

(D-KPOPT(1,3)=2, MUOPT(1,3)=2)

AKPL1= 1.01350E+02	AKPL2=-4.87840E-02	AKPL3= 4.24470E-06
AKPL4= 7.98818E-01	AKPL5= 4.50954E-01	AKPL6= 2.15988E-05
AKPG1= 2.31640E-02	AKPG2= 1.99610E-05	
BMUL1= 6.75520E-05	BMUL2= 9.23790E+02	BMUL3= 7.98818E-01
BMUL4= 2.55308E-06	BMUL5=-3.18826E-11	
BMUG1= 1.23750E-05	BMUG2= 4.48280E-09	
KPCRT= 5.16000E+00	MUCRT= 5.80000E-05	NF = 1
CSSL1= 2.40500E-01	CSSL2= 1.12600E+00	CSSL3= 1.00382E-02
DCPL1= 1.13560E-02	DCPL2=-3.29160E-02	DCPL3= 3.38130E-02
DCPL4=-1.52410E-02	DCPL5= 2.28360E-03	DCPL6= 1.36020E-03
CPMAX= 1.00000E+04		
EPSM = 7.12000E+02	SIGM = 3.92000E+00	

APPENDIX E

CONSTANTS AND DEFAULT DATA

Constants in SIMMER-III are uniquely defined in Subroutine INCNST, and they are used throughout the code. No numeric constant is directly used in the code except for integer constants.

Almost all the input variables are assigned defaulted values in Block Data DEFULT for the fluid dynamics and NEUDEF for the neutronics except for a few minimum set of input data to define a problem to run. The values defined represent present suggestion, and hence are subject to future change when new insight is obtained through code application.

The part of code listings of INCNST and DEFULT, and NEUDEF are attached in **Tables E-1, E-2, and E-3**, respectively, to show all the constants and default data.

Table E-1. Constants Defined in SIMMER-III.

C	LARGE	= 1.00000D+20
	SMALL	= 1.00000D-20
	TOSMAL	= 2.00000D-20
	TRESML	= 3.00000D-20
	FORSML	= 4.00000D-20
	FIVSML	= 5.00000D-20
	SIXSML	= 6.00000D-20
C	HALF	= 5.00000D-01
	ZERO	= 0.00000D+00
	ONE	= 1.00000D+00
	TWO	= 2.00000D+00
	THREE	= 3.00000D+00
	FOUR	= 4.00000D+00
	FIVE	= 5.00000D+00
	SIX	= 6.00000D+00
	SEVEN	= 7.00000D+00
	EIGHT	= 8.00000D+00
	RNINE	= 9.00000D+00
	TEN	= 1.00000D+01
	ELEVEN	= 1.10000D+01
	TWELV	= 1.20000D+01
C	CP1	= 1.00000D-01
	CP2	= 2.00000D-01
	CP3	= 3.00000D-01
	CP4	= 4.00000D-01
	CP5	= 5.00000D-01
	CP6	= 6.00000D-01
	CP7	= 7.00000D-01
	CP8	= 8.00000D-01
	CP9	= 9.00000D-01
C	C1M2	= 1.00000D-02
	C1M3	= 1.00000D-03
	C1M4	= 1.00000D-04

C1M5 = 1.00000D-05
 C1M6 = 1.00000D-06
 C17M1 = 1.70000D-01
 C24M1 = 2.40000D-01
 C1M7 = 1.00000D-07
 C1M8 = 1.00000D-08
 C1M9 = 1.00000D-09
 C1M10 = 1.00000D-10
 C1M11 = 1.00000D-11
 C1M12 = 1.00000D-12
 C1M15 = 1.00000D-15
 C1M18 = 1.00000D-18
 C8M2 = 8.00000D-02
 C5M2 = 5.00000D-02
 C5M3 = 5.00000D-03
 C2M5 = 2.00000D-05
 C5M5 = 5.00000D-05
 C98M4 = 9.80000D-04
 C7M1 = 7.00000D-01
 C71M1 = 7.10000D-01
 C98M1 = 9.80000D-01
 C95M2 = 9.50000D-02
 C72M1 = 7.20000D-01
 C23M1 = 2.30000D-01
 C23M2 = 2.30000D-02
 C55M1 = 5.50000D-01
 C75M1 = 7.50000D-01
 C25M1 = 2.50000D-01
 C25M2 = 2.50000D-02
 C26M1 = 2.60000D-01
 C11M1 = 1.10000D-01
 C15M1 = 1.50000D-01
 C16M1 = 1.60000D-01
 C33M1 = 3.30000D-01
 C43M1 = 4.30000D-01
 C44M2 = 4.40000D-02
 C30M2 = 3.00000D-02
 C105M2 = 1.05000D-02
 C84M2 = 8.40000D-02
 C35M1 = 3.50000D-01
 C19M3 = 1.90000D-03
 C809M1 = 8.09000D-01
 C157M1 = 1.57000D-01
 C562M1 = 5.62000D-01
 C45M1 = 4.50000D-01
 C49M3 = 4.90000D-03
 C63M4 = 6.30000D-04
 C215M7 = 2.15700D-07
 C264M5 = 2.64000D-05
 C267M6 = 2.69930D-06
 C719M1 = 7.19288D-01
 C743M1 = 7.43000D-01
 C924M1 = 9.24950D-01
 C886M1 = 8.86000D-01
 C546M2 = 5.46452D-02
 C207M3 = 2.07368D-03

 C316M1 = 3.16400D-01
 C116M1 = 1.16000D-01
 C125M1 = 1.25000D-01
 C766M1 = 7.76000D-01
 C148M1 = 1.48740D-01
 C524M1 = 5.24870D-01
 C773M1 = 7.73200D-01
 C758M2 = 7.58000D-02
 C292M1 = ONE-SQRT(HALF)
 C397M2 = 3.97887357D-02
 C201M4 = 2.01000D-04
 C812M1 = 8.12000D-01
 C567M8 = 5.67000D-08

C

C1E2 = 1.00000D+02
 C15E2 = 1.50000D+02
 C18E2 = 1.80000D+02
 C1E3 = 1.00000D+03
 C1E4 = 1.00000D+04
 C1E5 = 1.00000D+05
 C2E2 = 2.00000D+02
 C5E2 = 5.00000D+02
 C2E3 = 2.00000D+03
 C3E3 = 3.00000D+03
 C5E3 = 5.00000D+03
 C2E4 = 2.00000D+04
 C2E5 = 2.00000D+05
 C2E6 = 2.00000D+06
 C1E9 = 1.00000D+09
 C2E1 = 2.00000D+01
 C3E1 = 3.00000D+01
 C1E10 = 1.00000D+10
 C1E12 = 1.00000D+12
 C64E1 = 6.40000D+01
 C13E1 = 1.30000D+01
 C16E1 = 1.60000D+01
 C52E0 = 5.20000D+00
 C55E0 = 5.50000D+00
 C57E0 = 5.70000D+00
 C18E1 = 1.80000D+01
 C45E1 = 4.50000D+01
 C24E1 = 2.40000D+01
 C36E1 = 3.60000D+01
 C70E1 = 7.00000D+01
 C75E1 = 7.50000D+01
 C25E1 = 2.50000D+01
 C50E1 = 5.00000D+01
 C35E0 = 3.50000D+00
 C15E0 = 1.50000D+00
 C16E0 = 1.60000D+00
 C25E0 = 2.50000D+00
 C24E0 = 2.40000D+00
 C23E0 = 2.30000D+00
 C21E0 = 2.10000D+00
 C11E0 = 1.10000D+00
 C12E0 = 1.20000D+00
 C312E0 = 3.12000D+00
 C413E0 = 4.13000D+00
 C108E0 = 1.08000D+00
 C113E0 = 1.13000D+00
 C118E0 = 1.18000D+00
 C175E0 = 1.75000D+00
 C44E0 = 4.40000D+00
 C135E0 = 1.35000D+00
 C139E0 = 1.39000D+00
 C115E0 = 1.15049D+00
 C132E0 = 1.32000D+00
 C101E0 = 1.01000D+00
 C102E0 = 1.02000D+00
 C185E0 = 1.85200D+00
 C245E0 = 2.45000D+00
 C116E0 = 1.16145D+00
 C216E0 = 2.16178D+00
 C243E0 = 2.43787D+00
 C177E0 = 1.77000D+00
 C176E1 = 1.76700D+01
 C186E1 = 1.86700D+01
 C141E1 = 1.41000D+01
 C137E1 = 1.37000D+01
 C325E1 = 3.25000D+01
 C273E2 = 2.73160D+02
 C351E2 = 3.51000D+02
 C267E3 = 2.67000D+03
 C106E0 = 1.06036D+00
 C156M1 = 1.56100D-01

```

C193M1 = 1.93000D-01
C476M1 = 4.76350D-01
C103E0 = 1.03587D+00
C152E0 = 1.52996D+00
C176E0 = 1.76474D+00
C389E0 = 3.89411D+00
C266M2 = 2.66000D-02
C3M8 = 3.00000D-08
C5M8 = 5.00000D-08
C6M8 = 6.00000D-08
C387E5 = 3.87000D+05
C452E0 = 4.52000D+00
C771E0 = 7.71000D+00
C137E3 = 1.37000D+03
C98E5 = 9.80000D+05

C
C107 = 1.00000D+00 / 7.00000D+00
C106 = 1.00000D+00 / 6.00000D+00
C1024 = 1.00000D+00 / 2.40000D+01

C103 = 1.00000D+00 / 3.00000D+00
C403 = 4.00000D+00 / 3.00000D+00
C304 = 3.00000D+00 / 4.00000D+00
C407 = 4.00000D+00 / 7.00000D+00
C607 = 6.00000D+00 / 7.00000D+00
C803 = 8.00000D+00 / 3.00000D+00
C308 = 3.00000D+00 / 8.00000D+00
C203 = 2.00000D+00 / 3.00000D+00
C9016 = 9.00000D+00 / 1.60000D+01
C24031 = 2.40000D+01 / 3.10000D+01
C1504 = 1.50000D+01 / 4.00000D+00
C7106 = 7.10000D+01 / 6.00000D+00
C3706 = 3.70000D+01 / 6.00000D+00
C3106 = 3.10000D+01 / 6.00000D+00
C6506 = 6.50000D+01 / 6.00000D+00
C11003 = 1.10000D+02 / 3.00000D+00

C
LNTEN = LOG(TEN)
PI = ACOS(-ONE)
PIO2 = PI/TWO
TPI = TWO*PI
SQRT8 = SQRT(EIGHT)
SQRT22 = TWO*SQRT(TWO)
SQRT3 = SQRT(THREE)
CPSML = ONE - SMALL
CQLGE = 1.00000D+07
CQSML = 1.00000D-04
GRAV = 9.80665D+00
STEF = 5.66960D-08
RCGAS = 8.31447D+00

C
RBQSML(3) = ZERO
RBLESML(1) = FORSML
RBLESML(2) = TOSMAL
RBLESML(3) = TOSMAL
RBLESML(4) = FORSML
RBLESML(5) = TOSMAL
RBLESML(6) = TOSMAL
RBLESML(7) = FORSML

```

Table E-2. SIMMER-III Defaulted Variables for Fluid Dynamics.

```

C   DEFAULT THE CONTROL FLAGS.
C
DATA EOSOPT/100*0/ FPNOPT/100*0/ ERROPT/100*0/ RSTOPT/100*0/
DATA ALGOPT/ 0, 0, 0, 0, 1, 0, 0, 0, 1, 1
1      , 0, 0, 0, 1, 1, 1, 1, 1, 0
2      , 0, 0, 0, 0, 0, 0, 0, 0, 0
3      , 0, 0, 0, 0, 0, 0, 3, 0, 0
4      , 0, 0, 0, 0, 1, 0, 0, 0, 0
5      , 50*0 /
DATA HTCOPT/ 0, 0, 3, 1, 0, 0, 2, 0, 0, 0
1      , 1, 0, 0, 1, 0, 0, 0, 0, 0
3      , 80*0 /
DATA IFAOPT/ 1, 0, 3, 3, 0, 3, 3, 0, 0, 0
1      , 0, 0, 0, 0, 0, 0, 0, 0, 0
2      , 0, 0, 0, 0, 0, 0, 0, 0, 0
3      , 70*0 /
DATA HMOPT/ 1, 0, 0, 0, 51, 0, 1, 0, 1, 51
1      , 999, 0, 0, 0, 0, 2, 0, 0, 0, 0
2      , 1, 1, 1, 1, 1, 0, 0, 0, 0, 0
3      , 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
4      , 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
5      , 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
6      , 0, 0, 0, 0, 0, 1, 1, 0, 0, 0
7      , 0, 0, 0, 0, 0, 0, 0, 0, 0, 1
8      , 3, 1, 0, 0, 0, 0, 0, 0, 0, 0
9      , 10*0 /
DATA EDTOPT/ 10, 0, 2, 1, 0, 0, 0, 0, 0, 0
1      , 0, 0, 1, 0, 0, 0, 0, 0, 0, 0
2      , 80*0 /
DATA MXFOPT/ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0
1      , 90*0 /
C
C   INITIALIZE THE INTERFACIAL AREA DATA
C
DATA( ID(1,K),K=1,8 ) / 0, 1, 2, 3, 4, 5, 6, 7 /
DATA( ID(2,K),K=1,8 ) / 1, 0, 8, 9, 10, 11, 12, 13 /
DATA( ID(3,K),K=1,8 ) / 2, 8, 0, 14, 15, 16, 17, 18 /
DATA( ID(4,K),K=1,8 ) / 3, 9, 14, 0, 19, 20, 21, 22 /
DATA( ID(5,K),K=1,8 ) / 4, 10, 15, 19, 0, 23, 24, 25 /
DATA( ID(6,K),K=1,8 ) / 5, 11, 16, 20, 23, 0, 26, 27 /
DATA( ID(7,K),K=1,8 ) / 6, 12, 17, 21, 24, 26, 0, 28 /
DATA( ID(8,K),K=1,8 ) / 7, 13, 18, 22, 25, 27, 28, 0 /
C
DATA IVDL / 1, 2, 2, 1, 1, 2, 2, 3 /
DATA ISRCBB, ISRCDB, ISRCDD / 30*0 /
C
DATA ALPBUB ,ALPDSP / 0.3D+0 , 0.7D+0 /
DATA ALPB1 ,ALPB2 / 0.3D+0 , 0.7D+0 /
DATA ALPNC ,ALPNT / 7.0D-1 , 1.0D-2 /
DATA CBD / 1.0D+0 /
DATA CFDB ,CFDD / 1.0D+0 , 1.0D+0 /
DATA CFCB ,CFCD / 2.45D-1 , 2.45D-1 /
DATA CFL / 1.0D+0 /
DATA CFSB ,CFSD / 1.0D+0 , 1.0D+0 /
DATA CFT ,CFV / 1.0D+0 , 1.0D-4 /
DATA CGBS / 1.0D+0 /
DATA CGCS / 1.0D+0 /
DATA CNC / 1.0D+0 /
DATA CPTB ,CPTL / 1.0D+0 , 1.0D+0 /
DATA CRGB ,CRGL / 1.0D+0 , 1.0D+0 /
DATA CTTB ,CTTL / 1.0D+0 , 1.0D+0 /
DATA CTHETA / 1.0D+5 /
DATA CHYS / 1.0D+0 /
DATA DVRT / 0.2D+0 /
DATA MMIN ,MMAX / 1.0D+5 , 1.0D+11 /
DATA OMEGAB ,OMEGAD / 1.0D+0 , 1.0D+0 /
DATA THETA0 / 2.0D-3 /
DATA TAUNUC / 1.0D-4 /

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DATA CTWB          / 1.37D+1 /
DATA CTWD          / 3.25D+1 /
DATA WEB           ,WED    /10.0D+0 , 12.0D+0 /
DATA RPCNTL        / 5.0D-4 /
DATA CLDS
* / 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0 /
DATA CPSR          / 5.0D-2 /
DATA CLCS
* / 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0 /
DATA CLL
* / 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0,
* 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0 /
DATA CLG
* / 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0 /
DATA RLMIN
* / 5.0D-5, 5.0D-5, 5.0D-5, 5.0D-5, 5.0D-5, 5.0D-5, 5.0D-5 /
DATA RLMAX
* / 1.0D-2, 1.0D-2, 1.0D-2, 1.0D-2, 1.0D-2, 1.0D-2, 1.0D-2 /
DATA RGBMIN / 5.0D-5 /
DATA RGBMAX / 1.0D-2 /
DATA RLSBK / MCLRE*5.0D-4/ RLHMT /MCLRE*5.0D-4/
DATA RGSBK / 5.0D-4/
DATA RLINI / MCLRE*5.0D-3/ RGINI / 5.0D-3/
DATA CANG / 5.0D+1/
DATA FTHMIN / 5.0D-4 /
DATA FRTHKP / 1.0D-2 /
DATA CSSX / 1.0D+0 /

C
DATA CE1 ,CE2      / 7.00D-7 ,1.250D+0 /
DATA CE3 ,CE4      / 1.00D+0 ,45.00D+0 /
DATA CSFL ,CSF     / 1.00D+0 ,1.000D+0 /
DATA DHPOOL        / 1.00D+0 /
DATA DLB           / 3.00D-2 /
DATA JBEGIN,JSTOP  / 1.20D+0 ,4.000D-1 /

C
C
C THE TURBULENT VISCOSITY MODEL INPUTS.
C
DATA FACGOM        / 1.25D-1 /
DATA ALMNTU ,AGMNTU / 1.00D-3,1.00D-3/
DATA AGLIMIT       / 3.00D-1 /
DATA CMU           / 9.00D-1 /
DATA RATIOI,RATIOI / 1.00D-1,1.00D-1/
DATA XLARG         / 2.00D-1 /
DATA XBULLE        / 1.00D-2 /
DATA RPMXLB,RPMAXD / 1.00D+6,1.00D+4/

C
C
C DEFAULT THE TIME COMMON
C
DATA TSTART,TWFIN ,NDT0 / 0.0D+0 ,0.01D+0, 10/
DATA DTMAX ,DTMIN      / 1.0D-3 ,1.00D-6 /
DATA DTSTRT,DTINC     / 1.0D-5 ,1.05D+0 /
DATA DTHINI,FEDT      / 1.0D-1 ,0.50D+0 /
DATA DTHMIN,DTHMAX    / 1.0D-5 ,1.00D+0 /
DATA DTHPIN,THPIN,DTPN/ 1.0D-2 ,0.00D+0 ,0.0D+0/
DATA CYCFIN          / 10000000 /
DATA DTSE            / 1.0D+20 /
DATA IDTH            / 10 /
+<---- *IF DEF,DPIN,1
+----> DATA DTMPF          / 1.0D-5 /
+<---- *IF -DEF,URANUS,2
|
+----> DATA DTSH,DTSMAX    / 1.0D-4,0.01D+0 /
|
+----> DATA IWTF          / 0 /

C
C
C DEFAULT THE CPUTIM COMMON
C

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        DATA CPUTME ,GRNTIM ,SHLTIM ,PKDTIM ,OUTTIM
&      ,STPTIM ,STP1TM ,STP2TM ,STP3TM ,STP4TM
&      ,S11TIM ,EXFTIM ,HTCTIM ,HMTTIM ,S12TIM / 15*0.0D+0 /
+<--- *IF -DEF,DPIN,1
+---->      DATA SPINTM / 0.0D+0 /
+<--- *IF DEF,DPIN,1
+---->      DATA DPINTM / 0.0D+0 /
C
C      DEFAULT THE PARAM COMMON
C
        DATA G      ,COURTN      /-9.80665D+0 ,0.4D+0 /
        DATA GANG      / 0.0D+0 /
        DATA OPTPIT,MPIT      / 8,25 /
C
        DATA DPMK1 ,DTGMK1      / 1.00D+0 ,1.00D+0 /
        DATA DPMK4 ,DTGMK4      / 1.00D+0 ,1.00D+0 /
C
        DATA EPSSPN,MSIT / 1.0D-4,20 /
        DATA MAXITC      / 25 /
        DATA NSTEF      / 3 /
        DATA (ISTEF(I,1),I=1,6) / 0, 0, 0, 0, 0, 0 /
        DATA (ISTEF(I,2),I=1,6) / 1, 1, 1, 1, 1, 0 /
        DATA (ISTEF(I,3),I=1,6) / 1, 1, 1, 1, 1, 1 /
+<--- *IF DEF,RS6000,1
+---->      DATA FPSTAT      /32*.FALSE./
C
C      DEFAULT THE BOUND COMMON
C
        DATA IBOUV ,IBOUP ,IBOUT / MBCMOM*0, MBCS*0, MBCGLE*0 /
        DATA VTIM ,VVAR      / MBCMM*0.0D+0, MBCMM*0.0D+0 /
        DATA PTIM ,PVAR      / MBCMB*0.0D+0, MBCMB*0.0D+0 /
        DATA TTIM ,TVAR      / MBCME*0.0D+0, MBCME*0.0D+0 /
C
C      DEFAULT THE POWER DATA
C
+<--- *IF DEF,URANUS,4
|
|      DATA (FRTP(J),J=1,5) / 0.D+0,1.D+0,0.D+0,0.D+0,0.D+0 /
|      DATA DRAD      / IBM*1.00D+0 /
|      DATA DAX      / JBM*1.00D+0 /
+---->      DATA POW      / 0.00D+0 /
+<--- *IF DEF,DPIN,2
|
|      PARAMETER (KIM = NPBM*IBM)
+---->      DATA DPEL      / KIM*1.D+0 /
        DATA AMPTAB      / 1.D+0,1.D+0,38*-1.D+0 /
        DATA (TIMAMP(J),J=1,2) / 0.D+0,1.D+0 /
        DATA IPOW      / 0 /
C
C      DEFAULT THE HEAT AND MASS TRANSFER DATA
C
        DATA PHI      /1.0D-02/
        DATA EVCRG ,EVCE3 ,EVCTG /1.0D-06,1.0D-06,1.0D-06/
        DATA DVCRG ,DVCE3 ,DVCTG /1.0D-06,1.0D-06,1.0D-06/
        DATA FVCRG ,FVCE3 ,FVCTG /1.0D-06,1.0D-06,1.0D-06/
        DATA MIVC ,IVCHLG      /150,101/
C
C
        DATA FUND      /4.0D-01,6.0D-01,8.0D-01,1.0D+00/
        DATA FRG ,FEL ,FTG      /5.0D-01,1.1D+00,5.0D-01/
        DATA FMTLG      /0.0D+00/
        DATA FTSTL ,FTSTH      /6.0D-01,9.5D-01/
        DATA FPG4L ,FPG4K      /1.0D+00,1.0D+00/
        DATA (RBGMIN(M),M=1,MCGM1-1) /1.0D-10,1.0D-10,1.0D-10/
        DATA ACRMIN      /1.0D-05/
        DATA RGLMAX      /1.0D+00/
        DATA DTLMAX      /1.0D+03/
C
        DATA HLGMIN      /1.0D+06,1.0D+05,1.0D+04,1.0D+03,1.0D+02
*      ,1.0D+08/
        DATA ( TSUP(N,1),N=1,2)/ 0.00000D+00, 0.00000D+00/
        DATA ( TSUP(N,2),N=1,2)/ 0.00000D+00, 0.00000D+00/
        DATA ( TSUP(N,3),N=1,2)/ 0.00000D+00, 0.00000D+00/

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DATA (CPGMAX(N,2),N=1,2)/ 1.00000D+04, 1.00000D+04/
DATA (CPGMAX(N,3),N=1,2)/ 1.00000D+04, 1.00000D+04/
DATA (CPGMAX(N,4),N=1,2)/ 1.00000D+04, 1.00000D+04/
DATA (CPGMAX(N,5),N=1,2)/ 1.00000D+04, 1.00000D+04/
C
DATA ( NF(N,1),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( NF(N,2),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( NF(N,3),N=1,2)/ 1.00000D+00, 1.00000D+00/
DATA ( NF(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( NF(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA (TGMAX(N,1),N=1,2)/ 6.00000D+03, 6.00000D+03/
DATA (TGMAX(N,2),N=1,2)/ 6.00000D+03, 6.00000D+03/
DATA (TGMAX(N,3),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (TGMAX(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (TGMAX(N,5),N=1,2)/ 0.00000D+00, 1.00000D+03/
C
DATA (TLMAX(N,1),N=1,2)/ 1.06000D+04, 1.06000D+04/
DATA (TLMAX(N,2),N=1,2)/ 9.60000D+03, 9.60000D+03/
DATA (TLMAX(N,3),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (TLMAX(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (TLMAX(N,5),N=1,2)/ 0.00000D+00, 0.00000D+03/
C
DATA (NATOM(N,1),N=1,2)/ 3, 3/
DATA (NATOM(N,2),N=1,2)/ 1, 1/
DATA (NATOM(N,3),N=1,2)/ 1, 3/
DATA (NATOM(N,4),N=1,2)/ 5, 5/
DATA (NATOM(N,5),N=1,2)/ 1, 1/
C
DATA (MUOPT(N,1),N=1,2)/ 0, 0/
DATA (MUOPT(N,2),N=1,2)/ 0, 0/
DATA (MUOPT(N,3),N=1,2)/ 2, 2/
DATA (MUOPT(N,4),N=1,2)/ 0, 0/
DATA (MUOPT(N,5),N=1,2)/ 0, 1/
C
DATA (KPOPT(N,1),N=1,2)/ 1, 1/
DATA (KPOPT(N,2),N=1,2)/ 1, 1/
DATA (KPOPT(N,3),N=1,2)/ 2, 2/
DATA (KPOPT(N,4),N=1,2)/ 0, 0/
DATA (KPOPT(N,5),N=1,2)/ 0, 1/
C
DATA (AKPS(N,1,1),N=1,5)/ 3.69720D+00, 5.17160D+02, 8.35470D+03
*      , -2.29210D-03, 7.17150D-07/
*      ,(AKPS(N,2,1),N=1,5)/ 2.02070D+00, 4.68440D+03, -1.04430D+06
*      , -2.60310D-03, 8.93780D-07/
DATA (AKPS(N,1,2),N=1,5)/ 9.73500D+00, 0.00000D+00, 0.00000D+00
*      , 1.43400D-02, 0.00000D+00/
*      ,(AKPS(N,2,2),N=1,5)/ 9.73500D+00, 0.00000D+00, 0.00000D+00
*      , 1.43400D-02, 0.00000D+00/
DATA (AKPS(N,1,3),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
*      ,(AKPS(N,2,3),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
DATA (AKPS(N,1,4),N=1,5)/ 3.95450D+01, -1.17950D+04, 2.16930D+06
*      , -2.77400D-02, 7.64190D-06/
*      ,(AKPS(N,2,4),N=1,5)/ 3.95450D+01, -1.17950D+04, 2.16930D+06
*      , -2.77400D-02, 7.64190D-06/
DATA (AKPS(N,1,5),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
*      ,(AKPS(N,2,5),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
C
DATA (AKPL(N,1,1),N=1,6)/ 3.15000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(AKPL(N,2,1),N=1,6)/ 3.15000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (AKPL(N,1,2),N=1,6)/ 1.09810D+01, 3.21400D-03, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(AKPL(N,2,2),N=1,6)/ 1.09810D+01, 3.21400D-03, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/

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DATA (AKPL(N,1,3),N=1,6)/ 1.01350D+02,-4.87840D-02, 4.24470D-06
*      , 7.98818D-01, 4.50954D-01, 2.15988D-05/
*      ,(AKPL(N,2,3),N=1,6)/-2.80570D-01, 4.63990D-03,-5.57360D-06
*
*      , 9.27176D-01, 3.02036D-02,-1.60687D-06/
DATA (AKPL(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(AKPL(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (AKPL(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(AKPL(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA (AKPG(N,1,1),N=1,5)/ 2.74937D+02,-3.19190D+05,-8.96730D-02
*      , 1.28610D-05,-6.79170D-10/
DATA (AKPG(N,2,1),N=1,5)/ 2.74937D+02,-3.19190D+05,-8.96730D-02
*      , 1.28610D-05,-6.79170D-10/
DATA (AKPG(N,1,2),N=1,5)/-1.93570D+00,-2.38340D+03,-8.71460D-05
*      , 8.71000D-08,-7.10690D-12/
DATA (AKPG(N,2,2),N=1,5)/-1.93570D+00,-2.38340D+03,-8.71460D-05
*      , 8.71000D-08,-7.10690D-12/
DATA (AKPG(N,1,3),N=1,5)/ 2.31640D-02, 1.99610D-05, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
DATA (AKPG(N,2,3),N=1,5)/-5.51710D-03, 8.11940D-05, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
DATA (AKPG(N,1,4),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
DATA (AKPG(N,2,4),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
DATA (AKPG(N,1,5),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00/
DATA (AKPG(N,2,5),N=1,5)/-3.66590D+00,-1.37910D+02, 1.95490D-03
*      , -1.25570D-06, 4.16370D-10/
C
DATA (BMUL(N,1,1),N=1,5)/ 9.88000D-04, 4.62000D+03, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
*      ,(BMUL(N,2,1),N=1,5)/ 9.88000D-04, 4.62000D+03, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
DATA (BMUL(N,1,2),N=1,5)/ 2.93000D-05, 9.71500D+03, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
*      ,(BMUL(N,2,2),N=1,5)/ 2.93000D-05, 9.71500D+03, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
DATA (BMUL(N,1,3),N=1,5)/ 6.75520D-05, 9.23790D+02, 7.98818D-01
*      , 2.55308D-06,-3.18826D-11 /
*      ,(BMUL(N,2,3),N=1,5)/ 5.89150D-06, 1.48760D+03, 9.27176D-01
*      , 4.75264D-06,-5.90333D-10 /
DATA (BMUL(N,1,4),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
*      ,(BMUL(N,2,4),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
DATA (BMUL(N,1,5),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
*      ,(BMUL(N,2,5),N=1,5)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00 /
C
DATA (BMUG(N,1,1),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(BMUG(N,2,1),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (BMUG(N,1,2),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(BMUG(N,2,2),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (BMUG(N,1,3),N=1,3)/ 1.23750D-05, 4.48280D-09, 0.00000D+00/
*      ,(BMUG(N,2,3),N=1,3)/ 6.87070D-07, 3.09210D-08, 0.00000D+00/
DATA (BMUG(N,1,4),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(BMUG(N,2,4),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (BMUG(N,1,5),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,(BMUG(N,2,5),N=1,3)/ 3.60400D-06, 5.49720D-08,-1.59180D-11/
C
DATA (CSGL(N,1,1),N=1,3)/ 1.34800D+00, 2.77000D+00, 2.64185D-02/
*      ,(CSGL(N,2,1),N=1,3)/ 1.34800D+00, 2.77000D+00, 2.56608D-02/
DATA (CSGL(N,1,2),N=1,3)/ 1.70400D+00, 1.47700D+00, 6.32561D-02/
*      ,(CSGL(N,2,2),N=1,3)/ 1.70400D+00, 1.47700D+00, 6.32561D-02/

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C
C   DEFAULT THE HTC PROPERTIES
C
C *** COMMON CHTC.
  DATA HCDP / 1.0D+1, 1.0D+1, 1.0D+1, 1.0D+1, 1.0D+1,
*          1.0D+1, 1.0D+1, 1.0D+1 /
  DATA HCDLP / 2.0D+0, 2.0D+0, 2.0D+0 /
  DATA HCDGP / 2.0D+0 /
  DATA HCDLBS / 5.0D+0, 5.0D+0, 5.0D+0 /
  DATA HCDLAS / 2.0D+0, 2.0D+0, 2.0D+0 /
  DATA HCDGS / 5.0D+0 /
C
  DATA (HFCLP(N,1),N=1,5)/ 5.42D-1, 5.00D-1, 4.50D-1, 1.20D-2,
*                          3.33D-1 /
  DATA (HFCLP(N,2),N=1,5)/ 6.46D-1, 5.00D-1, 5.00D-1, 8.00D-3,
*                          3.33D-1 /
  DATA (HFCLP(N,3),N=1,5)/ 6.80D-1, 5.00D-1, 5.00D-1, 0.00D+0,
*                          0.00D+0 /
  DATA HFCGP / 5.42D-1, 5.00D-1, 4.50D-1, 1.20D-2,
*             3.33D-1 /
C
  DATA (HNCLP(N,1),N=1,3)/ 4.74D-1, 2.50D-1, 1.44D+0 /
  DATA (HNCLP(N,2),N=1,3)/ 5.30D-1, 2.50D-1, 1.74D+0 /
  DATA (HNCLP(N,3),N=1,3)/ 6.20D-1, 2.50D-1, 1.91D+0 /
  DATA HNCGP / 4.74D-1, 2.50D-1, 1.44D+0 /
C
  DATA (HFCLS(N,1),N=1,3)/ 2.30D-2, 8.00D-1, 3.00D-1 /
  DATA (HFCLS(N,2),N=1,3)/ 2.50D-2, 8.00D-1, 8.00D-1 /
  DATA (HFCLS(N,3),N=1,3)/ 2.50D-2, 8.00D-1, 8.00D-1 /

  DATA HFCGS / 2.30D-2, 8.00D-1, 3.00D-1 /
  DATA (HFCXS(N,1),N=1,3)/ 2.30D-2, 8.00D-1, 3.00D-1 /
  DATA (HFCXS(N,2),N=1,3)/ 2.50D-2, 8.00D-1, 8.00D-1 /
  DATA (HFCXS(N,3),N=1,3)/ 2.50D-2, 8.00D-1, 8.00D-1 /
  DATA (HFCXS(N,4),N=1,3)/ 2.30D-2, 8.00D-1, 3.00D-1 /
  DATA (HRSMUL(N),N=1,11)/ 11*1.00D+0 /
  DATA HGSMUL / 1.00D+0 /
  DATA HGLMUL / 1.00D+0, 1.00D+0, 1.00D+0, 1.00D+0,
*             1.00D+0, 1.00D+0, 1.00D+0 /
  DATA HLG MUL / 1.00D+0, 1.00D+0, 1.00D+0 /
  DATA HRTMUL / 1.00D+0, 1.00D+0, 1.00D+0, 1.00D+0,
*             1.00D+0, 1.00D+0, 1.00D+0, 1.00D+0,
*             1.00D+0, 1.00D+0, 1.00D+0, 1.00D+0,
*             1.00D+0, 1.00D+0 /
  DATA HPTMUL / 1.00D+0, 1.00D+0, 1.00D+0, 1.00D+0 /
  DATA HAFMUL / 1.00D+0 /
C
  DATA HREIC ,HREOS / 5.00D+1, 3.00D+2 /
  DATA HOSLDP / 2.70D+0, 2.70D+0, 2.70D+0 /
  DATA HOSGBU / 2.70D+0 /
C
  DATA (HICLCP(N,1),N=1,6)/ 1.13D+0, 5.00D-1, 2.89D+0, 2.15D+0,
*                          6.40D-1, 5.00D-1 /
  DATA (HICLCP(N,2),N=1,6)/ 1.13D+0, 5.00D-1, 2.89D+0, 2.15D+0,
*                          6.40D-1, 5.00D-1 /
  DATA (HICLCP(N,3),N=1,6)/ 1.13D+0, 5.00D-1, 2.89D+0, 2.15D+0,
*                          6.40D-1, 5.00D-1 /
C
  DATA (HICLDP(N,1),N=1,3)/ 8.420D-1, 1.025D+0, 2.000D+2 /
  DATA (HICLDP(N,2),N=1,3)/ 8.420D-1, 1.025D+0, 2.000D+2 /
  DATA (HICLDP(N,3),N=1,3)/ 8.420D-1, 1.025D+0, 2.000D+2 /
C
  DATA HCDMXS ,HKEXP / 5.00D+0, -0.20D+0 /
C
C *** COMMON FBC.
  DATA FFB / 1.0D+0 /
  DATA CMFB / 5.5D-1 /
  DATA CDNB / 1.0D-1 /
  DATA BESLIP / 3.0D+0 /

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DATA BESLP2          / 3.0D+0 /
DATA FILMIN          / 1.4D-4 /
DATA EHTECFB        / 5.0D-2 /
C
C   DEFAULT FILM BOILING INDEX
C
DATA (KMCLRE(N,1),N=1,3) / 2,1,1 /
DATA (KMCLRE(N,2),N=1,3) / 3,3,2 /
DATA (KMCLRE(N,3),N=1,3) / 4,4,4 /
DATA (KMCLRE(N,4),N=1,3) / 5,5,5 /
DATA (KMCLRE(N,5),N=1,3) / 7,7,7 /
C
DATA (JKMCLR(N,1),N=1,3) / 1,1,2 /
DATA (JKMCLR(N,2),N=1,3) / 1,2,2 /
C
DATA (IHOT (N,1),N=1,3) / 1,1,1 /
DATA (IHOT (N,2),N=1,3) / 1,2,2 /
DATA (IHOT (N,3),N=1,3) / 4,4,4 /
DATA (IHOT (N,4),N=1,3) / 5,5,5 /
DATA (IHOT (N,5),N=1,3) / 7,7,7 /
C
DATA (ICOO (N,1),N=1,3) / 2,2,3 /
DATA (ICOO (N,2),N=1,3) / 3,3,3 /
DATA (ICOO (N,3),N=1,3) / 1,2,3 /
DATA (ICOO (N,4),N=1,3) / 1,2,3 /
DATA (ICOO (N,5),N=1,3) / 1,2,3 /
C
DATA (KHRT (N,1),N=1,3) / 1,7,13 /
DATA (KHRT (N,2),N=1,3) / 2,8,14 /
C
DATA (INVFLG(N,1),N=1,3) / 2,1,1 /
DATA (INVFLG(N,2),N=1,3) / 2,2,1 /
DATA (INVFLG(N,3),N=1,3) / 0,1,1 /
DATA (INVFLG(N,4),N=1,3) / 0,0,1 /
DATA (INVFLG(N,5),N=1,3) / 0,1,1 /
C
C   DEFAULT THE VALUES OF EPSILON BLOCK
C
DATA EPSVEL,EPSP      / 1.0D-4,10.0D+0 /
DATA EPSRO ,EPST      / 1.0D-4,1.0D+03 /
DATA EPSPCV          / 1.D-04/
DATA FXR              / 5.00000D-1, 9.99999D-1, 9.99999D-1
&                      ,9.99999D-1, 9.99999D-1, 5.00000D-1 /
DATA FXE              / 1.0D+10, 1.0D+10, 1.0D+10, 1.0D+10
&                      , 1.0D+10, 2.0D+00 /
DATA EITRF            / 1.D-6 /
DATA NITRF            / 100 /
DATA FCOUPG,FCOUP    / -1.0D-10, 1.0D-10 /
DATA ALPEXC          / 1.0D-10 /
DATA FVCCF1           / 1.D+0 /
DATA EXPPR1           / 1.D+0 /
C
C   DEFAULT THE EDIT COMMON
C
DATA TCPRT            / MNTEC*1.0D+20 /
DATA TCPPF            / MNTEC*1.0D+20 /
DATA TCDMP            / MNTEC*1.0D+20 /
DATA DTPRT            / MNTEC*1.0D+10 /
DATA DTPPF            / MNTEC*1.0D+10 /
DATA DTDMP            / MNTEC*1.0D+10 /
DATA PRTC,DMPC,PPFC,BSFC/50,100,25,10/
DATA IVBF/0/
DATA NSPRNT           / 0 /
DATA NAME              / 'SIMMER 3 TEST PROBLEM' /
DATA PCGRP             / MNGRP*0 /
DATA PPGRP             / MNPP *0 /
DATA PRCEL             / 250 *0 /
DATA LPRGN             / 270 *0 /
DATA NPRINT            / MNMAT*1 /
DATA TCBSF / MNTEC*1.0D20 /
DATA DTBSF / MNTEC*1.0D10 /

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DATA SN / 200* ' ' /
+<--- *IF DEF,DPIN,1
+---> DATA SF / 200* ' ' /
C
C DEFAULT THE EOS DATA
C
C ### MTAB IS A TABLE THAT CORRELATES THE 3 DENSITY FIELDS
C (SOLID, LIQUID, AND VAPOR) TO THE MATERIALS.
C
C MECTAB IS A TABLE THAT CORRELATES THE 3 ENERGY FIELDS
C (STRUCTURE, LIQUID, AND VAPOR) TO THE DENSITIES.
C
C MLGTAB IS A TABLE THAT CORRELATES THE 3 CONDENSIBLE VAPORS
C (FUEL, STEEL, AND SODIUM) TO THE LIQUID ENERGY COMPONENT.
C
C ### MATERIAL 1 IS FERTILE AND FISSILE FUEL.
C MATERIAL 2 IS STEEL FOR THE CLADDING AND CAN WALLS.
C MATERIAL 3 IS SODIUM FOR THE COOLANT.
C MATERIAL 4 IS THE CONTROL MATERIAL.
C MATERIAL 5 IS THE FISSION GAS.
C
DATA (MTAB (I,1),I=1, MCSR) /1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 4/
DATA (MTAB (I,2),I=1,MCLR) /1, 1, 2, 3, 1, 1, 2, 4, 1, 1, 5, 5, 5/
DATA (MTAB (I,3),I=1, MCGR) /1, 1, 2, 3, 5/
DATA (MECTAB(J,1),J=1,MCSRE) /1, 3, 5, 7, 8, 9,10,11,12/
DATA (MECTAB(J,2),J=1,MCLRE) /1, 3, 4, 5, 7, 8, 9/
DATA (MECTAB(J,3),J=1,MCGM1) /1, 3, 4, 5/
DATA (MLGTAB(J) ,J=1,MCLM3) /1, 2, 3/
C
DATA MFUEL,MST,MNA,MCON,MFG /1, 2, 3, 4, 5/
DATA MLDCVF/ 1, 1, 2, 2, 1, 1, 1, 2, 2, 2, 1, 1, 2 /
DATA MLECVF/ 1, 2, 2, 1, 1, 2, 2 /
C
DATA ALPHA0, EPSTG , EPSEN , EPSSV , EPSPG /
* 1.0D-2, 1.0D-6, 1.0D-6, 1.0D-6, 1.0D-6/
C
DATA (ESOLUS(N,1),N=1,2)/ 1.05162D+06, 1.12157D+06/
DATA (ESOLUS(N,2),N=1,2)/ 9.12379D+05, 9.12379D+05/
DATA (ESOLUS(N,3),N=1,2)/ 2.06717D+05, -1.04750D+05/
DATA (ESOLUS(N,4),N=1,2)/ 9.46500D+06, 9.46500D+06/
DATA (ESOLUS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA (ELIQUS(N,1),N=1,2)/ 1.31829D+06, 1.39871D+06/
DATA (ELIQUS(N,2),N=1,2)/ 1.25158D+06, 1.25158D+06/
DATA (ELIQUS(N,3),N=1,2)/ 2.06717D+05, -1.04750D+05/
DATA (ELIQUS(N,4),N=1,2)/ 1.13580D+07, 1.13580D+07/
DATA (ELIQUS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( ECRT(N,1),N=1,2)/ 4.99290D+06, 4.99290D+06/
DATA ( ECRT(N,2),N=1,2)/ 8.20580D+06, 8.20580D+06/
DATA ( ECRT(N,3),N=1,2)/ 4.17692D+06, 1.91253D+06/
DATA ( ECRT(N,4),N=1,2)/ 2.27160D+07, 2.27160D+07/
DATA ( ECRT(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( ELIQG(N,1),N=1,2)/ 2.98033D+06, 3.04328D+06/
DATA ( ELIQG(N,2),N=1,2)/ 7.73961D+06, 7.73961D+06/
DATA ( ELIQG(N,3),N=1,2)/ 4.57699D+06, 2.28449D+06/
DATA ( ELIQG(N,4),N=1,2)/ 2.00000D+07, 2.00000D+07/
DATA ( ELIQG(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA (TSOLUS(N,1),N=1,2)/ 3.00200D+03, 3.12000D+03/
DATA (TSOLUS(N,2),N=1,2)/ 1.71300D+03, 1.71300D+03/
DATA (TSOLUS(N,3),N=1,2)/ 3.71000D+02, 2.73160D+02/
DATA (TSOLUS(N,4),N=1,2)/ 5.00000D+03, 5.00000D+03/
DATA (TSOLUS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA (TLIQUS(N,1),N=1,2)/ 3.04100D+03, 3.12000D+03/
DATA (TLIQUS(N,2),N=1,2)/ 1.75300D+03, 1.75300D+03/
DATA (TLIQUS(N,3),N=1,2)/ 3.71000D+02, 2.73160D+02/
DATA (TLIQUS(N,4),N=1,2)/ 6.00000D+03, 6.00000D+03/
DATA (TLIQUS(N,5),N=1,2)/ 1.61250D+02, 7.88000D+01/

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C
DATA ( TCRT(N,1),N=1,2)/ 1.06000D+04, 1.06000D+04/
DATA ( TCRT(N,2),N=1,2)/ 9.60000D+03, 9.60000D+03/
DATA ( TCRT(N,3),N=1,2)/ 2.50370D+03, 6.47126D+02/
DATA ( TCRT(N,4),N=1,2)/ 1.20000D+04, 1.20000D+04/
DATA ( TCRT(N,5),N=1,2)/ 2.89730D+02, 1.32500D+02/

C
DATA (VSOLUS(N,1),N=1,2)/ 1.00230D-04, 1.04656D-04/
DATA (VSOLUS(N,2),N=1,2)/ 1.36168D-04, 1.36168D-04/
DATA (VSOLUS(N,3),N=1,2)/ 1.08029D-03, 1.00022D-03/
DATA (VSOLUS(N,4),N=1,2)/ 3.96800D-04, 3.96800D-04/
DATA (VSOLUS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/

C
DATA (VLIQUS(N,1),N=1,2)/ 1.08814D-04, 1.12867D-04/
DATA (VLIQUS(N,2),N=1,2)/ 1.41420D-04, 1.41420D-04/
DATA (VLIQUS(N,3),N=1,2)/ 1.08029D-03, 1.00022D-03/
DATA (VLIQUS(N,4),N=1,2)/ 3.96800D-04, 3.96800D-04/
DATA (VLIQUS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/

C
DATA ( ROCRT(N,1),N=1,2)/ 1.56000D+03, 1.56000D+03/
DATA ( ROCRT(N,2),N=1,2)/ 1.14300D+03, 1.14300D+03/
DATA ( ROCRT(N,3),N=1,2)/ 2.19000D+02, 3.22000D+02/
DATA ( ROCRT(N,4),N=1,2)/ 2.52000D+03, 2.52000D+03/
DATA ( ROCRT(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/

C
DATA ( PCRT(N,1),N=1,2)/ 1.57873D+08, 1.57873D+08/
DATA ( PCRT(N,2),N=1,2)/ 4.56760D+08, 4.56760D+08/
DATA ( PCRT(N,3),N=1,2)/ 2.56406D+07, 2.18859D+07/
DATA ( PCRT(N,4),N=1,2)/ 1.00000D+10, 1.00000D+10/
DATA ( PCRT(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/

C
DATA ( RUGM(N,1),N=1,2)/ 3.07945D+01, 3.07945D+01/
DATA ( RUGM(N,2),N=1,2)/ 1.48646D+02, 1.48646D+02/
DATA ( RUGM(N,3),N=1,2)/ 3.61661D+02, 4.61520D+02/
DATA ( RUGM(N,4),N=1,2)/ 2.51000D+02, 2.51000D+02/
DATA ( RUGM(N,5),N=1,2)/ 6.33293D+01, 2.87004D+02/

C
DATA ( WM(N,1),N=1,2)/ 2.70000D+02, 2.70000D+02/
DATA ( WM(N,2),N=1,2)/ 5.59354D+01, 5.59354D+01/
DATA ( WM(N,3),N=1,2)/ 2.29898D+01, 1.80152D+01/
DATA ( WM(N,4),N=1,2)/ 5.53000D+01, 5.53000D+01/
DATA ( WM(N,5),N=1,2)/ 1.31290D+02, 2.89700D+01/

C
DATA (SUPHEA(N,1),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (SUPHEA(N,2),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (SUPHEA(N,3),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (SUPHEA(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (SUPHEA(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/

C
DATA TAUST / 1.00000D-03, 1.00000D-03, 1.00000D-03
*      , 1.00000D-03, 1.00000D-03/

C
DATA ( PTS(N,1),N=1,2)/ 0.10000D+00, 0.10000D+00/
DATA ( PTS(N,2),N=1,2)/ 0.18000D+00, 0.18000D+00/
DATA ( PTS(N,3),N=1,2)/ 0.50000D+00, 0.50000D+00/
DATA ( PTS(N,4),N=1,2)/ 0.10000D+00, 0.10000D+00/
DATA ( PTS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/

C
DATA ( TLBND(N,1),N=1,2)/ 1.00000D+04, 8.50000D+03/
DATA ( TLBND(N,2),N=1,2)/ 8.00000D+03, 8.00000D+03/
DATA ( TLBND(N,3),N=1,2)/ 2.30000D+03, 6.05000D+02/
DATA ( TLBND(N,4),N=1,2)/ 1.20000D+04, 1.20000D+04/
DATA ( TLBND(N,5),N=1,2)/ 2.89730D+02, 1.32500D+02/

C
DATA ( CVG(N,1),N=1,2)/ 3.06427D+02, 3.01247D+02/
DATA ( CVG(N,2),N=1,2)/ 2.22969D+02, 2.22969D+02/
DATA ( CVG(N,3),N=1,2)/ 4.60613D+02, 1.63536D+03/
DATA ( CVG(N,4),N=1,2)/ 5.00000D+02, 5.00000D+02/
DATA ( CVG(N,5),N=1,2)/ 9.50710D+01, 7.21200D+02/

C
DATA (ELIQGD(N,1),N=1,2)/ 2.98034D+06, 3.04329D+06/

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DATA ( ELIQGD(N,2),N=1,2)/ 7.73961D+06, 7.73961D+06/
DATA ( ELIQGD(N,3),N=1,2)/ 4.57844D+06, 2.28457D+06/
DATA ( ELIQGD(N,4),N=1,2)/ 2.00000D+07, 2.00000D+07/
DATA ( ELIQGD(N,5),N=1,2)/-1.30152D+04,-1.58195D+05/
C
DATA ( PSMIN(N,1),N=1,2)/ 2.19149D-05, 2.19149D-05/
DATA ( PSMIN(N,2),N=1,2)/ 1.96268D-11, 1.96268D-11/
DATA ( PSMIN(N,3),N=1,2)/ 3.27460D-09, 2.88335D-01/
DATA ( PSMIN(N,4),N=1,2)/ 1.00000D-20, 1.00000D-20/
DATA ( PSMIN(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( DTDPS(N,1),N=1,2)/ 5.85547D-08, 5.52486D-08/
DATA ( DTDPS(N,2),N=1,2)/ 1.92381D-08, 1.92381D-08/
DATA ( DTDPS(N,3),N=1,2)/ 9.51892D-08, 8.37753D-09/
DATA ( DTDPS(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( DTDPS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( DVDPS(N,1),N=1,2)/-5.46331D-16,-5.46331D-16/
DATA ( DVDPS(N,2),N=1,2)/-6.58746D-16,-6.58746D-16/
DATA ( DVDPS(N,3),N=1,2)/-1.85485D-13,-7.70118D-15/
DATA ( DVDPS(N,4),N=1,2)/-1.00000D-16,-1.00000D-16/
DATA ( DVDPS(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( DTDPC(N,1),N=1,2)/ 1.91288D-05, 1.91288D-05/
DATA ( DTDPC(N,2),N=1,2)/ 6.06817D-06, 6.06817D-06/
DATA ( DTDPC(N,3),N=1,2)/ 2.11232D-05, 2.82109D-06/
DATA ( DTDPC(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( DTDPC(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( BETA(N,1),N=1,2)/-1.00000D+00,-1.00000D+00/
DATA ( BETA(N,2),N=1,2)/-1.00000D+00,-1.00000D+00/
DATA ( BETA(N,3),N=1,2)/ 1.50000D-01,-1.00000D+00/
DATA ( BETA(N,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( BETA(N,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( AS(N,1,1),N=1,3)/ 4.68166D-01, 5.24030D-01,-9.59833D-02/
* ( AS(N,2,1),N=1,3)/ 4.44390D-01, 4.89576D-01,-2.83438D-02/
DATA ( AS(N,1,2),N=1,3)/ 8.56796D-01,-3.28896D-01, 2.92311D-01/
* ( AS(N,2,2),N=1,3)/ 8.56796D-01,-3.28896D-01, 2.92311D-01/
DATA ( AS(N,1,3),N=1,3)/ 1.00000D+00, 0.00000D+00, 0.00000D+00/
* ( AS(N,2,3),N=1,3)/ 1.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( AS(N,1,4),N=1,3)/ 1.00000D+00, 0.00000D+00, 0.00000D+00/
* ( AS(N,2,4),N=1,3)/ 1.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( AS(N,1,5),N=1,3)/ 1.00000D+00, 0.00000D+00, 0.00000D+00/
* ( AS(N,2,5),N=1,3)/ 1.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA ( BS(N,1,1),N=1,3)/-6.48590D-03,-1.62062D-01, 7.27906D-02/
* ( BS(N,2,1),N=1,3)/-1.44971D-01,-7.36914D-03, 2.60596D-02/
DATA ( BS(N,1,2),N=1,3)/-9.08374D-02, 4.23217D-02,-1.96932D-02/
* ( BS(N,2,2),N=1,3)/-9.08374D-02, 4.23217D-02,-1.96932D-02/
DATA ( BS(N,1,3),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
* ( BS(N,2,3),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( BS(N,1,4),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
* ( BS(N,2,4),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( BS(N,1,5),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
* ( BS(N,2,5),N=1,3)/ 0.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA ( AL(N,1,1),N=1,6)/ 8.41923D-01,-1.69174D-02, 1.47156D-02
* , 3.68955D+00, 2.89670D+01,-1.66741D+02/
* ( AL(N,2,1),N=1,6)/ 8.81083D-01,-2.04486D-02, 1.86174D-02
* , 3.47820D+00, 2.95237D+01,-1.69116D+02/
DATA ( AL(N,1,2),N=1,6)/ 1.02425D+00,-6.82077D-02, 6.60477D-03
* , 6.00388D+00, 5.95140D+00, 0.00000D+00/
* ( AL(N,2,2),N=1,6)/ 1.02425D+00,-6.82077D-02, 6.60477D-03
* , 6.00388D+00, 5.95140D+00, 0.00000D+00/
DATA ( AL(N,1,3),N=1,6)/ 5.76094D-01,-2.33486D-02, 4.72888D-04
* , 1.99989D+01,-1.08409D+02, 8.96169D+03/
* ( AL(N,2,3),N=1,6)/-8.35175D-02, 7.85859D-05, 3.81615D-05
* , -1.55949D+01, 5.19998D+00,-1.71742D+01/
DATA ( AL(N,1,4),N=1,6)/ 1.00000D+00, 0.00000D+00, 0.00000D+00

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*           , 2.00000D+00, 0.00000D+00, 0.00000D+00/
*   ,( AL(N,2,4),N=1,6)/ 1.00000D+00, 0.00000D+00, 0.00000D+00
*           , 2.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( AL(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*   ,( AL(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA ( BL(N,1,1),N=1,4)/ 2.17296D+01, 4.42327D-04,-7.99342D+04
*           ,-8.88130D+00 /
*   ,( BL(N,2,1),N=1,4)/ 2.17296D+01, 4.42327D-04,-7.99342D+04
*           ,-8.88130D+00 /
DATA ( BL(N,1,2),N=1,4)/ 2.37361D+01, 1.54890D-04,-5.07204D+04
*           ,-3.30628D+00 /
*   ,( BL(N,2,2),N=1,4)/ 2.37361D+01, 1.54890D-04,-5.07204D+04
*           ,-3.30628D+00 /
DATA ( BL(N,1,3),N=1,4)/ 2.21057D+01, 0.00000D+00,-1.26337D+04
*           ,-4.67200D-01 /
*   ,( BL(N,2,3),N=1,4)/ 2.20110D+01, 1.10023D-02,-7.91404D+03
*           ,-1.20208D+01 /
DATA ( BL(N,1,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
*   ,( BL(N,2,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
DATA ( BL(N,1,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
*   ,( BL(N,2,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
C
DATA ( CL(N,1,1),N=1,4)/-4.16525D+01, 9.47848D+01,-7.88238D+01
*           , 1.97832D+01 /
*   ,( CL(N,2,1),N=1,4)/-3.51500D+01, 6.72600D+01,-4.70436D+01
*           , 8.08263D+00 /
DATA ( CL(N,1,2),N=1,4)/-9.23249D+00,-1.74176D+01, 3.84477D+01
*           ,-1.89791D+01 /
*   ,( CL(N,2,2),N=1,4)/-9.23249D+00,-1.74176D+01, 3.84477D+01
*           ,-1.89791D+01 /
DATA ( CL(N,1,3),N=1,4)/-2.42195D+01, 2.99496D+01,-3.39662D+00
*           ,-8.16499D+00 /
*   ,( CL(N,2,3),N=1,4)/-5.32832D+00,-2.07178D+01, 3.66287D+01
*           ,-1.57712D+01 /
DATA ( CL(N,1,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
*   ,( CL(N,2,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
DATA ( CL(N,1,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
*   ,( CL(N,2,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00 /
C
DATA ( DL(N,1,1),N=1,6)/ 3.72680D-01,-1.67343D-01, 1.44446D-01
*           , 3.06379D+00,-1.55974D+00, 2.09893D+00/
*   ,( DL(N,2,1),N=1,6)/ 3.93703D-01,-1.81812D-01, 1.74487D-01
*           , 2.89613D+00,-1.54733D+00, 2.07800D+00/
DATA ( DL(N,1,2),N=1,6)/ 1.81594D-01,-6.22683D-03, 8.98282D-03
*           , 5.17704D+00,-1.62972D+00, 2.71165D+00/
*   ,( DL(N,2,2),N=1,6)/ 1.81594D-01,-6.22683D-03, 8.98282D-03
*           , 5.17704D+00,-1.62972D+00, 2.71165D+00/
DATA ( DL(N,1,3),N=1,6)/ 6.27665D-02,-2.21705D-03, 2.27740D-04
*           , 1.70725D+01,-1.26722D+00, 2.59838D+00/
*   ,( DL(N,2,3),N=1,6)/-5.90421D-03, 6.46334D-04,-6.48209D-05
*           ,-1.49738D+01,-1.47461D+00, 3.58713D+00/
DATA ( DL(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 2.00000D+00, 0.00000D+00, 0.00000D+00/
*   ,( DL(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 2.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( DL(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*   ,( DL(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 0.00000D+00, 0.00000D+00, 0.00000D+00/
C

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DATA ( FL(N,1,1),N=1,6)/-1.32899D-12, 1.90472D-01,-1.42352D+01
*      , 2.15440D+01,-1.93115D+01,-1.42655D-11/
*      ,( FL(N,2,1),N=1,6)/-3.61402D-12,-4.22202D-02,-1.68215D+01
*      , 3.17194D+01,-2.92392D+01,-1.42655D-11/
DATA ( FL(N,1,2),N=1,6)/-2.58082D-13, 1.01637D+00,-1.55026D+01
*      , 4.54114D+01,-4.07002D+01,-1.01686D-12/
*      ,( FL(N,2,2),N=1,6)/-2.58082D-13, 1.01637D+00,-1.55026D+01
*      , 4.54114D+01,-4.07002D+01,-1.01686D-12/
DATA ( FL(N,1,3),N=1,6)/-3.09510D-12, 5.59746D-01,-4.64421D+00
*      , 4.33770D+00,-3.36198D+00,-1.46413D-10/
*      ,( FL(N,2,3),N=1,6)/-2.19863D-11, 2.10295D-01,-1.30727D+01
*      , 3.19227D+01,-2.57188D+01,-5.18389D-11/
DATA ( FL(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,( FL(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( FL(N,1,5),N=1,6)/ 1.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,( FL(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA ( AG(N,1,1),N=1,4)/ 1.41301D-04, 2.94299D+02, 2.85846D-04
*      , 2.00000D-01 /
*      ,( AG(N,2,1),N=1,4)/ 1.41301D-04, 2.94299D+02, 2.85846D-04
*      , 2.00000D-01 /
DATA ( AG(N,1,2),N=1,4)/ 1.51243D-04, 2.02244D+03, 6.50753D-04
*      , 2.57346D-01 /
*      ,( AG(N,2,2),N=1,4)/ 1.51243D-04, 2.02244D+03, 6.50753D-04
*      , 2.57346D-01 /
DATA ( AG(N,1,3),N=1,4)/ 2.93447D-04, 1.23634D+04, 1.96134D-02
*      , 4.92937D-01 /
*      ,( AG(N,2,3),N=1,4)/ 3.19124D-04, 2.05417D+03, 4.64886D-03
*      , -1.43266D+00 /
DATA ( AG(N,1,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 1.00000D+00
*      , 0.00000D+00 /
*      ,( AG(N,2,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 1.00000D+00
*      , 0.00000D+00 /
DATA ( AG(N,1,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 1.00000D+00
*      , 0.00000D+00 /
*      ,( AG(N,2,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 1.00000D+00
*      , 0.00000D+00 /
C
DATA ( BG(N,1,1),N=1,6)/ 3.90118D-01, 2.64047D+00, 1.79946D+00
*      , 9.17799D+00, 2.31365D+01, 6.07538D+01/
*      ,( BG(N,2,1),N=1,6)/ 3.90118D-01, 2.64047D+00, 1.79946D+00
*      , 9.17799D+00, 2.31365D+01, 6.07538D+01/
DATA ( BG(N,1,2),N=1,6)/-1.19877D-01, 4.83281D+00,-1.04117D+00
*      , 1.28107D+01, 9.77240D+00, 6.14938D+01/
*      ,( BG(N,2,2),N=1,6)/-1.19877D-01, 4.83281D+00,-1.04117D+00
*      , 1.28107D+01, 9.77240D+00, 6.14938D+01/
DATA ( BG(N,1,3),N=1,6)/ 2.42590D-01, 7.33754D+00,-3.20191D+00
*      , 1.88331D+01, 3.94583D+00, 7.19859D+01/
*      ,( BG(N,2,3),N=1,6)/-5.55561D-01, 8.97592D+00,-8.04305D-01
*      , 2.29085D+01, 3.17568D+01, 1.51944D+02/
DATA ( BG(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,( BG(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( BG(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,( BG(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA ( CG(N,1,1),N=1,6)/ 3.02512D+02, 2.41081D-03,-8.14218D-07
*      , 9.69623D-01, 4.17946D-04,-8.32298D-08/
*      ,( CG(N,2,1),N=1,6)/ 2.97266D+02, 2.35586D-03,-8.26332D-07
*      , 9.69434D-01, 4.22861D-04,-8.11911D-08/
DATA ( CG(N,1,2),N=1,6)/ 2.15388D+02, 9.04415D-03,-2.83239D-06
*      , 8.33333D-01, 2.19035D-03,-8.43355D-09/
*      ,( CG(N,2,2),N=1,6)/ 2.15388D+02, 9.04415D-03,-2.83239D-06
*      , 8.33333D-01, 2.19035D-03,-8.43355D-09/

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DATA ( CG(N,1,3),N=1,6)/ 3.35053D+02,-4.36960D-01, 1.83657D-04
*      , 6.98966D-01, 6.74084D-03,-1.09662D-07/
*      ,( CG(N,2,3),N=1,6)/ 1.44656D+03, 3.06421D+00,-1.81241D-02
*      , 8.65365D-01, 4.15257D-02,-8.95715D-06/
DATA ( CG(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,( CG(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 1.00000D+00, 0.00000D+00, 0.00000D+00/
DATA ( CG(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*      ,( CG(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 1.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA ( DG(N,1,1),N=1,2)/ 0.00000D+00, 0.00000D+00/
*      ,( DG(N,2,1),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( DG(N,1,2),N=1,2)/ 0.00000D+00, 0.00000D+00/
*      ,( DG(N,2,2),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( DG(N,1,3),N=1,2)/-2.14845D+01, 9.21571D+03/
*      ,( DG(N,2,3),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( DG(N,1,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
*      ,( DG(N,2,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA ( DG(N,1,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
*      ,( DG(N,2,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA ( FG(N,1,1),N=1,4)/ 5.57168D-01, 2.78675D+00, 1.85168D+00
*      , 1.07188D+01 /
*      ,( FG(N,2,1),N=1,4)/ 5.57168D-01, 2.78675D+00, 1.85168D+00
*      , 1.07188D+01 /
DATA ( FG(N,1,2),N=1,4)/ 3.48245D-01, 4.39524D+00,-7.32274D-01
*      , 1.43431D+01 /
*      ,( FG(N,2,2),N=1,4)/ 3.48245D-01, 4.39524D+00,-7.32274D-01
*      , 1.43431D+01 /
DATA ( FG(N,1,3),N=1,4)/ 9.50847D-01, 6.26498D+00, 9.88924D+00
*      , 2.19575D+01 /
*      ,( FG(N,2,3),N=1,4)/ 8.34432D-01, 1.39037D+01, 1.68331D+01
*      , 2.79382D+02 /
DATA ( FG(N,1,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
*      ,( FG(N,2,4),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
DATA ( FG(N,1,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
*      ,( FG(N,2,5),N=1,4)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
C
DATA (ASAT(N,1,1),N=1,4)/ 4.50854D-04,-1.57919D-05, 1.69876D-07
*      ,-1.76528D-08 /
*      ,(ASAT(N,2,1),N=1,4)/ 4.50854D-04,-1.57919D-05, 1.69876D-07
*      ,-1.76528D-08 /
DATA (ASAT(N,1,2),N=1,4)/ 5.77921D-04,-2.08089D-05,-1.61242D-08
*      ,-6.56103D-09 /
*      ,(ASAT(N,2,2),N=1,4)/ 5.77921D-04,-2.08089D-05,-1.61242D-08
*      ,-6.56103D-09 /
DATA (ASAT(N,1,3),N=1,4)/ 1.80128D-03,-8.05016D-05, 4.82697D-08
*      ,-8.53040D-09 /
*      ,(ASAT(N,2,3),N=1,4)/ 4.71948D-03,-1.49028D-04,-2.68050D-06
*      , 2.18431D-08 /
DATA (ASAT(N,1,4),N=1,4)/ 1.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
*      ,(ASAT(N,2,4),N=1,4)/ 1.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
DATA (ASAT(N,1,5),N=1,4)/ 1.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
*      ,(ASAT(N,2,5),N=1,4)/ 1.00000D+00, 0.00000D+00, 0.00000D+00
*      , 0.00000D+00 /
C
DATA (BSAT(N,1,1),N=1,6)/-1.03373D-04,-1.47509D-10,-4.25199D-16
*      , 9.43396D-01, 2.30701D-02, 1.25429D-07/
*      ,(BSAT(N,2,1),N=1,6)/-1.03384D-04,-1.48030D-10,-3.78342D-16
*      , 8.01887D-01, 2.53025D-02, 7.62684D-08/
DATA (BSAT(N,1,2),N=1,6)/-9.11919D-05, 0.00000D+00, 0.00000D+00

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*           , 8.33333D-01, 4.03621D-02, 1.86344D-08/
*   , (BSAT(N,2,2),N=1,6)/-9.11919D-05, 0.00000D+00, 0.00000D+00
*           , 8.33333D-01, 4.03621D-02, 1.86344D-08/
DATA (BSAT(N,1,3),N=1,6)/-2.57567D-04, 3.02115D-08,-2.75445D-11
*           , 9.18640D-01, 5.35439D-02, 4.88971D-08/
*   , (BSAT(N,2,3),N=1,6)/-2.60256D-04,-1.20933D-06,-3.93217D-09
*           , 9.34903D-01, 1.69003D-01,-6.74881D-05/
DATA (BSAT(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*   , (BSAT(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (BSAT(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*   , (BSAT(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA (CSAT(N,1,1),N=1,6)/ 5.20115D+02, 4.38079D-04,-7.99968D-07
*           , 9.81132D-01, 1.93566D-03, 2.74910D-08/
*   , (CSAT(N,2,1),N=1,6)/ 5.14152D+02, 5.84459D-04,-8.30648D-07
*           , 9.81132D-01, 1.91882D-03, 2.59729D-08/
DATA (CSAT(N,1,2),N=1,6)/ 6.80662D+02, 3.91671D-02,-2.32314D-06
*           , 8.33333D-01, 4.14974D-03, 1.79897D-08/
*   , (CSAT(N,2,2),N=1,6)/ 6.80662D+02, 3.91671D-02,-2.32314D-06
*           , 8.33333D-01, 4.14974D-03, 1.79897D-08/
DATA (CSAT(N,1,3),N=1,6)/ 9.98522D+02, 1.14342D-01, 1.40119D-04
*           , 9.98522D-01, 2.76460D-03, 1.18490D-05/
*   , (CSAT(N,2,3),N=1,6)/ 4.76409D+03,-2.40058D+00, 1.06644D-02
*           , 9.42629D-01, 1.73392D-02, 2.85586D-05/
DATA (CSAT(N,1,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*   , (CSAT(N,2,4),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
DATA (CSAT(N,1,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
*   , (CSAT(N,2,5),N=1,6)/ 0.00000D+00, 0.00000D+00, 0.00000D+00
*           , 1.00000D+00, 0.00000D+00, 0.00000D+00/
C
DATA (BSL (N,1,1),N=1,2)/ 3.19439D-11, 2.05900D-01/
*   , (BSL (N,2,1),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (BSL (N,1,2),N=1,2)/ 8.62126D-12, 2.48538D-01/
*   , (BSL (N,2,2),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (BSL (N,1,3),N=1,2)/ 1.71700D-10, 3.26820D+00/
*   , (BSL (N,2,3),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (BSL (N,1,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
*   , (BSL (N,2,4),N=1,2)/ 0.00000D+00, 0.00000D+00/
DATA (BSL (N,1,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
*   , (BSL (N,2,5),N=1,2)/ 0.00000D+00, 0.00000D+00/
C
DATA (IFREE(N,1),N=1,2)/ 0, 0/
DATA (IFREE(N,2),N=1,2)/ 0, 0/
DATA (IFREE(N,3),N=1,2)/ 0, 0/
DATA (IFREE(N,4),N=1,2)/ 0, 0/
DATA (IFREE(N,5),N=1,2)/ 0, 0/
C
DATA (ISPN(N,1),N=1,2)/ 2, 2/
DATA (ISPN(N,2),N=1,2)/ 2, 2/
DATA (ISPN(N,3),N=1,2)/ 2, 2/
DATA (ISPN(N,4),N=1,2)/ 0, 0/
DATA (ISPN(N,5),N=1,2)/ 0, 0/
C
DATA (IMRK(N,1),N=1,2)/ 0, 0/
DATA (IMRK(N,2),N=1,2)/ 0, 0/
DATA (IMRK(N,3),N=1,2)/ 1, 0/
DATA (IMRK(N,4),N=1,2)/ 0, 0/
DATA (IMRK(N,5),N=1,2)/ 0, 0/
C
DATA (ISAE(N,1),N=1,2)/ 0, 0/
DATA (ISAE(N,2),N=1,2)/ 0, 0/
DATA (ISAE(N,3),N=1,2)/ 0, 0/
DATA (ISAE(N,4),N=1,2)/ 0, 0/

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DATA (ISAE(N,5),N=1,2)/ 0, 0/
C
C
C   DEFAULT DATA OF STRUCTURE INPUT
C
DATA FMELT ,CMELT ,WMELT / 0.5D+0 ,0.0D+0 ,0.0D+0/
DATA XCSTR           /1.0D+00/
DATA HKMUL           /1.0D+00 ,1.0D+00 ,1.0D+00/
DATA XWSTR           /1.0D+00/
DATA DWFAL           /2.0D-03/
DATA TWFAL           /1.541D+03/
DATA BETACW          /1.000D-01/
DATA TCRMIN          /3.000D-04/
DATA OHMF            /9.0D-01/
DATA OHMC            /1.8D-01/
+---- *IF DEF,BLOW,13
|
| DATA JGPL1,JGPL2   /IBM*0,IBM*0/
| DATA JGPU1,JGPU2   /IBM*0,IBM*0/
| DATA PGPL,PGPU     /IBM*1.0D+07,IBM*1.0D+07/
| DATA TGPL,TGPU     /IBM*1.0D+03,IBM*1.0D+03/
| DATA AGLS          /2.00D-06/
| DATA DHGB          /1.00D-04/
| DATA TMFAIL        /1.50D+02/
| DATA RJGB          /6.33293D+05/
| DATA GAMGB         /1.50D+00/
| DATA UOGB          /6.25D-04/
| DATA TOGB          /726.85D0/
| DATA AFRGB         /7.915D-02/
+----> DATA BFRGB         /-2.5D-01/
|
| DATA TL11G5,FL11G5 / 1.0D-3,1.0D+0 /
| DATA TL12G5,FL12G5 / 1.0D-2,1.0D+0 /
| DATA TL13G5,FL13G5 / 1.0D-2,1.0D+0 /
| DATA AKGAP         / 5.11043D-1 /
| DATA AHGAP         / 5.67826D+3 /
| DATA AHGMIN        / 1.00000D+2 /
| DATA AHGMAX        / 4.00000D+4 /
+---- *IF DEF,DPIN,6
|
| DATA FP34 ,FC34, TC34 / 0.1D+0 ,1.0D+0, 1.0D-03 /
| DATA PMELT         / 0.0D+0 ,1.0D+0 /
| DATA FAFAIL        / 0.0D+0, 0.8D+0, 0.5D+0 /
| DATA ES4ST, SGUTS0, FCT /7.82354D+05, 7.66D+8,-5.06D+5/
| DATA FEJ           / 0.50D+0 /
+----> DATA FRICT         / 1.0D+0 /
|
| DATA INPFLG        / NIPFLG*0/
| DATA LABORT        / .FALSE. /
C
C   DEFAULT DATA OF EOSREGION
C
DATA REGN             / 1 /
DATA MATEOS           / MNEOS*1 /
+---- *IF DEF,SW
C ---- SW PROBLEM
|
| DATA FMOL / 0.75D+0/
| DATA FKCR / 0.10D+0/
| DATA FLIMITER / 1.0D-3,1.0D-3,1.0D-6,1.0D-6/
| DATA HEATOPT / 0 /
| DATA QNAOH / 189.0D3 /
| DATA QNA20 / 176.0D3 /
| DATA WMNA,WMH ,WMO
| * / 23.0D+0, 1.0D+0, 16.0D+0 /
| DATA MAXITR / 30 /
| DATA EPSTR / 1.0D-4 /
+----> *EI
C

```

Table E-3. SIMMER-III Defaulted Variables for Neutronics.

```

+<---- *IF -DEF,URANUS
C
COMMON/SHLOCL/NOT1ST,SECOND
LOGICAL      NOT1ST,SECOND
DATA  NOT1ST/.FALSE./SECOND/.FALSE./
C
C 20 'NCNTL':  OPTIONAL SETTING NEUTRONICS
C
DATA NIOPT / 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0
&          , 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
&          , 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
&          , 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0
&          , 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
&          ,10*0, 10*0, 10*0, 10*0, 10*0
&          , 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0
&          , 88*0 /
C
C 21 'NPAR':  SIZE OF ARRAYS, NEUTRONICS MESH STRUCTURE
C           AND MISCELLANEOUS INTEGERS
C
* NCRAD,NCAXI, IT,JT ; NO INTIAL VALUE.
* NREGB, IXSREG, NEZFLG ; NO INTIAL VALUE.
* NFRAD, NFAXI ; SETS INITIAL VALUE BY CLRDIM ROUTINE.
C
DATA ISNT,IGM,IGD,NDKGRP,MT,LNISIP,NRXS/4,18,6,6,5,5,1/
DATA ITR,ICOS,IDIVR                      /0,0,1/
C
C 22 'NEDT':  EDITING CONTROL DATA
C
* LCELPT ; SETS INITIAL VALUE BY CLRDIM ROUTINE.
* IRGBND ; NO INTIAL VALUE.
C
DATA NEUPRI,IEDXST,IEDSFT,INVPRT,INVREG/1,0,0,0,0/
C
C 23 'NINI':  INITIAL CONDITION
C
* POWER, RAMPT, RCRATE, DSPECT ; NO INTIAL VALUE.
* RHOIN, GENTIN, OM ; SET TO ZERO BY NEIPRT. (ITR=0)
* ETAINP,BETINP ; NO INTIAL VALUE.
* DKHETI ; SETS INITIAL VALUE BY CLRDIM ROUTINE.
C
DATA IRAMPT                               /0/
DATA (DECAY(I),I=1,6) /0.13000D-01,0.31100D-01,0.13400D+00
&          ,0.34700D+00,0.14000D+01,0.37500D+01/
DATA (BETAD(I),I=1,6) /0.74200D-04,0.77670D-03,0.66800D-03
&          ,0.13674D-02,0.63970D-03,0.17530D-03/
DATA DKYLDs                               /0.0D+0/
DATA (DKYLD(I),I=1,6) / 1789.0D-05,23078.0D-06, 1282.0D-05
&          ,6987.0D-06, 939.0D-06, 3881.0D-06/
DATA (DKLAM(I),I=1,6) /19854.0D-05,14366.0D-06, 9362.0D-07
&          ,762.0D-07, 9725.0D-06, 8875.0D-10/
C
C 24 'NQUS':  QUASI-STATIC DATA
C
* IWTF,DTSH,DTSMAX ; SETS INITIAL VALUE BY DEFAULT BLOCK DATA.
C
DATA LIPSTP,ITGAMM,IQUASI,IFXUDL          /7,5,0,0/
DATA EPSG,EPSPHY                          /1.0D-5 ,1.0D-5/
DATA EPS4,EPS5,EPS6,EPS7,EPS8
& /0.02D+0, 5.0D+0, 1.0D+0, 1.0D+0, 1.0D+6/
DATA EPS9,EPS10,EPS11,EPS12,EPS13
& / 5.0D-1, 1.0D-2, 5.0D-1, 5.0D-1, 5.0D-1/
DATA EPS14,EPS15,EPS16,EPS17,EPS18
1 /2.50D-1, 2.50D-1, 2.50D-1, 0.08516D+0, 1.0D+1/
C
C 25 'NCNV':  ITERATION LIMITS AND CONVERGENCE CRITERIA
C
DATA ITLMOU,ITLMIN                        /200,50/
DATA EPSO,EPSPT,EPSFAC,EPSMIN,ERRFXU

```

```

      1 /1.0D-5 ,1.0D-5 ,1.5D+1 ,1.0D-6 ,1.0D-6/
C
C 26 'NSHL': SHIELDING FLAGS AND ITERATION LIMITS
C
C * NOXSCL ; SETS INITIAL VALUE BY CLRDIM ROUTINE.
C
      DATA ISHLD,ITLMBG                /0,10/
+<-- *IF -DEF,ISOTOPE,1
+-->      DATA ITEMIP                    /0/
      DATA EPSEBK                       /1.0D-3/
+<-- *IF DEF,ISOTOPE,1
+-->      DATA ISIGOD,ITEMOD            /2,2/
C
C 27 'NISO': ISOTOPE NAME
C
C * ISOTOP, NCMIX, LNMN ,LMC, AVDENS; NO INTIAL VALUE.
C * THDENS ; SET TO ZERO BY CLRDIM.
C
+<-- *IF1 DEF,ISOTOPE
C
C 28 'NHET': HETERO CROSS SECTION DATA
C
C * IHETE, INUCF ; SETS INITIAL VALUE BY CLRDIM ROUTINE.
C
      DATA RPEL,RCOOL                    /0.0D+0,0.0D+0/
+--> *EI1
C
C 29 'NFIK': POSDIF AND AWDD OPTION
C
      DATA (WDAMPA(N),N=1,NEIGM)        / NEIGM*0.D+0 /
      DATA (WDAMPR(N),N=1,NEIGM)        / NEIGM*0.D+0 /
C
C 30 'NSOU': SOURCE-INPUT
C
      DATA NSOUTM,ISOUTM,IITLAD,ISOUPR   /0,1,1,0/
      DATA GAMMAZ,EVAD,EVMAD,XLALAD,XLAHAD,XLAXAD,PODAD
& /1.0D+0 ,0.0D+0 ,1.0D+2 ,1.0D-2 ,5.0D-1 ,1.0D-3 ,1.0D+0/
      DATA (SOUSPE(N),N=1,NEIGM)        / NEIGM*0.0D+0 /
      DATA ((SOURCF(I,J),I=1,NEI),J=1,NEJ) / NEIJ*0.0D+0 /
      DATA (SOUPR(N),N=1,NSOUPR)         / NSOUPR*0.0D+0 /
      DATA (SOUTM(N),N=1,NSOUMX)         / NSOUMX*0.0D+0 /
      DATA (SOUMX(N),N=1,NSOUMX)         / NSOUMX*0.0D+0 /
C
+--> *EI

```

APPENDIX F

POST-PROCESSING FILE DESCRIPTION

The structure of a post-processing file (PPF) is based on AFDM, in other words a T6P format. However, SIMMER-III PPF has some differences from the previous codes. First, the mixed use of 4 byte words and 8 byte words in the AFDM PPF or SIMMER-III TAPE04 causes tedious treatment in processing the files. Therefore, all the word lengths in the SIMMER-III PPF were changed to 4 bytes. This will require some corrections to the existing post-processing programs such as T6P. Second, the fluid-dynamic models and variables are completely different from AFDM, the variable assignment to individual record types is changed from the AFDM PPF.

The list of record types currently in use is given in **Table F-1** with the numbers of FORTRAN records and brief descriptions. The list of all the variables assigned different record types is given **Table F-2**. If all the record types are dumped on a one file, the resultant PPF tends to become very large. Also the fluid dynamics and the neutronics dump variables at different intervals. Thus SIMMER-III currently dumps two PPFs, SIMPF for the fluid dynamics and SIMNP for the neutronics. Assignment of record types to the two PPFs is indicated in **Table F-1**. The nine record types 1-9 are dumped on SIMNP, and the rest on SIMPF.

Since the SIMPF format consists of all the component data of same physical variable, such as macroscopic density, it occupies useless file space even in analyzing a simple one- or two-component system. For example, all the liquid densities are output even in the case where only the sodium density is required for a sodium boiling analysis. Therefore, another post-processing file with a simpler format, called "base file" and named SIMBF, is prepared and can optionally be dumped. The user can specify each fluid dynamic variable to be output to this file, depending on his/her needs. The file format is indicated in **Table F-3**.

From the experience in SIMMER-II, SIMNP can become very large and complex to be handled portably. Many users are interested in quickly looking at the minimum neutronics results such as power and reactivity as soon as a calculation is finished. For this reason, an

additional PPF, named as SIMPK, is dumped, containing the neutronics time step summary information. The content of SIMPK is essentially the same as the record type 1 in SIMNP, but has a simple file structure of one un-formatted record per reactivity step. The list of variables stored in SIMPK is given in **Table F-4**.

The detailed pin model DPIN introduces some new variables related to the description of the fuel pin. The values of these variables can be saved by the user at specified time in a binary SIMFF file. A similar approach to what was adopted for the SIMBF file has been chosen to generate the SIMFF file. The file format is listed in **Table F-5**.

In the standard use of the PPF files, data are dumped as unformatted binary records. To make PPF files more portable in any computer installation, an option is available for writing files in a text format, except for SIMBF. This option is invoked by a user-specified flag in XCNTL (EDTOPT(3) > 0).

Table F-1. List of Record Types of Post-processing File.

Record type No.	PPF file	FORTTRAN Records	Contents
# 1	SIMNP	5	: Neutronics time step summary.
# 2	SIMNP	LNSIP+3	: Cell-wise number densities..
# 3	SIMNP	7	: Cell-wise data of effective macroscopic cross-sections.
# 4	SIMNP	11	: Geometries and isotopes.
# 5	SIMNP	9	: Cell-wise data of reactivity components.
# 6	SIMNP	6	: Cell-wise data of material density and temperature.
# 7	SIMNP	IGM*2+4	: Adjoint flux distribution.
# 8	SIMNP	IGM*2+3	: Real flux distribution.
# 9	SIMNP	4	: Reactivity components.
#10			: Not used.
#11			: Not used.
#12			: Not used.
#13	SIMPF	1	: Radius and axis for the fluid dynamics calculation.
#14	SIMPF	10+1	: Structure-field volume fractions.
#15	SIMPF	12+1	: Macroscopic densities of structure-field components.
#16	SIMPF	9+1	: Temperatures of structure-field components.
#17	SIMPF	9+1	: Specific volumes of structure-field components.
#18	SIMPF	9+1	: Specific internal energies of structure-field components.
#19	SIMPF	7+1	: Liquid-field volume fractions.
#20	SIMPF	13+1	: Macroscopic densities of liquid-field components.
#21	SIMPF	7+1	: Temperatures of liquid-field components.
#22	SIMPF	7+1	: Specific volumes of liquid-field components.
#23	SIMPF	7+1	: Specific internal energies of liquid-field components.
#24	SIMPF	7+1	: Temperature and macroscopic densities of vapor-field components.
#25	SIMPF	5+1	: Specific internal energy and volumes of vapor-field components.
#26	SIMPF	6+1	: Convectible interfacial areas of real liquid components.
#27	SIMPF	1+1	: Convectible interfacial area of the vapor mixture.
#28	SIMPF	4+1	: Convectible interfacial areas of particles.
#29	SIMPF	3+1	: Pressure, hydraulic diameter and virtual mass.
#30	SIMPF	3+1	: Axial velocities.
#31	SIMPF	3+1	: Radial velocities.
#32	SIMPF	1+1	: The virtual wall

- | | | | |
|-----|-------|-----|--|
| #33 | SIMPF | 5+1 | : Volume fraction, temperature, specific internal energy and macroscopic densities of fuel pin interior. |
| #34 | SIMPF | 7+1 | : Radii of liquid droplets, particles and bubbles in the bubbly flow region. |
| #35 | SIMPF | 7+1 | : Radii of liquid droplets and particles in the dispersed flow region. |

Table F-2. SIMMER-III Variables Stored in Post-processing Files.

(SIMNP for Record Types 1-9, and SIMPF for the rest)

FORTTRAN**Records No. No.Variable****Contents****Record type #1****:****Neutronics time step summary.**

(Integer type: 1 word = 4 bytes)

(Real type: 1 word = 8 bytes)

1.	1.	ID	Record-ID = 1.	
	2.	IR	Number of other FORTRAN records = 4.	
	3.	NIOPT	Time step flag. (=1: reactivity , =2:flux shape.)	
	4.	NDIM	Number of geometrical dimensions = 2.	
2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IGD	Number of delayed neutron groups.	
	2.	IDKGRP	Number of decay heating groups.	
4.	1.	DTH	Reactivity time step	(s)
	2.	DTSH	Flux shape time step.	(s)
	3.	XX	Reactivity in dollar.	(\$)
	4.	RAMP	Reactivity ramp rate.	(\$/s)
	5.	POWFS	Prompt fission power amplitude.	(-)
	6.	POWDK	Decay power amplitude.	(s)
	7.	PHY	Total power amplitude (POWFS+POWDK).	(-)
	8.	PINTG	Integrated amplitude.	(-)
	9.	TPOW	Total reactor power.	(W)
	10.	PINT	Integrated reactor power (neutronic energy).	(J)
	11.	REACT	Reactivity.	($\Delta k/k$)
	12.	TEBETA	Total effective delayed neutron fraction.	(-)
	13.	GENTIM	Neutron generation time.	(s)
	14.	OM	Inverse period.	(1/s)
5.	1.	EFBETA(1)	Effective delayed neutron fraction for each delayed neutron precursor group.	(-)
	:	:	:	
	IGD.	EFBETA(IGD)	(IGD : Number of delayed neutron groups)	
	IGD+1.	CUCT(1)	Delayed precursor concentration for each delayed neutron group.	(-)
	:	:	:	
	2*IGD.	CUCT(IGD)	(IGD : Number of delayed neutron groups)	
	1+2*IGD..	DKHET(1)	Decay heat fraction for each decay heating group.(-)	
	:	:	:	
	2*IGD.	DKHET	(IDKGRP : Number of decay heating groups)	

+IDKGRP. (IDKGRP)

Record type #2	:	Cell-wise number densities.
		(Integer type: 1 word = 4 bytes) (Real type: 1 word = 8 bytes)
1.	1.	ID Record-ID = 2.
	2.	IR Number of other FORTRAN records = LNISIP+2.
	3.	NIOPT Time step flag. (>0: flux shape time step.)
	4.	NDIM Number of geometrical dimensions = 2.
2.	1.	TH Time. (s)
	2.	KSTEP Flux shape time step number.
	3.	IRSTEP Reactivity time step number.
3.	1.	IT Total number of neutronics radial mesh cells.
	2.	JT Total number of neutronics axial mesh cells.
	3.	LNISIP Number of isotopes (or isotopic mixtures).
4.	1.	DENISO(1,ij) Number densities of isotope 1. (1/barn-m)
:	:	: (ij= 1,IT*JT; mesh cell)
3+LNISIP.	1.	DENISO(LNISIP,ij) Number densities of isotope LNISIP.

Record type #3	:	Cell-wise data of effective macroscopic cross-sections.
		(Integer type: 1 word = 4 bytes) (Real type: 1 word = 8 bytes)
1.	1.	ID Record-ID = 3.
	2.	IR Number of other FORTRAN records = 6.
	3.	NIOPT Time step flag. (>0: flux shape time step.)
	4.	NDIM Number of geometrical dimensions = 2.
2.	1.	TH Time. (s)
	2.	KSTEP Flux shape time step number.
	3.	IRSTEP Reactivity time step number.
3.	1.	IT Total number of neutronics radial mesh cells.
	2.	JT Total number of neutronics axial mesh cells.
	3.	IGM Number of neutron energy groups.
	4.	IGU Total number of up-scattering groups.
	5.	IGSCAT Number of scattering matrix elements (=IGM*2).
4.	1.	CELTOT(ij,g) Macroscopic total cross-section. (1/m) (ij= 1,IT*JT:mesh cell, g=1,IGM:energy group.)
5.	1.	CELFIS(ij,g) Macroscopic $v\Sigma_f$ cross-section. (1/m) (ij= 1,IT*JT:mesh cell, g=1,IGM:energy group.)
6.	1.	CELABS(ij,g) Macroscopic absorption cross-section. (1/m) (ij= 1,IT*JT:mesh cell, g=1,IGM:energy group.)
7.	1.	CELTMX(ij,g,g') Macroscopic scattering cross-section. (1/m) (ij= 1,IT*JT:mesh cell, g=1,IGM, g'=1,IGM:energy group.)

Record type #4 : **Geometries and isotopes.**

(Integer type: 1 word = 4 bytes)
(Real type: 1 word = 8 bytes)

1.	1.	ID	Record-ID = 4	
	2.	IR	Number of other FORTRAN records = 10.	
	3.	NIOPT	Time step flag. (>0)	
	4.	NDIM	Number of geometrical dimensions = 2.	
2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IT	Total number of neutronics radial mesh cells.	
	2.	JT	Total number of neutronics axial mesh cells.	
	3.	MHSO	Number of heat-source material components.	
	4.	LNISIP	Number of isotopes (or isotopic mixtures).	
	5.	MT	Number of materials.	
	6.	NRXS	Number of isotopic cross-section regions.	
4.	1.	XMECHB(itp)	Neutronics radial noding. (itp=1,IT+1: mesh cell boundary)	(m)
5.	1.	ZMECHB(jtb)	Neutronics axial noding. (jtp=1,JT+1: mesh cell boundary)	(m)
6.	1.	VOLUME(ij)	Neutronics mesh cell volume. (ij= 1,IT*JT:mesh cell)	(m ³)
7.	1.	NCMIX(mc,nx)	Material identification number. (mc=1,MHSO nx=1,NRXS)	
8.	1.	IXSREG(4,nx)	Cross-section region boundaries. (4:left, right, bottom, top, nx=1,NRXS)	
9.	1.	LNMN(m)	Number of isotopes in the material. (m=1,MT)	
10.	1.	LMC(n, m)	Isotope identification number. (n=1,LNISIP, m=1,MT)	
11.	1.	AISONAM(n)	Names of isotopes (or isotopic mixtures). (n=1,LNISIP)	

Record type #5 : **Cell-wise data of reactivity components.**
(Integer type: 1 word = 4 bytes)
(Real type: 1 word = 8 bytes)

1.	1.	ID	Record-ID = 5	
	2.	IR	Number of other FORTRAN records = 8.	
	3.	NIOPT	Time step flag. (=1: reactivity, =2:flux shape.)	
	4.	NDIM	Number of geometrical dimensions = 2.	
2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IT	Total number of neutronics radial mesh cells.	

	2.	JT	Total number of neutronics axial mesh cells.	
4.	1.	RHOCEL(ij)	Cell-wise net reactivity. (ij= 1,IT*JT)	(\$)
5.	1.	RHOPFS(ij)	Cell-wise reactivity due to prompt fissions. (ij= 1,IT*JT)	(\$)
6.	1.	RHODFS(ij)	Cell-wise reactivity due to delayed fissions. (ij= 1,IT*JT)	(\$)
7.	1.	RHOSCT(ij)	Cell-wise reactivity due to scatterings. (ij= 1,IT*JT)	(\$)
8.	1.	RHOTOT(ij)	Cell-wise reactivity due to total cross-section. (ij= 1,IT*JT)	(\$)
9.	1.	RHOLKG(ij)	Cell-wise reactivity due to leakage. (ij= 1,IT*JT)	(\$)

Record type #6 : Cell-wise data of material density and temperature.

(Integer type: 1 word = 4 bytes)
(Real type: 1 word = 8 bytes)

1.	1.	ID	Record-ID = 6	
	2.	IR	Number of other FORTRAN records = 5.	
	3.	NIOPT	Time step flag. (=1: reactivity , =2:flux shape.)	
	4.	NDIM	Number of geometrical dimensions = 2.	
2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IT	Total number of neutronics radial mesh cells.	
	2.	JT	Total number of neutronics axial mesh cells.	
	3.	MHSO	Number of heat-source material components.	
4.	1.	ROBR(ij,n)	Component density. (ij=1, IT*JT: mesh cell, n=1,MHSO : component number)	
	:			
	:			
5.	1.	TMBR(ij,n)	Component temperature. (ij=1, IT*JT: mesh cell, n=1,MHSO : component number)	(K)
	:			
	:			
6.	1.	ENERGY(ij,n)	Component energy. (ij=1, IT*JT: mesh cell, n=1,MHSO : component number)	(W/kg)
	:			
	:			

Record type #7 : Adjoint flux distribution.

(Integer type: 1 word = 4 bytes)
(Real type: 1 word = 8 bytes)

1.	1.	ID	Record-ID = 7.	
	2.	IR	Number of other FORTRAN records = IGM*2+3.	
	3.	NIOPT	Time step flag. (>0)	
	4.	NDIM	Number of geometrical dimensions = 2.	

2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IT	Total number of neutronics radial mesh cells.	
	2.	JT	Total number of neutronics axial mesh cells.	
	3.	IGM	Number of neutron energy groups.	
	4.	NDIR	Number of directions for negative flux fixup.	
4.	1.	ENGBND(g)	Neutron energy boundary.	(eV)
			(g=1,IGM+1: neutron energy boundary)	
5.	1.	ADFLUX(ij,1)	Adjoint flux for energy group 1.	(1/m ² *s)
	:	:	(ij=1,IT*JT : mesh cell.)	
4+IGM.	1.	ADFLUX(ij,IGM)	Adjoint flux for energy group IGM.	(1/m ² *s)
5+IGM.	1.	XXNEGF(ij,4,1)	The negative flux fixup percentage table for energy group 1.	
	:	:	(ij=1,IT*JT : mesh cell. 4:up, right,,down,left)	
4+IGM*2.	1.	XXNEGF(ij,4,IGM)	The negative flux fixup percentage table for energy group IGM.	

Record type #8 : **Real flux distribution.**
 (Integer type: 1 word = 4 bytes)
 (Real type: 1 word = 8 bytes)

1.	1.	ID	Record-ID = 8.	
	2.	IR	Number of other FORTRAN records = IGM*2+2.	
	3.	NIOPT	Time step flag. (>=1: flux shape time step.)	
	4.	NDIM	Number of geometrical dimensions = 2.	
2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IT	Total number of neutronics radial mesh cells.	
	2.	JT	Total number of neutronics axial mesh cells.	
	3.	IGM	Number of neutron energy groups.	
	4.	NDIR	Number of directions for negative flux fixup.	
4.	1.	CUFLUX(ij, 1)	Real flux for energy group 1.	(1/m ² *s)
	:	:	(ij=1,IT*JT : mesh cell)	
3+IGM.	1.	CUFLUX(ij, IGM)	Real flux for energy group IGM.	(1/m ² *s)
4+IGM.	1.	XXNEGF(ij,4,1)	Negative flux fixup percentage table for energy group 1.	
	:	:	(ij=1,IT*JT : mesh cell. 4:up, right,,down,left)	
3+IGM*2.	1.	XXNEGF(ij,4,IGM)	Negative flux fixup percentage table for energy group IGM.	

Record type #9 : **Reactivity components.**
 (Integer type; 1 word = 4 bytes)
 (Real type; 1 word = 8 bytes)

1.	1.	ID	Record-ID = 9
----	----	----	---------------

	2.	IR	Number of other FORTRAN records = 3.	
	3.	NIOPT	Time step flag. (=1: reactivity, =2:flux shape.)	
	4.	NDIM	Number of geometrical dimensions = 2.	
2.	1.	TH	Time.	(s)
	2.	KSTEP	Flux shape time step number.	
	3.	IRSTEP	Reactivity time step number.	
3.	1.	IT	Total number of neutronics radial mesh cells.	
	2.	JT	Total number of neutronics axial mesh cells.	
4.	1.	DPFIS	Reactivity due to prompt fissions.	(\$)
	2.	DDFIS	Reactivity due to delayed fissions.	(\$)
	3.	DSCAT	Reactivity due to scatterings.	(\$)
	4.	DTOTL	Reactivity due to total cross-section.	(\$)
	5.	DLEAK	Reactivity due to leakage.	(\$)
	6.	REAPRG	External reactivity.	(\$)

Record type #10-#12 : **Not used.**

Record type #13 : **Radius and axis for the fluid dynamics calculation (dumped from INIPP).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 13.0	
	2.	IBAR	Total number of radial mesh cells.	
	3.	JBAR	Total number of axial mesh cells.	
	4.	DRC(i)	The radial mesh size. (i= 1, IBAR)	(m)
	5.	DZC(j)	The axial mesh size. (j= 1, JBAR)	(m)
	6.	COLOUR(i)	Array of colors for plotting. (i= 1, 4)	
	7.	NAME(i)	Problem title. (i= 1, 18)	

Record type #14 : **Structure-field volume fractions (dumped from WTSTR).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 14.0	
	2.	IR	Number of other FORTRAN records = 10.	
	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	ALPSK1(i,j)	Volume fraction of pin fuel surface. (i = 1,IBAR, j= 1,JBAR)	(-)
3.	1.	ALPSK2(i,j)	Volume fraction of left crust fuel. (i = 1,IBAR, j= 1,JBAR)	(-)
4.	1.	ALPSK3(i,j)	Volume fraction of right crust fuel. (i = 1,IBAR, j= 1,JBAR)	(-)
5.	1.	ALPSK4(i,j)	Volume fraction of cladding.	(-)

			(i = 1,IBAR, j= 1,JBAR)	
6.	1.	ALPSK5(i,j)	Volume fraction of left can wall surface.	(-)
			(i = 1,IBAR, j= 1,JBAR)	
7.	1.	ALPSK6(i,j)	Volume fraction of left can wall interior.	(-)
			(i = 1,IBAR, j= 1,JBAR)	
8.	1.	ALPSK7(i,j)	Volume fraction of right can wall surface.	(-)
			(i = 1,IBAR, j= 1,JBAR)	
9.	1.	ALPSK8(i,j)	Volume fraction of right can wall interior.	(-)
			(i = 1,IBAR, j= 1,JBAR)	
10.	1.	ALPSK9(i,j)	Volume fraction of control.	(-)
			(i = 1,IBAR, j= 1,JBAR)	
11.	1.	ALPS0(i,j)	Volume fraction of total structure-field.	(-)
			(ALPS1+2+3+4+6+8+9+ALPINK+ALPNFK1+2+3+)	
			(i = 1,IBAR, j= 1,JBAR)	

Record type #15 : **Macroscopic densities of structure-field components (dumped from WTSTR).**
 (1 word = 4 bytes)

1.	1.	ID	Record-ID = 15.0	
		2.	IR	Number of other FORTRAN records = 12.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	RBSK1 (i,j)	Macroscopic density of fertile pin fuel surface.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
3.	1.	RBSK2 (i,j)	Macroscopic density of fissile pin fuel surface.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
4.	1.	RBSK3 (i,j)	Macroscopic density of left fertile crust fuel.(kg/m ³)	
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	RBSK4 (i,k,j j)	Macroscopic density of left fissile crust fuel.(kg/m ³)	
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	RBSK5 (i,j)	Macroscopic density of right fertile crust fuel.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
7.	1.	RBSK6 (i,j)	Macroscopic density of right fissile crust fuel.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
8.	1.	RBSK7 (i,j)	Macroscopic density of cladding.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
9.	1.	RBSK8 (i,j)	Macroscopic density of left can wall surface.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
10.	1.	RBSK9 (i,j)	Macroscopic density of left can wall interior.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
11.	1.	RBSK10 (i,j)	Macroscopic density of right can wall surface.	

		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
12.	1.	RSBK11 (i,j)	Macroscopic density of right can wall interior.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
13.	1.	RBSK12 (i,j)	Macroscopic density of control.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)

Record type #16 : **Temperatures of structure-field components (dumped from WTSTR).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 16.0	
		2. IR	Number of other FORTRAN records = 9.	
		3. T	Time.	(s)
		4. CYCLE	Fluid dynamics time step number.	(-)
2.	1.	TSK1(i,j)	Temperature of pin fuel surface.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	TSK2(i,j)	Temperature of left crust fuel.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	TSK3(i,j)	Temperature of right crust fuel.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	TSK4(i,j)	Temperature of cladding.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	TSK5(i,j)	Temperature of left can wall surface.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	TSK6(i,j)	Temperature of left can wall interior.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	TSK7(i,j)	Temperature of right can wall surface.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
9.	1.	TSK8(i,j)	Temperature of right can wall interior.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
10.	1.	TSK9(i,j)	Temperature of control.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #17 : **Specific volumes of structure-field components (dumped from WTSTR).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 17.0	
		2. IR	Number of other FORTRAN records = 9.	
		3. T	Time.	(s)
		4. CYCLE	Fluid dynamics time step number.	(-)
2.	1.	SVSK1(i,j)	Specific volume of pin fuel surface.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	SVSK2(i,j)	Specific volume of left crust fuel.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	SVSK3(i,j)	Specific volume of right crust fuel.	(m ³ /kg)

		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	SVSK4(i,j)	Specific volume of cladding.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	SVSK5(i,j)	Specific volume of left can wall surface.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	SVSK6(i,j)	Specific volume of left can wall interior.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	SVSK7(i,j)	Specific volume of right can wall surface.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
9.	1.	SVSK8(i,j)	Specific volume of right can wall interior.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
10.	1.	SVSK9(i,j)	Specific volume of control.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #18 : **Specific internal energies of structure-field components (dumped from WTSTR).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 18.0	
		2. IR	Number of other FORTRAN records = 9.	
		3. T	Time.	(s)
		4. CYCLE	Fluid dynamics time step number.	(-)
2.	1.	SIESK1(i,j)	Specific internal energy of pin fuel surface.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	SIESK2(i,j)	Specific internal energy of left crust fuel.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	SIESK3(i,j)	Specific internal energy of right crust fuel.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	SIESK4(i,j)	Specific internal energy of cladding.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	SIESK5(i,j)	Specific internal energy of left can wall surface.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	SIESK6(i,j)	Specific internal energy of left can wall interior.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	SIESK7(i,j)	Specific internal energy of right can wall surface.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
9.	1.	SIESK8(i,j)	Specific internal energy of right can wall interior.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
10.	1.	SIESK9(i,j)	Specific internal energy of control.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #19 : **Liquid-field volume fractions (dumped from WPPF).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 19.0	
		2. IR	Number of other FORTRAN records = 6.	

	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	ALPLK1(i,j)	Volume fraction of liquid fuel.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	ALPLK2(i,j)	Volume fraction of liquid steel.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	ALPLK3(i,j)	Volume fraction of liquid sodium.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	ALPLK4(i,j)	Volume fraction of solid fuel particles.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	ALPLK5(i,j)	Volume fraction of solid steel particles.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	ALPLK6(i,j)	Volume fraction of control particles.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	ALPLK7(i,j)	Volume fraction of fuel chunks.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #20 : **Macroscopic densities of liquid-field components (dumped from WPPF).**

(1 word = 4 bytes)

1.	1.	ID	Record-ID = 20.0	
	2.	IR	Number of other FORTRAN records = 10.	
	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	RBLK1 (i,j)	Macroscopic density of liquid fertile fuel.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	RBLK2 (i,j)	Macroscopic density of liquid fissile fuel.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	RBLK3 (i,j)	Macroscopic density of liquid steel.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	RBLK4 (i,j)	Macroscopic density of liquid sodium.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	RBLK5 (i,j)	Macroscopic density of fertile fuel particles.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	RBLK6 (i,j)	Macroscopic density of fissile fuel particles.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	RBLK7 (i,j)	Macroscopic density of steel particles.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
9.	1.	RBLK8 (i,j)	Macroscopic density of control particles.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
10.	1.	RBLK9 (i,j)	Macroscopic density of fertile fuel chunks.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
11.	1.	RBLK10 (i,j)	Macroscopic density of fissile fuel chunks.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
12.	1.	RBLK11 (i,j)	Macroscopic density of fission gas in liquid fuel.	

		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
13.	1.	RBLK12(i,j)	Macroscopic density of fission gas in fuel particles.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)
14.	1.	RBLK13(i,j)	Macroscopic density of fission gas in fuel chunks.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)

Record type #21 : **Temperatures of liquid-field components
(dumped from WPPF).** (1 word = 4 bytes)

1.	1.	ID	Record-ID = 21.0	
		2.	IR	Number of other FORTRAN records = 6.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	TLK1(i,j)	Temperature of liquid fuel. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	TLK2(i,j)	Temperature of liquid steel. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	TLK3(i,j)	Temperature of liquid sodium. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	TLK4(i,j)	Temperature of fuel particles. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	TLK5(i,j)	Temperature of steel particles. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	TLK6(i,j)	Temperature of control particles. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	TLK7(i,j)	Temperature of fuel chunks. (K)	
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #22 : **Specific volumes of liquid-field components
(dumped from WPPF).** (1 word = 4 bytes)

1.	1.	ID	Record-ID = 22.0	
		2.	IR	Number of other FORTRAN records = 6.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	SVLK1(i,j)	Specific volume of liquid fuel. (m ³ /kg)	
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	SVLK2(i,j)	Specific volume of liquid steel. (m ³ /kg)	
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	SVLK3(i,j)	Specific volume of liquid sodium. (m ³ /kg)	
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	SVLK4(i,j)	Specific volume of fuel particles. (m ³ /kg)	
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	SVLK5(i,j)	Specific volume of steel particles. (m ³ /kg)	
		:	(i = 1,IBAR, j= 1,JBAR)	

7.	1.	SVLK6(i,j)	Specific volume of control particles.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	SVLK7(i,j)	Specific volume of fuel chunks.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #23 : **Specific internal energies of liquid-field components (dumped from WPPF).**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 23.0	
		2.	IR	Number of other FORTRAN records = 6.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	SIELK1(i,j)	Specific internal energy of liquid fuel.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	SIELK2(i,j)	Specific internal energy of liquid steel.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	SIELK3(i,j)	Specific internal energy of liquid sodium.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	SIELK4(i,j)	Specific internal energy of fuel particles.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	SIELK5(i,j)	Specific internal energy of steel particles.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	SIELK6(i,j)	Specific internal energy of control particles.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	SIELK7(i,j)	Specific internal energy of fuel chunks.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	

Record type #24 : **Temperature and macroscopic densities of vapor-field components (dumped from WPPF)**
(1 word = 4 bytes)

1.	1.	ID	Record-ID = 24.0	
		2.	IR	Number of other FORTRAN records = 7.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	ALPGK(i,j)	Vapor volume fraction.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	TGK(i,j)	Temperature of vapor.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	RBGK1(i,j)	Macroscopic density of fertile fuel vapor.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	RBGK2(i,j)	Macroscopic density of fissile fuel vapor.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	RBGK3(i,j)	Macroscopic density of steel vapor.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	RBGK4(i,j)	Macroscopic density of sodium vapor.	(kg/m ³)

		:	(i = 1,IBAR, j= 1,JBAR)	
8.	1.	RBGK5(i,j)	Macroscopic density of fission gas.	(kg/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)	
Record type #25		:	Specific internal energy and volumes of vapor-field components (dumped from WPPF).	
				(1 word = 4 bytes)
1.	1.	ID	Record-ID = 25.0	
		2.	IR	Number of other FORTRAN records = 5.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	SIEGK(i,j)	Specific internal energy of vapor.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	SVGK1(i,j)	Specific volume of fuel vapor.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	SVGK2(i,j)	Specific volume of steel vapor.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	SVGK3(i,j)	Specific volume of sodium vapor.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	SVGK4(i,j)	Specific volume of fission gas.	(m ³ /kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
Record type #26		:	Convectible interfacial areas of real liquid components (dumped from WPPF).	
				(1 word = 4 bytes)
1.	1.	ID	Record-ID = 26.0	
		2.	IR	Number of other FORTRAN records = 6.
		3.	T	Time. (s)
		4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	SALMBK1(i,j)	Convectible interfacial area of liquid fuel in the bubbly region.	(1/m)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	SALMBK2(i,j)	Convectible interfacial area of liquid steel in the bubble region.	(1/m)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	SALMBK3(i,j)	Convectible interfacial area of liquid sodium in the bubbly region.	(1/m)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	SALMDK1(i,j)	Convectible interfacial area of liquid fuel in the dispersed region.	(1/m)
		:	(i = 1,IBAR, j= 1,JBAR)	
6.	1.	SALMDK2(i,j)	Convectible interfacial area of liquid steel in the dispersed region.	(1/m)
		:	(i = 1,IBAR, j= 1,JBAR)	
7.	1.	SALMDK3(i,j)	Convectible interfacial area of liquid sodium in the dispersed region.	(1/m)

	:		(i = 1,IBAR, j= 1,JBAR)
Record type #27	:		Convectible interfacial area of the vapor mixture (dumped from WPPF). (1 word = 4 bytes)
1.	1.	ID	Record-ID = 27.0
		2.	IR
		3.	T
		4.	CYCLE
2.	1.	SAGBK(i,j)	Fluid dynamics time step number. (-)
		:	Convectible interfacial area of the vapor mixture. (i = 1,IBAR, j= 1,JBAR) (1/m)
Record type #28	:		Convectible interfacial areas of particles (dumped from WPPF). (1 word = 4 bytes)
1.	1.	ID	Record-ID = 28.0
		2.	IR
		3.	T
		4.	CYCLE
2.	1.	SALMBK4 (i,j)	Number of other FORTRAN records = 3.
		:	Time. (s)
3.	1.	SALMBK5(i,j)	Fluid dynamics time step number. (-)
		:	Convectible interfacial area of fuel particles. (1/m)
4.	1.	SALMBK6(i,j)	(i = 1,IBAR, j= 1,JBAR)
		:	Convectible interfacial area of steel particles. (1/m)
5.	1.	SALMBK7(i,j)	(i = 1,IBAR, j= 1,JBAR)
		:	Convectible interfacial area of control particles. (i = 1,IBAR, j= 1,JBAR) (1/m)
		:	Convectible interfacial area of fuel chunks. (1/m)
		:	(i = 1,IBAR, j= 1,JBAR)
Record type #29	:		Pressure, hydraulic diameter and virtual mass (dumped from WPPF). (1 word = 4 bytes)
1.	1.	ID	Record-ID = 29.0
		2.	IR
		3.	T
		4.	CYCLE
2.	1.	PK(i,j)	Number of other FORTRAN records = 3.
		:	Time. (s)
3.	1.	DHK(i,j)	Fluid dynamics time step number. (-)
		:	Pressure. (Pa)
4.	1.	VMK(i,j)	(i = 1,IBAR, j= 1,JBAR)
		:	Hydraulic diameter. (m)
		:	(i = 1,IBAR, j= 1,JBAR)
		:	Virtual mass (Pa/m ³)
		:	(i = 1,IBAR, j= 1,JBAR)
Record type #30	:		Axial velocities (dumped from WPPF) (1 word = 4 bytes)
1.	1.	ID	Record-ID = 30.0
		2.	IR
			Number of other FORTRAN records = 3.

	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	VK1(i,j)	Axial velocity of liquid field 1.	(m/s)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	VK2(i,j)	Axial velocity of liquid field 2.	(m/s)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	VKG(i,j)	Axial velocity of vapor field.	(m/s)
		:	(i = 1,IBAR, j= 1,JBAR)	
Record type #31		:	Radial velocities (dumped from WPPF).	
				(1 word = 4 bytes)
1.	1.	ID	Record-ID = 31.0	
	2.	IR	Number of other FORTRAN records = 3.	
	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	UK1(i,j)	Radial velocity of liquid field 1.	(m/s)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	UK2(i,j)	Radial velocity of liquid field 2.	(m/s)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	UKG(i,j)	Radial velocity of vapor field.	(m/s)
		:	(i = 1,IBAR, j= 1,JBAR)	
Record type #32		:	The virtual wall (dumped from WPPF).	
				(1 word = 4 bytes)
1.	1.	ID	Record-ID = 32.0	
	2.	IR	Number of other FORTRAN records = 1.	
	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	WALLK	The virtual wall	(-)
Record type #33		:	Volume fraction, temperature, specific internal energy and macroscopic densities of pin fuel interior (dumped from WPPF).	
				(1 word = 4 bytes)
1.	1.	ID	Record-ID = 33.0	
	2.	IR	Number of other FORTRAN records = 5.	
	3.	T	Time.	(s)
	4.	CYCLE	Fluid dynamics time step number.	(-)
2.	1.	ALPINK(i,j)	Volume fraction of pin fuel interior.	(-)
		:	(i = 1,IBAR, j= 1,JBAR)	
3.	1.	TIPINK(i,j)	Temperature of pin fuel interior.	(K)
		:	(i = 1,IBAR, j= 1,JBAR)	
4.	1.	EIPINK(i,j)	Specific internal energy of pin fuel interior.	(J/kg)
		:	(i = 1,IBAR, j= 1,JBAR)	
5.	1.	RBIK1(i,j)	Macroscopic density of fertile pin fuel interior.	
		:	(i = 1,IBAR, j= 1,JBAR)	(kg/m ³)

6.	1.	RBIK2(i,j) :	Macroscopic density of fissile pin fuel interior. (i = 1,IBAR, j= 1,JBAR) (kg/m ³)
Record type #34		:	Radii of droplets, particles and bubbles in the bubbly flow region (dumped from WPPF). (1 word = 4 bytes)
1.	1.	ID	Record-ID = 34.0
	2.	IR	Number of other FORTRAN records = 7.
	3.	T	Time. (s)
	4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	RGBK(i,j) :	Radius of bubbles in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
3.	1.	RLMBK1(i,j) :	Radius of liquid fuel droplets in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
4.	1.	RLMBK2(i,j) :	Radius of liquid steel droplets in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
5.	1.	RLMBK3(i,j) :	Radius of liquid sodium droplets in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
6.	1.	RLMBK4(i,j) :	Radius of fuel particles in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
7.	1.	RLMBK5(i,j) :	Radius of steel particles in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
8.	1.	RLMBK6(i,j) :	Radius of control particles in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
9.	1.	RLMBK7(i,j) :	Radius of fuel chunks in the bubbly flow region. (m) (i = 1,IBAR, j= 1,JBAR)
Record type #35		:	Radii of droplets and particles in the dispersed flow region (dumped from WPPF). (1 word = 4 bytes)
1.	1.	ID	Record-ID = 35.0
	2.	IR	Number of other FORTRAN records = 6.
	3.	T	Time. (s)
	4.	CYCLE	Fluid dynamics time step number. (-)
2.	1.	RLMDK1(i,j) :	Radius of liquid fuel droplets in the dispersed flow region. (m) (i = 1,IBAR, j= 1,JBAR)
3.	1.	RLMDK2(i,j) :	Radius of liquid steel droplets in the dispersed flow region. (m) (i = 1,IBAR, j= 1,JBAR)

4.	1.	RLMDK3(i,j)	Radius of liquid sodium droplets in the dispersed flow region. (m)
		:	(i = 1,IBAR, j= 1,JBAR)
5.	1.	RLMDK4(i,j)	Radius of fuel particles in the dispersed flow region. (m)
		:	(i = 1,IBAR, j= 1,JBAR)
6.	1.	RLMDK5(i,j)	Radius of steel particles in the dispersed flow region. (m)
		:	(i = 1,IBAR, j= 1,JBAR)
7.	1.	RLMDK6(i,j)	Radius of control particles in the dispersed flow region. (m)
		:	(i = 1,IBAR, j= 1,JBAR)
8.	1.	RLMDK7(i,j)	Radius of fuel chunks in the dispersed flow region. (m)
		:	(i = 1,IBAR, j= 1,JBAR)

Table F-3. List of Record Types of Base File (SIMBF).

The base file consists of 2 parts, i.e. header part and data substances. The header part appears at the beginning of SIMBF and contains the information on the geometry, number of variables, and the names of variables. The data substances are repeated until the end of the calculational time and contains the time, cycle, and the variable values at each time point.

Header part

Record	Variables
#1	CASE
#2	IB, JB, DR (IB), DZ (JB), I1, I2, J1, J2
#3	NV, MV, IV
#4	SN(1),FN,....., SN(NV) ,FN

Data substance

Record	Variables
#1	TIMEC, NCYCC
#2	((DATAC(i, j, 1), i=I1,I2) , j=J1,J2)
.....	
#1+Nv	((DATAC(i, j, NV), i=I1,I2) , j=J1,J2)
#2+Nv	((VB(i, j, l), i=1,IB) , l=1,IV) *1
#3+Nv	((UL(i, j, l), j=1,JB) , l=1,IV) *1
*1	This record exists only if $IV \geq 1$.

Variable	description
CASE	Case identification.
IB	Number of radial meshes.
JB	Number of axial meshes.
DR	Radial mesh width.
DZ	Axial mesh width.
I1	Left-most address of the rectangular region which is output to this file.
I2	Right-most address of the rectangular region which is output to this file.
J1	Lower-most address of the rectangular region which is output to this file.
J2	Upper-most address of the rectangular region which is output to this file.
NV	Number of variables output to this file.
MV	Not used.
IV	Number of velocity fields which bottom and right boundary velocities are written as VB and UL respectively.
FN	Blank card (64 byte).

TIMEC	Calculational time for DATAC.
NCYCC	Calculational cycle for DATAC.
DATAC	Calculated variable at TIMEC and CYCC
VB	Bottom boundary velocities.
UL	Left boundary velocities.

The variables to be sent to base file is specified by input variable SN in NAMELIST group XEDT. The same variable names in the record type #14 up to #34 in **Table F-2** can be used to specify the variable. In addition, the following variables which are frequently required in interpreting the calculated results are included.

PSAT1	Saturation pressure of fuel at its liquid temperature.
PSAT2	Saturation pressure of steel at its liquid temperature.
PSAT3	Saturation pressure of sodium at its liquid temperature.
TSATI1	Saturation temperature of fuel at the steel vapor partial pressure.
TSATI2	Saturation temperature of steel at the steel vapor partial pressure.
TSATI3	Saturation temperature of sodium at the steel vapor partial pressure.
TSAT1	Saturation temperature of fuel at the cell pressure.
TSAT2	Saturation temperature of steel at the cell pressure.
TSAT3	Saturation temperature of sodium at the cell pressure.
PGMK1	Partial pressure of fuel vapor.
PGMK2	Partial pressure of steel vapor.
PGMK3	Partial pressure of sodium vapor.
PGMK4	Partial pressure of non-condensable gas.
ALPGE	Effective void fraction.
UMQ1	Radial momentum of velocity field 1.
UMQ2	Radial momentum of velocity field 2.
UMQ3	Radial momentum of velocity field 3.
VMQ1	Axial momentum of velocity field 1.
VMQ2	Axial momentum of velocity field 2.
VMQ3	Axial momentum of velocity field 3.
FALRAT	Mechanical failure fraction for the code option DPIN.
RBCA1	Macroscopic density of fertile fuel in cavity for the code option DPIN.
RBCA2	Macroscopic density of fissile fuel in cavity for the code option DPIN.
RBCA3	Macroscopic density of dissolved fission gas in cavity for the code option DPIN.
RBCA4	Macroscopic density of free fission gas in cavity for the code option DPIN.
PC	Cavity pressure for the code option DPIN.
ECA	Specific internal energy of cavity mixture for the code option DPIN.
TC	Cavity temperature for the code option DPIN.

GPC	Fuel mass transfer from solid fuel to the cavity for the code option DPIN.
RCAV	Fuel pin cavity radius for the code option DPIN.
VCA	Axial velocity of fuel and gas mixture in cavity for the code option DPIN.
GAPC	Mass transfer rate between fuel pellet and cavity for the code option DPIN.
QPC	Energy transfer rate between fuel pellet and cavity for the code option DPIN.
FCAV	Fuel melt fraction for the code option DPIN.
HGS	Gas-side heat transfer coefficient between gas and structure.
PRAG	Prandtl number of gas mixture.
REYG	Reynolds number of gas mixture in axial direction.
VISG	Viscosity of gas mixture.
CPG	Specific heat of gas mixture.
KPG	Thermal conductivity of gas mixture.
VQG	Axial velocity of velocity field q_3 .
DHG	Hydraulic diameter.
VSG	Specific volume of gas mixture.
HRSO	Sodium-side heat transfer coefficient between sodium and structure.

Table F-4. SIMMER-III Variables Stored in Post-processing File.
(SIMPk for Neutronics Time Step Summary)

FORTTRAN			
Records No.	No.	Variable	Contents
			(1 word = 4 bytes)
1.	1.	TH	Reactivity time. (s)
	2.	DTH	Reactivity time step. (s)
	3.	CYCLE	Fluid dynamics time step number. (-)
	4.	XX	Reactivity in dollar. (\$)
	5.	RAMP	Reactivity ramp rate. (\$/s)
	6.	POWFS	Prompt fission power amplitude. (-)
	7.	POWDK	Decay power amplitude. (-)
	8.	PHY	Total power amplitude (POWFS+POWDK). (-)
	9.	PINTG	Integrated amplitude. (-)
	10.	TPOW	Total reactor power. (W)
	11.	PINT	Integrated reactor power (neutronic energy). (J)
	12.	REACT	Reactivity. ($\Delta k/k$)
	13.	TEBETA	Total effective delayed neutron fraction. (-)
	14.	GENTIM	Neutron generation time. (s)
	15.	OM	Inverse period. (1/s)

**Table F-5. List of Record Types of Post-processing File (SIMFF).
(SIMFF for Detailed Pin Model)**

Similar to the base file (SIMBF), SIMFF consists of 2 parts, i.e. header part and data substances. The header part appears at the beginning of the file and contains the information on the geometry, number of variables, and the names of variables. The data substances are repeated until the end of the calculational time and contain the time, cycle, and the variable values at each time point.

The user can select each one of the fuel variables to be saved by specifying the input variables SF in NAMELIST group XEDT. The variables will be dumped every cycle based on BSFC in NAMELIST group XEDT at the same frequency as done for the dumping in the SIMBF file.

Header part

Record	Variables
#1	CASE
#2	IB, JB, ICL, JCR, JCB, JCT, NPB, DR (IB), DZ (JB)
#3	NSF
#4	SF(1), FN, •••••, SF(NV), FN

Data substance

Record	Variables
#1	TIMEC, NCYCC
#2	((DATA(n, i, j), n=1,NPB+1), i=ICL,ICR) , j=JCB,JCT)

Variable	description
CASE	Case identification.
IB	Number of radial meshes.
JB	Number of axial meshes.
ICL	Left-most address of the rectangular region which is output to this file.
ICR	Right-most address of the rectangular region which is output to this file.
JCB	Lower-most address of the rectangular region which is output to this file.
JCT	Upper-most address of the rectangular region which is output to this file.
NPB	Number of radial nodes in the fuel.
DR	Radial mesh width.
DZ	Axial mesh width.
NV	Number of variables output to this file.

SF	Name of fuel variables to be dumped in SIMFF. The variables to be sent to file is specified by input variable SF in NAMELIST group XEDT.
FN	Blank card (64 byte).
TIMEC	Calculational time for DATAC.
NCYCC	Calculational cycle for DATAC.
DATAC	Calculated variable at TIMEC and CYCC. These variables are;
RP	Fuel radius.
RBPIP	Fuel macroscopic density.
EP	Fuel specific internal energy.
TPIP	Fuel temperature.
SVPIP	Fuel specific volume.
EPP	Fuel porosity.
HPIP	Heat transfer coefficient.
ARSIP	Heat transfer area.
QHPIP	Fuel nuclear power (specific internal energy generation rate).

APPENDIX G

INPUT MANUAL (Version 3.A)

The input for SIMMER-III (S-III) is in a NAMELIST style. In this format, the input variables are divided into classes that correspond to different NAMELISTs. Namely, each class is distinguished by a different NAMELIST name. In an input stream, NAMELIST classes can be freely ordered except that the first three classes, START, XCNTL and XMSH, must be specified in this order at the beginning of an input deck. Also the input variables may be freely ordered in each NAMELIST class:

XCNTL, XMSH, XTME, XRGN, XCWD, XEDT, XEOS, XMXF, XIFA, XHTC, XBND, XTPP, XSOS, XHMT, XSTR, XMSC, XERG, XSWC, NCNTL, NPAR, NEDT, NINI, NQUS, NCVN, NSHL, NISO, NHET and NSOU.

All the variables, except for the mesh-cell variables, are given their default values. Any number of comment cards may be entered between NAMELIST groups, since they are simply ignored.

There is a special integer input class in the NAMELIST XCNTL containing option control flags, so that all the problem control inputs are specified and listed in a concise table. These are sub-divided into several option flag variables: ALGOPT for the fluid-dynamics algorithm; EOSOPT for the EOS; and so forth. Also available is an integer input class in the NAMELIST NCNTL containing option control flags for the neutronics.

Fluid-dynamics mesh-cell variables are specified by cell regions (XRGN). Region boundaries can overlap one another, and in this case later input overrides the former specification. In addition, all the cell variables can also be specified mesh-cell-wise through XCWD. The cell-wise input overrides the region-wise specification. Many of the input variables have dimensions. Definition of the dimension indexes used in S-III is attached to this input manual (Attachment 1). Edit control input variables for the fluid dynamics need a detailed description, which is also given in the attachment to this appendix (Attachment 2). Finally the alphabetic index of input variables is given in Attachment 3, providing a cross-reference between variables and NAMELIST classes.

List of NAMELIST Names

	<u>Page</u>	<u>Name</u>	<u>Description</u>
1.	3	START	The first input card, to specify whether the run is new or whether the run is restarting from a dump (not in NAMELIST format).
2.	4	XCNTL	Control and option input variables.
3.	29	XMSH	Fluid-dynamics mesh input variables.

These first three input classes must be entered in the above order. The remaining NAMELIST classes may be entered in any order and, if desired, several times.

4.	30	XTME	Time and time-step control.
5.	31	XRGN	Fluid-dynamics region-dependent input variables.
6.	35	XCWD	Fluid-dynamics mesh-cell-wise input variables.
7.	39	XEDT	Edit and output control input variables.
8.	41	XEOS	Equation-of-state model input variables.
9.	45	XXMF	Momentum exchange model input variables.
10.	50	XIFA	Interfacial-area model input variables.
11.	55	XHTC	Heat-transfer coefficients model input variables.
12.	58	XBND	Boundary conditions input variables.
13.	62	XTPP	Thermophysical properties input variables.
14.	64	XSOS	Heat source input variables (URANUS option only).
15.	65	XHMT	Heat and mass transfer model input variables.
16.	69	XSTR	Structure model input variables.
17.	73	XMSC	Miscellaneous input variables.
18.	76	XERG	Material region input variables.
19.	78	XSWC	The Sodium-Water reaction input variables.
20.	79	NCNTL	Neutronics option flag input variables.
21.	83	NPAR	Neutronics integer control input variables.
22.	85	NEDT	Neutronics edit control input variables.
23.	86	NINI	Neutronics initialization input variables.
24.	87	NQUS	Neutronics quasi-static method control input variables.
25.	89	NCNV	Neutron flux shape convergence control input variables.
26.	90	NSHL	Shielding factor related input variables.
27.	91	NISO	Isotope and cross-section related input variables.
28.	92	NHET	Additional input variables for treating heterogeneity and up-scattering.
29.	93	NSOU	The neutronics input variables for source-driven reactors.

List of Attachments to the NAMELISTs

<u>Page</u>	<u>Description</u>
94	Attachment 1: Definition of Dimension Indexes.
97	Attachment 2: Description of Output Control Variables.
104	Attachment 3: Index of Input Variables.

1. The First Card of the Input Deck

The first card of the input deck begins with either the word **START** (for starting a run) or else with the word **RESTART** (for restarting the run from a dump). If this card does not begin with **RESTART**, the run is regarded as a **START**. This card has 80 characters at most and must be given for every run. On the **RESTART** card, the last field is **NDMP** (the previous dump file sequential number to use for the restart). If **NDMP** > 0, the run is restarted from dump **NDMP**. If **NDMP** < 0, the run is restarted from the last dump on the file. If **NDMP** = 0, the run is restarted from the first dump on the file. Although the user has the freedom to change all input data items when restarting from a dump, care should be taken not to cause unwanted inconsistencies since the mesh variables are not re-initialized.

FORMAT:

- a. **START** : a S-III run is started from a new set of input data.
- b. **RESTART** : S-III is restarted from the previous dump **NDMP**.

2. XCNTL

Run control and option control input variables. This NAMELIST class is further subdivided into several option flag variables that can be ordered freely. All the standard or recommended input values are now defaulted, and hence the options in this NAMELIST class need be explicitly defined only when special controls are required.

Variable	Dimension	Default	Description
ALGOPT	(100)		Code control option flags for fluid-dynamics algorithm.
	1	0	Option for the pressure matrix solver. =0 : Direct banded-matrix inversion method. ≠0 : Preconditioned conjugate gradient (PCG) method, which is faster than the direct method when the number of cells is greater than about 1000 and EITRF (NAMELIST /XMSC/) is 10^7 . =1 : ILUCR (Incomplete Lower and Upper decomposition Conjugate Residuals). =2 : Modified ILUCR, where the weighting parameters for diagonal and off-diagonal columns are used in the LU decomposition (subroutine NDECMP). =3 : ILUBCG (Incomplete Lower and Upper decomposition Bi-Conjugate Gradient). =4 : Modified ILUBCG (recommended when the PCG solver is used).
	2	0	Flag to select the initial guess for the PCG solver. ≠0 : The previous solution is used as the initial guess. =0 : The initial guess is zero. '0' is recommended when the PCG solver is selected because the initial guess was found to have only a minor effect on convergence.
	3	0	Option to use the relaxation method to reduce the error from source-term decoupling. =1 : Use source term decoupling relaxation Method-1. =0 : Do not use the relaxation method. '0' is recommended.
	4	0	Time-step control options for reducing the source-term splitting error. =0 : No restriction on time-step size. =±1 : If the source-term splitting error is large at a cycle, the cycle is re-calculated with its time step halved. =±2 : If the source-term splitting error is large at a cycle, the time-step in the next cycle is set to be $\Delta t/DTINC$, depending on the source-term splitting error, where DTINC is a variable in the NAMELIST /XTME/.

Variable	Dimension	Default	Description
			<p><0 : The time-step control status is printed.</p> <p>The source-term splitting error is large if the following condition is satisfied in any two-phase cell:</p> $ P_{EOS}^{Step 2} - P_{Cell}^{Step 4} / P_{Cell}^{Step 2} > DPMK4,$ $ T_G^{Step 2} - T_G^{Step 1} / T_G^{Step 1} > DTGMK1, \text{ or}$ $ T_G^{Step 2} - T_G^{Step 4} / T_G^{Step 2} > DTGMK4,$ <p>where DPMK1, DPMK4, DTGMK1, and DTGMK4 are variables in the NAMELIST /XMSC/.</p>
5	1	1	<p>Options for the slope calculation in the higher-order differencing scheme.</p> <p>=1 : Original (the same as AFDM).</p> <p>=2 : Corrected slope for the original.</p> <p>=3 : Monotonized central differencing replaced by MINMOD function.</p> <p>=4 : Monotonized central differencing replaced by van Leer slope.</p>
6	0	0	<p>Option to select the convergence criterion for the pressure iteration in STEP3.</p> <p>=1 : Convergence is achieved when <i>Criterion(1)</i> or <i>Criterion(2)</i>.</p> <p>=0 : Convergence is achieved when <i>Criterion(1)</i> only is met.</p>
7			Not currently used.
8	0	0	<p>Option to specify the velocity fields between which drag is calculated. The option is used in subroutines VITERP and VITER, which are called by STEP2 and STEP4, respectively.</p> <p>=1 : Solve the “drag interaction” between velocity fields q2 and q3.</p> <p>=0 : Solve the “drag interaction” between velocity fields q1, q2 and q3.</p>
9*	1	1	<p>Flag to determine the type of differencing scheme used to solve the mass and momentum equations.</p> <p>=1 : Higher order differencing is used.</p> <p>=0 : Donor cell differencing is used.</p>
10*	1	1	<p>Flag to determine the type of differencing scheme used to solve the energy equation.</p> <p>=1 : Higher order differencing is used.</p>

Variable	Dimension	Default	Description
			=0 : Donor cell differencing is used.
			*) These two control variables should normally be either on or off simultaneously.
11	0	0	Flag to specify how the velocity gradient is evaluated. This is used in subroutines DFDR and DFDZ to evaluate the turbulent effect on the IFA source terms. =1 : Second order evaluation of the gradient. =0 : First order evaluation of the gradient.
12	0	0	Flag to force donor cell differencing. =1 : The differencing scheme is forced to be donor cell, even when ALGOPT(9)=1 and/or ALGOPT(10)=1, by setting the slope to zero in subroutines RSLOPE and ASLOPE. =0 : Donor cell differencing is not forced (the type of differencing scheme depends on the values of ALGOPT(9) and ALGOPT(10)).
13	0	0	Option to use a remedy in subroutines RSLOPE and ASLOPE to avoid a numerical error. =0 : Use the remedy. =1 : Do not use the remedy.
14-19			Not currently used.
20	0	0	Option to calculate the pressure-volume work due to intra-cell mass transfer in STEP1. =1 : The STEP1 pressure-volume work is calculated. =0 : Pressure-volume work is not calculated.
21			Not currently used.
22	0	0	Option to calculate the energy dissipation due to structure friction (in subroutine EAJHIQ). =1 : Energy dissipation due to the structure friction is calculated. =0 : Energy dissipation is not calculated.
23	0	0	Control variable to prevent the vapor specific internal energy from becoming too low due to convection calculation. This option must be applied very carefully because it may affect the vapor temperature greatly. =0 : No restriction on vapor energy. =1 : Non-negative restriction on vapor energy.
24, 25			Control variable to select the remedy for spurious pressure generation in a single phase cell. In some cases, volume changes due to mass transfer and temperature change in STEP1 cause spurious pressure spike which results in a very small time step size and/or pressure iteration failure

Variable	Dimension	Default	Description
			especially if the cell is single phase. This is because the volume changes in STEP1 are not taken into account in the convection calculation in STEP2. These flags select the remedy to this problem.
24		0	<p>=0 : No remedy is taken.</p> <p> ALGOPT(24) =1 : The excessive volumes of liquid fuel and liquid steel are transferred to the neighboring upper cell.</p> <p> ALGOPT(24) =2 : The excessive volumes of liquid fuel, liquid steel and particles are transferred to the neighboring upper cell.</p> <p>ALGOPT(24)<0 : Print a message on the volume adjustment.</p> <p>'0' is the default value, but '1' is also recommended if the time step size tends to be very small due to numerical instabilities.</p>
25		0	<p>=0 : The excessive volume of sodium is simply removed to avoid FCI in the upper cell when ALGOPT(24) =1 or 2.</p> <p>=1 : The excessive volume of sodium is also transferred to the neighboring upper cell when ALGOPT(24) =1 or 2.</p>
26-29			Not currently used.
30		0	<p>Flag to control the calculation of viscous-drag term in the momentum equations. This models the viscous shear between the fluid flows in the adjacent mesh cells. See also control option MXFOPT(3) in NAMELIST /XCNTL/.</p> <p>=1 : Calculate the viscous-drag term.</p> <p>=0 : Do not calculate.</p>
31		0	<p>Control variable to delay the increase in time-step size.</p> <p>=n : The time-step size is not increased until the (m+n)-th cycle, whenever the time step is increased at the m-th cycle by whatever reason.</p> <p>'0' is the default value, but n=2~5 is recommended</p>
32			Not currently used.
33		0	<p>Control variable to prevent the vapor temperature from falling too low in the pressure iteration. See also TGMIN parameter in NAMELIST /XEOS/.</p> <p>=1 : Restriction on vapor temperature.</p> <p>=0 : No restriction on vapor temperature.</p>
34-36			Not currently used.
37		3	Number of iterations for solving the equation of macroscopic density, $\bar{\rho}_\epsilon$. This option is used in the relaxation method against source-term decoupling, Method-1.
38-40			Not currently used.

Variable	Dimension	Default	Description
	41	0	Flag to select the method of time-step control. =0 : Standard time-step control. =1 : Random time-step control (see also FRAND and SEED parameters in NAMELIST /XMSC/).
	42-44		Not currently used.
	45	1	Option to control the procedure to prevent the mass being negative in the convection calculation. =0: The mass flux at each cell interface is modified so as to keep the mass in the cell positive. =1: The time step is recalculated with the halved time step size.
	49	0	Flag to apply the inner boundary condition. See also parameters in NAMELIST /XBND/. =0 : Do not apply. >0 : Apply.
	50	0	Flag to apply a sodium-water chemical reaction model in liquid or vapor state. Used only when HISTORIAN code option SW is on. See also input variables in NAMELIST /XSWC/. =0 : Do not apply. >0 : Apply.
Variable	Dimension	Default	Description
EOSOPT	(100)		Code control option flags for the equations of state.
	1	0	Initialization option for the thermodynamic state of vapor field. This option determines the state of the vapor components of the real liquids in a cell, <u>unless</u> the partial pressures or specific volumes of the corresponding condensable gases are explicitly specified by input variables PGMINB and VGMINB in NAMELIST /XRGN/ or PGMC and VGMC in NAMELIST /XCWD/. =0 : The condensable-gas pressures are defined as the saturation pressures of the real liquids in a cell. =1 : The condensable-gas pressures are calculated from the saturated pressure equations using the vapor temperature (TGINB in NAMELIST /XRGN/ or TGC in NAMELIST /XCWD/) instead of the liquid temperatures.
	2	0	Initialization option for the assignment of macroscopic densities. =0 : For liquid- and structure-field components, the volume fractions are specified by input variables ASMINB and ALMINB in NAMELIST /XRGN/ or ASC and ALC in NAMELIST /XCWD/. The specific volumes are calculated from the equation of state functions using the temperatures.

Variable	Dimension	Default	Description
			<p>For the vapor field, the effective volume fraction is calculated by subtracting the liquid-field, structure-field, and no-flow volume fractions from the cell volume. The specific volumes of the vapor components are calculated from the equation of state functions using the vapor temperature and the partial pressures. The macroscopic densities of the vapor components are then the ratio of the volume fractions and the specific volumes, $\bar{\rho}_{Gm} = \alpha_{g\ell} / \nu_{Gm}$.</p> <p>=1 : For single-phase cells, the macroscopic densities of vapor-, liquid-, and structure-field components are calculated in the same way as for EOSOPT(2)=0. For two-phase cells, the macroscopic densities of real liquids and vapor components are calculated so as to conserve the mass of each material component in a cell. The mass of the liquid plus vapor phases of each component are calculated from the real-liquid macroscopic densities, which are defined in the same way as for EOSOPT(2)=0. Then the specified volume fractions of the real liquids in the two-phase cell are decreased to compensate for the mass of the component in the vapor phase. If the volume fraction of a real liquid becomes negative by this method, the volume fraction of the real liquid is set to zero.</p>
	3-9		Not currently used.
	10	0	<p>Option to set the vapor temperature to the temperature of real liquid component which has the maximum volume fraction if the vapor temperature falls below the minimum temperature specified by input variable TGMIN in NAMELIST /XEOS/. This option may help the situation in which the vapor temperature in a two-phase cell with very small void fraction becomes unstable due to numerical problem.</p> <p>=0 : Do not adjust the vapor temperature.</p> <p>=1 : Adjust the vapor temperature.</p>
	11-40		Not currently used.
	41	0	<p>Option to print the mesh-cell number if the iteration for vapor temperature fails in STEP1 or STEP4.</p> <p>=1 : Print a message.</p> <p>=0 : Do not print a message.</p>
	42	0	<p>Option to print the mesh-cell number if the iteration for vapor temperature fails in STEP1 or STEP4 because the vapor temperature falls below the minimum temperature specified by input variable TGMIN in NAMELIST /XEOS/.</p> <p>=1 : Print a message.</p> <p>=0 : Do not print a message.</p>
	43	0	Option to print information in the event of the liquid internal

Variable	Dimension	Default	Description
			energy exceeding the critical energy in subroutine EOST. =1 : Print a message. =0 : Do not print a message.
Variable	Dimension	Default	Description
TPPOPT	(100) 1-100		Code control option flags for the thermophysical properties. Not currently used.
Variable	Dimension	Default	Description
HTCOPT	(100)		Code control option flags for the heat-transfer coefficients (HTCs). Not currently used.
	1		Not currently used.
	2	0	Option to print values of HTCs and debug information from subroutine HTC in STEP1 (output is printed every long print). =0 : Do not print. =n : Print for cell n only. =999 : Print for all cells.
	3	3	Flag to select whether a natural convection heat transfer correlation is used to calculate an HTC in a continuous phase (CP) liquid or gas which is exchanging heat with particles and droplets. Natural convection heat transfer in the CP fluid is calculated using the input variables HNCLP and HNCGP in NAMELIST /XHTC/. =0 : A natural convection HTC is not calculated. =1 : Natural convection heat transfer is calculated only for CP liquids to droplets. =2 : Natural convection heat transfer is calculated for CP liquids to droplets and solid particles. =3 : Natural convection heat transfer is calculated for CP liquids, and for a gas/vapor mixture in dispersed flow, to droplets and solid particles.
	4	1	Option to calculate HTCs between droplets in the dispersed flow regime from a transient conduction formulation which uses a droplet-droplet contact time calculated from the relative velocities of the droplets. =0 : A steady-state HTC is used. =1 : The HTC is calculated from transient contact between droplets.
	5-6		Not currently used.
	7	2	Option to calculate internal and external HTCs for fluid particles which take account of internal circulation and oscillation of the particles. Heat transfer in both the

Variable	Dimension	Default	Description
			<p>continuous phase (CP) and discontinuous phase (DP) fluids are enhanced according to the input variables HREIC, HREOS, HICLCP, HICLDP, HOSLDP and HOSGBU in NAMELIST /XHTC/.</p> <p>=0 : CP fluid-particle HTCs are calculated using rigid particle correlations only.</p> <p>=1 : The HTCs in the CP fluids only are enhanced due to internal circulation and oscillation of the DP droplets and bubbles.</p> <p>=2 : The HTCs in both the CP and DP fluids are enhanced due to internal circulation and oscillation of the DP droplets and bubbles.</p>
	8-9		Not currently used.
	10-14		Flags to control the calculation of “boiling” HTCs, and the film boiling model in particular. A boiling HTC can be calculated if the interface temperature between two liquid-field components exceeds the saturation temperature of the volatile liquid. HTCOPT(12) to HTCOPT(14) are used only if HTCOPT(10) for particles or HTCOPT(11) for real liquids has a non-zero value.
	10	0	<p>Option to calculate a boiling HTC between particle and liquid components. This option should be used to select the film boiling model for solid particles.</p> <p>=0 : No boiling HTCs (i.e. HTCs are calculated as if no mass transfer occurs).</p> <p>=1 : Boiling HTCs are calculated.</p>
	11	1	<p>Option to calculate a boiling HTC between two liquid components. This option should be used to select the film boiling model.</p> <p>=0 : No boiling HTCs (i.e. HTCs are calculated as if no mass transfer occurs).</p> <p>=1 : Boiling HTCs are calculated if the topology is suitable for the film boiling model (i.e. hot droplets in a continuous phase volatile liquid).</p> <p>=2 : Boiling HTCs are calculated for all topologies (i.e. including droplets of volatile liquids in a continuous phase hot liquid).</p>
	12	0	<p>Option to calculate the surface temperature of the hot liquid component in the case of film boiling. The surface temperature is set to either a contact temperature due to transient wetting by the coolant, or else simply to the temperature of the hot component (i.e. assuming no wetting).</p> <p>=0 : The hot liquid surface temperature is set to a transient wetting contact temperature</p>

Variable	Dimension	Default	Description
			=1 : The surface temperature is set to the temperature of the liquid energy component.
	13		Not currently used.
	14	1	Flag to select the film boiling heat transfer area for a droplet to account for a possible reduction in heat transfer in the vapor removal region. The heat transfer areal fraction of the droplet is set by either input data variable FFB in NAMELIST /XHTC/, or else by a droplet size criterion. The criterion sets a fraction of '1' for "large" droplets and '0.5' for "small" droplets (i.e. heat transfer over a hemisphere). =0 : The heat transfer area is set by the droplet size criterion. =1 : The heat transfer area is set by input data. The recommended value is '1', with FFB = 1.0.
	15-19		Not currently used.
	20	0	Flag to select the method for calculating the gap conductance of the pin. =0 : An input constant value of the gap conductance is used. See also AHGAP parameter in NAMELIST /XSTR/. =1 : The gap conductance is calculated as the heat-transfer coefficient for conduction through the gas in the fuel-cladding gap using an input constant value of thermal conductivity of the gas in the gap and the fuel-cladding gap predicted by the pin model. See also AKGAP, AHGMIN, and AHGMAX parameters in NAMELIST /XSTR/. =2 : The gap conductance is calculated as the heat-transfer coefficient for conduction through the gas in the fuel-cladding gap using the temperature-dependent thermal conductivity of the gas in the gap, which is evaluated by the thermophysical property model, and the fuel-cladding gap predicted by the pin model. See also control option HTCOPT(21) in NAMELIST/XCNTL/ and AHGMIN and AHGMAX parameters in NAMELIST /XSTR/.
	21	0	Flag to use the gap conductance derived from the model of the PAPS2S code. Active only when HTCOPT(20)=2. =0 : Do not use. =1 : Use.
	22	0	Flag to consider the radiation heat transfer in calculating the gap conductance. See also input variables OHMF and OHMC in NAMELIST /XSTR/. =0 : Do not consider. =1 : Consider.
	23-100		Not currently used.

Variable	Dimension	Default	Description
IFAOPT	(100)		Code control option flags for the interfacial areas.
	1	1	Not currently used.
	2	0	Flag to select the type of flow model. =0 : The selection of pool or channel flow is based on the flooding criterion. =1 : The channel flow model is used regardless of the existence of the structure components. =2 : The pool flow model is used regardless of the existence of the structure components.
	3	3	Flag to control the definition of $A_{CP,B \rightarrow D}$ by convection. $A_{CP,B \rightarrow D}$ is an interfacial area of the continuous phase (CP) component which is transferred from the bubbly flow region to the dispersed flow region due to the convection between two cells which have different void fraction and/or flow regime. =0 : $A_{CP,B \rightarrow D} = 0$. =1 : the same radius of the existing CP droplet is assumed to the transferred CP component. =2 : $A_{CP,B \rightarrow D} = \frac{A_{G,B}}{\alpha_{G,B}} \alpha_{CP,B \rightarrow D}$, where $A_{G,B}$ is the interfacial area of bubbles, $\alpha_{G,B}$ is the volume fraction of bubbles, and $\alpha_{CP,B \rightarrow D}$ is the volume fraction of CP component transferred from bubbly flow region to dispersed flow region. This option compensates the loss of $A_{G,B}$ which is caused by the reduction of bubbly flow region and forces the total interfacial area between CP component and vapor be conserved through the transfer. =3 : $A_{CP,B \rightarrow D} = \frac{A_{G,B}}{\alpha_{G,B}} \alpha_{CP,B \rightarrow D} f_B$, where f_B is the volumetric fraction of bubbly flow region. By multiplying this factor, the compensation in the option No. 2 becomes dependent on the amount of the bubbly flow region.
4	3	Flag to control the definition of $A_{G,D \rightarrow B}$ by convection. $A_{G,D \rightarrow B}$ is an interfacial area of the vapor which is transferred from the dispersed flow region to the bubbly flow region due to the convection between two cells which have different void fraction and/or flow regime. =0 : $A_{G,D \rightarrow B} = 0$. =1 : the same radius of the existing bubble is assumed for the transferred vapor component. =2 : $A_{G,D \rightarrow B} = \frac{A_{CP,D}}{\alpha_{CP,D}} \alpha_{G,D \rightarrow B}$, where $A_{CP,D}$ and $\alpha_{CP,D}$ are the interfacial area and volume fraction of CP components	

Variable	Dimension	Default	Description
			<p>in the dispersed flow region respectively, and $\alpha_{G,D \rightarrow B}$ is the volume fraction of vapor transferred from dispersed flow region to bubbly flow region. This option compensates the loss of $A_{CP,D}$ which is caused by the reduction of dispersed flow region and forces the total interfacial area between CP component and vapor be conserved through the transfer.</p> <p>=3 : $A_{G,D \rightarrow B} = \frac{A_{CP,D}}{\alpha_{CP,D}} \alpha_{G,D \rightarrow B} f_D$, where f_D is the volumetric fraction of dispersed flow region. By multiplying this factor, the compensation in the option No. 2 becomes dependent of the amount of the dispersed flow region.</p>
5		0	<p>Flag to control the calculation of compression term for $A_{G,B}$.</p> <p>=0 : Calculate the compression term (recommended value), and</p> <p>=1 : Do not calculate.</p>
6		3	<p>Flag to control the definition of $A_{CP,B \rightarrow D}$ by intra-cell mass transfer. The objective of this option is same as IFAOPT(3), but this option concerns $A_{CP,B \rightarrow D}$ by intra-cell mass transfer.</p> <p>=0 : $A_{CP,B \rightarrow D} = 0$.</p> <p>=1 : the same radius of the existing CP droplet is assumed</p> <p>=2 : $A_{CP,B \rightarrow D} = \frac{A_{G,B}}{\alpha_{G,B}} \alpha_{CP,B \rightarrow D}$.</p> <p>=3 : $A_{CP,B \rightarrow D} = \frac{A_{G,B}}{\alpha_{G,B}} \alpha_{CP,B \rightarrow D} f_B$.</p>
7		3	<p>Flag to control the definition of $A_{G,D \rightarrow B}$ by intra-cell mass transfer. The objective of this option is same as IFAOPT(4), but this option concerns $A_{G,D \rightarrow B}$ by intra-cell mass transfer.</p> <p>=0 : $A_{G,D \rightarrow B} = 0$.</p> <p>=1 : the same radius of the existing bubble is assumed.</p> <p>=2 : $A_{G,D \rightarrow B} = \frac{A_{CP,D}}{\alpha_{CP,D}} \alpha_{G,D \rightarrow B}$.</p> <p>=3 : $A_{G,D \rightarrow B} = \frac{A_{CP,D}}{\alpha_{CP,D}} \alpha_{G,D \rightarrow B} f_D$.</p>
8		0	<p>Flag to determine whether the limit to the maximum droplet size by the real liquid volume is applied or not. This limit is calculated by the following equation.</p> $r_{Lm,max} = \left(\frac{3V_{cell}\alpha_{Lm}}{4\pi} \right)^{1/3},$ <p>where V_{cell} is the cell volume and α_{Lm} is the volume fraction of the liquid component.</p>

Variable	Dimension	Default	Description
			=0 : Do not apply. =1 : Apply.
	9-19		Not currently used.
	20	0	Flag to select formula of IFA source terms. =0 : Linearized formula are used. =1 : Differential formula are used.
	21	0	Flag to select the correlation of time constant for the Weber breakup of droplets. =0 : Taylor-type correlations. See also CTWB and CTWD parameters in NAMELIST /XIFA/. =1 : Pilch and Erdman's correlation.
	22	0	Flag to select whether an effect of decrease of the velocity difference between droplets and continuous fluid are taken into account after droplet fragmentation. =0 : The effect is ignored. =1 : The effect is taken into account.
	23-24		Not currently used.
	25	0	Flag to select the method for the bubble nucleation. =0 : AFDM-type model. =1 : Wall nucleation model for flashing flow.

Variable	Dimension	Default	Description
HMTOPT	(100)		Code control option flags for the heat and mass transfer.
	1	1	Option to reduce the liquid-fuel, liquid-steel, and particles-side heat-transfer coefficients in the event of excessive heat transfer in the M/F calculation. =1 : Heat transfer coefficients are reduced. =0 : Heat transfer coefficients are not reduced.
	2-4		Not currently used.
	5	51	Flag to reduce the HTC's only for the explicitly updated components in the event of excessive heat transfer in the V/C calculation. = n : HTC's are reduced after the n-th V/C iteration step. = 0 : HTC's are not reduced.
	6	0	Flag to reduce the interfacial areas or the heat-transfer coefficients in the event of excessive heat transfer in the V/C calculation. =n : Interfacial areas are reduced after the n-th V/C iteration step. =-n : Heat-transfer coefficients are reduced after the n-th V/C

Variable	Dimension	Default	Description
			iteration step.
			=0 : Interfacial areas and heat-transfer coefficients are not reduced.
7	1	1	Flag to apply the equilibrium freezing model for liquid steel into structures. =0 : Do not apply. =1 : Apply.
8	0	0	Option to skip the v/c calculation for the cell where the convergence is not achieved. =0: The V/C calculation is not skipped. =1: The V/C calculation is skipped.
9	1	1	Flag to determine whether the supersaturated vapor is forced into condensation or not by calling the subroutine VCESUB. =0 : No supersaturated vapor is forced condensation. =1 : No subcooled vapor is forced into condensation. >1 : Selected supersaturated vapor components are forced into condensation. The selections are made by =2 : fuel and steel, =3 : fuel and sodium, =4 : steel and sodium, =5 : fuel, =6 : steel, and =7 : sodium. HMTOPT(9)>1 may be used with flags to suppress the V/C mass transfers. See also NGAMVC and NGAMIK input variables in NAMELIST /XHMT/.
10	51	51	Option to halve the time-step size if the number of V/C iterations exceeds a specified value. =n : The time-step size is halved for the next cycle if the number of V/C iterations exceeds n. =0 : Time-step size is not restricted.
11	999	999	Option to consider gas-diffusion effects on V/C phase transition. = 0 : No gas-diffusion effect is considered. (i.e. V/C is calculated based on the heat-transfer limited model). ≠ 0 : Gas-diffusion effects are considered. HMTOPT(11) is the maximum number of iterations to calculate the interface temperature. If HMTOPT(11)>0, Sherwood numbers are calculated based on the heat- and mass-transfer analogy, i.e. Prandtl numbers in Nusselt

Variable	Dimension	Default	Description
			number correlations are replaced with Schmidt numbers for the calculation of Sherwood numbers. If HMTOPT(11)<0, Schmidt number = Prandtl number is assumed.
	12	0	Option to consider vapor-side HTCs under mass transfer. This option is active only if HMTOPT(11) ≠ 0. = 0 : Vapor-side HTCs for sensible heat are used. = 1 : Vapor-side HTCs under mass transfer are used.
	13	0	Option to control the treatment of liquid component with small mass in V/C calculation. See also FMTLG parameter in NAMELIST /XHMT/. =0: Transfer the liquid component with small mass to vapor. =1: Set the HTC and IFA between the liquid component with small mass and vapor to zero.
	14-20		Not currently used.
	21-25	1, 1, 1, 1, 1	If HMTOPT(20+n)=1, Steffensen's method is applied to the residual of the n-th independent variable in the V/C iteration. The independent variables are: (21): macroscopic density of fuel vapor, (22): macroscopic density of steel vapor, (23): macroscopic density of sodium vapor, (24): specific internal energy of liquid sodium, and (25): vapor mixture temperature.
	26-30		Not currently used.
	31	0	Option to switch off the non-equilibrium M/F model. Non-equilibrium M/F is calculated in subroutine MFHMT in STEP1. =0 : Call the subroutine MFHMT. =1 : MFHMT is not called.
	32	0	Option to switch off the non-equilibrium V/C model. Non-equilibrium V/C is calculated in subroutine VCHMT in STEP1. =0 : Call the subroutine VCHMT. =1 : VCHMT is not called.
	33-40		Not currently used.
	41-45		Debug print options in subroutine VCHMT. The cell variables to be printed are specified by the input variable PRCEL in the NAMELIST /XEDT/.
	41	0	=n : Print the EOS variables every n-th V/C iteration.
	42	0	=n : Print the derivatives of EOS variables every n-th V/C iteration.
	43	0	=n : Print the mass transfer rates and their derivatives every

Variable	Dimension	Default	Description
			n-th V/C iteration.
44		0	=n : Print the interfacial temperatures and their derivatives every n-th V/C iteration.
45		0	=n : Print the V/C matrix elements every n-th V/C iteration.
46		0	Option to print an error message in the event that interfacial areas or heat-transfer coefficients are reduced in V/C iteration. =1 : Print the error message. =0 : Nothing printed.
47		0	Option to print information in the event of steel wall breakup. =1 : Print a message. =0 : Nothing printed.
48		0	Option to print information in the event of crust breakup. =1 : Print a message. =0 : Nothing printed.
49-50			Not currently used.
51		0	Option to print information in the event of V/C iteration failure. =1 : Print an error message. =2 : Print the vapor temperature, pressure, and vapor volume fraction with the error message. =0 : Nothing printed.
52		0	Option to print information in the event of the excessive vapor temperature change in the V/C iteration. See the input variable FDTGMX in NAMELIST /XHMT/. =1 : Print an error message. =2 : Print the vapor temperature, pressure, and vapor volume fraction with the error message. =0 : Nothing printed.
53		0	Option to print a message in the event of a successful V/C iteration. =1 : Print the message. =0 : Nothing printed.
54		0	Option to print an error message in the event that subcooled vapor cannot be removed in V/C iteration. =1 : Print the error message. =0 : Nothing printed.
55-62			Not currently used.
63		0	Flag to control the breakup of a "thin" can wall.

Variable	Dimension	Default	Description
			<p>=0 : Breakup the can wall if it is thin.</p> <p>=1 : Suppress the breakup of can wall even if it is thin.</p> <p>'0' is the recommended value.</p>
64	0	0	<p>Option to select the can-wall breakup conditions.</p> <p>=0 : Only the thermal breakup criterion is applied to can-wall failure. See also WMELT parameter in NAMELIST /XSTR/.</p> <p>=1 : Both the thermal and mechanical breakup criteria are applied to can-wall failure. See also DWFAL and TWFAL parameters in NAMELIST /XSTR/.</p>
65	0	0	<p>Flag to control the breakup of fuel crust formed on a can wall. See also TCRMIN parameter in NAMELIST /XSTR/.</p> <p>=0 : Breakup the fuel crust when the can-wall thermal failure is predicted under the crust.</p> <p>=1 : Breakup the fuel crust when the can-wall thermal failure or the can-wall melting is predicted under the crust.</p>
66	1	1	<p>Option to select the breakup conditions of fuel pellet which are added to thermal breakup.</p> <p>=0 : The fuel pellet does not break up until the thermal breakup condition is met.</p> <p>=1 : The fuel pellet breaks up when the cladding is lost.</p> <p>=2 : The fuel pellet breaks up when the cladding and the can walls are lost.</p> <p>=3 : The fuel pellet breaks up when the cladding is lost and the pin structure in the lower cell does not exist.</p> <p>=4 : The fuel pellet breaks up when the cladding and the can walls are lost, and the pin structure in the lower cell does not exist.</p>
67	1	1	<p>Option to select the breakup conditions of control pellet which are added to thermal breakup.</p> <p>=0 : No breakup of the control pellet.</p> <p>=1 : The control pellet breaks up when the cladding is lost.</p> <p>=2 : The control pellet breaks up when the cladding and the can walls are lost.</p> <p>=3 : The control pellet breaks up when the cladding is lost and the pin structure in the lower cell does not exist.</p> <p>=4 : The control pellet breaks up when the cladding and the can walls are lost, and the pin structure in the lower cell does not exist.</p>
68			Not currently used.
69	0	0	Flag to consider chunk formation when the fuel pellet breaks

Variable	Dimension	Default	Description
			up and to apply chunk model in the momentum-exchange function calculation.
			=0 : Do not consider. The fuel particle is formed instead of the fuel chunk.
			=1 : Consider.
70			Not currently used.
71	0		Flag to apply the inter-cell heat transfer.
			=0 : Do not call the subroutine ITCHTR, which calculates the inter-cell heat transfer.
			=1 : Call ITCHTR.
72	0		Flag to apply the inter-cell heat transfer in liquid field components. Active only when HMTOPT(71)=1.
			=0 : Do not calculate.
			=1 : Calculate the inter-cell heat transfer in real liquids.
			=2 : Calculate the inter-cell heat transfer in real liquids and solid particles.
73	0		Flag to apply the inter-cell heat transfer in vapor. Active only when HMTOPT(71)=1.
			=0 : Do not calculate.
			=1 : Calculate.
74	0		Flag to apply the axial inter-cell heat transfer in cladding and can wall. Active only when HMTOPT(71)=1.
			=0 : Do not calculate.
			=1 : Calculate.
75			Not currently used.
76	0		Flag to apply the axial inter-cell axial heat transfer between fluids and lower/upper structures. The equilibrium melting of can-wall interior occurs when its energy exceeds the solidus energy. See also input variables CSSX in NAMELIST /XIFA/ and HFCXS in NAMELIST /XHTC/. Active only when HMTOPT(71)=1.
			=0 : Do not calculate.
			=1 : Calculate.
77-79			Not currently used.
80	0		Flag to select routines containing M/F modeling.
			=0 : Original coding containing classical bulk freezing model.
			=1 : Modified M/F subroutines.
81	0		Flag to select the melting/freezing "model".
			=0 : Classical bulk freezing model.
			=1 : General model: user can choose from HMTOPT(83) to

Variable	Dimension	Default	Description
			HMTOPT(88). =2 : Interface resistance with bulk freezing model (see also HMTOPT(91)). =3 : Fuel caps freezing model. The liquid fuel-steel wall interface temperature is automatically determined by experimental correlation, while The liquid steel-steel wall interface temperature can be specified by HMTOPT(87). See also input parameters CASC, PSC1 and PSC2 in NAMELIST /XHMT/.
82	0	0	Option to specify the velocity used to calculate the contact density of the first CP liquid (i.e. the continuous phase liquid with the highest volume fraction): =0 : The instantaneous velocity is used. =1 : The maximum velocity of bubbly flow CP liquid in the mesh cell is used. =2 : The initial velocity of bubbly flow CP liquid in the mesh cell is used.
83	0	0	Flag to select the HTC's for liquid fuel-steel wall contact (for HMTOPT(81)=1; otherwise there are restrictions on this option): =0 : "Standard" convection/conduction HTC's are used. =1 : Interface resistance HTC's are used (function of contact point density).
84	0	0	Flag to select the HTC's for liquid steel-steel wall contact (for HMTOPT(81)=1; otherwise there are restrictions on this option): =0 : "Standard" convection/conduction HTC's are used. =1 : Interface resistance HTC's are used (function of contact point density).
85	0	0	Flag to specify the type of gap heat transfer coefficient between fuel crust and steel wall (for HMTOPT(81)=1; otherwise there are restrictions on this option): =0 : No gap; perfect contact. =1 : An interface resistance is calculated from the density of contact points for liquid fuel at the instant of crust formation. =2 : Input variable HCRGAP of NAMELIST /XHMT/ is used. Active only when HMTOPT(81) ≠ 3.
86	0	0	Option to define the liquid fuel-steel wall interface temperature (for HMTOPT(81)=1; otherwise there are restrictions on this option): =0 : Conduction-limited interface temperature (original model).

Variable	Dimension	Default	Description
			=1 : No non-equilibrium phase change. =2 : Input variable TILFW of NAMELIST /XHMT/ is used.
87		0	Option to define the liquid steel-steel wall interface temperature (for HMTOPT(81)=1; otherwise there are restrictions on this option): =0 : Steel melting point (original model). =1 : No non-equilibrium phase change. =2 : Input variable TILSW of NAMELIST /XHMT/ is used. =3 : Experimental correlation is used.
88		0	Option to define the liquid fuel-fuel crust interface temperature (for HMTOPT(81)=1; otherwise there are restrictions on this option): =0 : Fuel melting point (original model). =1 : No non-equilibrium phase change. =2 : Input variable TILFC of NAMELIST /XHMT/ is used.
89-90			Not currently used.
91		0	The interface resistance bulk freezing model (HMTOPT(81)=2) uses: =0 : Modified coding and input variables. =1 : Hard-coded variables (original coding).
92		0	Option to select the heat-transfer model of the can wall and the crust. =0 : The slab geometry heat-transfer model is applied. =1 : The cylindrical heat-transfer model is applied.
Variable	Dimension	Default	Description
EDTOPT	(100)		Code control option flags for the printer output.
	1	10	Flag to select the print frequency of the header of the "short print". =n : The header is printed every n-th short print (values of n less than 5 are ignored).
	2	0	Option to print integral and conservation information about cells, from subroutine PRTINT. =1 : Nothing printed. =0 : Integral and conservation information is printed.
	3	2	Flag to select the format of the post-processing file. =0 : Post-processing file is written in binary format. =1 : Post-processing file is written in card image (i.e. ASCII format). =2 : Post-processing file is not outputted.

Variable	Dimension	Default	Description
	4	1	Flag to select the print frequency of the “short print”. =n : The time-step information (the “short print”) is written every n-th cycle.
	5	0	Option to print the cover page which lists the HISTORIAN options and the code control options from NAMELIST /XCNTL/. =1 : List of options are printed. =0 : Options are not printed.
	6	0	Flag to determine the EOS tables’ format. =0 : Nothing printed. =1 : Print the EOS tables (the range and scale of temperature to be printed are automatically defined by the code). =2 : Print the EOS tables (the range and scale of temperature to be printed are specified by the input variable DTEOS in NAMELIST /XEDT/).
	7	0	Flag to determine the TPP tables’ format. =0 : Nothing printed. =1 : Print the TPP tables (the range and scale of temperature to be printed are automatically defined by the code). =2 : Print the TPP tables (the range and scale of temperature to be printed are specified by the input variable DTPP in NAMELIST /XEDT/).
	8	0	Option to print the size of erasable arrays required by the subroutines in STEP1. =1 : The size of the arrays is printed. =0 : The size is not printed.
	9	0	Option to print the values of variables at the start of a run. =0 : The initial information is printed. =1 : The initial information is not printed.
	10		Not currently used.
	11	0	Option to echo user specified input. =1 : User specified input data is printed. =0 : User specified input is not echoed.
	12	0	Option to print information on the mass and energy conservation in STEP1. =0 : No conservation information is printed. =1 : The cell-wise and total integrated deviations of mass and energy during STEP1 are printed. =2 : In addition to the above information, the cell-wise deviations of mass and energy in each cycle are printed.

Variable	Dimension	Default	Description
			<p>=3 : In addition to the above information, the cell-wise fractional deviations with respect to the beginning of the time-step values are printed.</p> <p>=4 : In addition to the above information, the mass and energy deviations for each component are printed.</p> <p>=5 : In addition to the above information, the fractional deviations of mass and energy with respect to the beginning of the time-step values are printed.</p> <p>=6 : In addition to the above information, the end of time-step mass and energy in each cell are printed.</p> <p>=7 : In addition to the above information, the beginning of time-step mass and energy in each cell are printed.</p>
13	1	1	<p>Option to include boundary cell values in the “global variable” listing.</p> <p>=1 : Print the boundary cell values in the global variable listing.</p> <p>=0 : Boundary cell values are not printed.</p>
14	0	0	<p>Flag to select the format for the “global variable” listing.</p> <p>=0 : In the global variable listing, the vertical axis is printed as a column if the radial cell number ≤ 3. If the radial cell number > 3, the radial axis is printed as a column.</p> <p>=1 : The radial axis is printed as a column.</p> <p>=2 : The vertical axis is printed as a column.</p> <p>=3 : The axis which has the largest cell number is printed as a column.</p>
15	0	0	<p>Option to print the mass and energy summation in each input sub-region (refer to NAMELIST /XRGN/).</p> <p>=0 : The summation is not printed.</p> <p>=1 : The summation is printed.</p>
16	0	0	<p>Option to restore the set-over can wall, which is moved by the structure configuration model, to an original cell in which the can wall actually exists. This option is effective only for post-processing and base file dumps.</p> <p>=0 : Set-over can wall is not restored.</p> <p>=1 : Set-over can wall is restored.</p>
17	0	0	<p>Flag to control the debug information from pressure iteration. Debug information is printed if the pressure iteration number exceeds this input.</p>
18-19			Not currently used.
20	0	0	<p>Number of restart dump files created during the run. This option is effective only for UNIX workstations.</p>

Variable	Dimension	Default	Description
			=1 : Restart dump is output to one file sequentially. =2 : Restart dump is output to the files named SIMDFn cyclically, where the maximum number of n is given by EDTOPT(20). Each restart dump overwrites the previous one (see also DMPC in NAMELIST/XEDT/).
	21-50		Not currently used.
	51	0	Option to print debug information which can help to identify NAMELIST variables which are spelled incorrectly. =0 : Nothing printed. =1 : Print the debug information.
	52	0	Option to echo cell-wise input data. =0 : Cell-wise data is not printed. =1 : Cell-wise data is echoed.
	53-79		Not currently used.
	80	0	Option to output more detailed information from TWODANT. =0 : No additional information is output. =1 : Additional information is printed to file (SIMDI: FORTRAN logical file number: 80).

Variable	Dimension	Default	Description
MXFOPT	(100)		Code control option flags for the momentum exchange functions.
	1	2	Flag to apply Ueda's model for evaluating the two-phase pressure drop in the bubbly flow region. The model uses input variables CFRS1 ~ CFRS3 and CANUL1 ~ CANUL3 in NAMELIST /XMXF/. =2 : Ueda's model is applied for all channel flow regimes. =1 : Ueda's model is applied only for bubble flow. =0 : Ueda's model is not applied.
	2	0	Flag to apply the particle viscosity model to the momentum diffusion model. =0 : Apply. =1 : Do not apply.
	3	0	Flag to take account of the turbulence-diffusion effect on the viscous-drag term in the momentum equations. Active only if control option ALGOPT(3)=1 in NAMELIST /XCNTL/. See also parameters in NAMELIST /XMXF/. =0 : Calculate the viscous-drag term only due to the molecular diffusion. =1 : Take account of the turbulence-diffusion effect.

Variable	Dimension	Default	Description
	4	0	Flag to select the characteristic length compared with a particle diameter in a liquid-structure momentum exchange process: =0 : Hydraulic diameter is used. =1 : Input variable PVSCL of NAMELIST /XMXF/ is used.
	5	0	Option flag to apply the model for the droplet-liquid momentum coupling under film boiling condition. =0: Do not apply the model. =1: Apply the model.
	6	0	Option for chunk model. =0 : Chunk model is applied for solid particles. ≠0 : Chunk model is not applied for solid particles.
	7	0	Flag to select the formulation of the particle viscosity model. =0 : The effective volume fraction of particles $\frac{\alpha_p}{1-\alpha_s}$ is used to calculate the particle viscosity. =1 : The particle viscosity by $\frac{\alpha_p}{1-\alpha_s}$ and $\frac{\alpha_p}{\alpha_L + \alpha_p}$ are compared and the larger value is used.
	8	0	Flag to apply the momentum coupling for the flow which cross the arrays of cylinder (pin bundles) to the horizontal direction. See also parameters CWST, CWSL, DTUBE and CWMXF in NAMELIST /XMXF/. =0 : Apply the original model. =1 : Do not apply. =2 : Take account of the momentum coupling for arrays of cylinder.
	9	0	Option to determine the arrays of cylinder. Used only if MXFOPT(8)=2. =1 : Square array. =2 : Triangular array.
	10	0	Flag to determine whether the particle viscosity model is applied to the momentum exchange function between fluids or not. The effective volume fraction of particles is calculated by $\frac{\alpha_p}{1-\alpha_s}$. =0 : The particle viscosity model is not applied. =1 : The particle viscosity model is applied.
	11	0	Flag to control the appliance of particle jamming model to the

Variable	Dimension	Default	Description
			velocity field 1.
			=0 : Apply the particle jamming model. The volume fractions of all particle components are summed to calculate the particle volume fraction regardless of the velocity field assignment.
			=1 : Apply the particle jamming model. The volume fractions of particle components are summed to calculate the particle volume fraction if the particle belongs to the 1st velocity field.
			=2 : Do not apply the particle jamming model.
	12	0	Flag to control the appliance of particle jamming model to the velocity field 2.
			=0 : Apply the particle jamming model. The volume fractions of all particle components are summed to calculate the particle volume fraction regardless of the velocity field assignment.
			=1 : Apply the particle jamming model. The volume fractions of particle components are summed to calculate the particle volume fraction if the particle belongs to the 2nd velocity field.
			=2 : Do not apply the particle jamming model.
	95	0	Flag to apply the drag coefficient interpolated between ellipsoidal bubble's and cap bubble's. See also parameter DHINP in NAMELIST /XMXF/.
			=0 : Do not apply.
			=1 : Apply.

Variable	Dimension	Default	Description
FPNOPT	(100)		Code control option flags for the DPIN model.
	1	0	Flag to specify whether fuel mass average melt fraction or area melt fraction is used for the pin failure.
			=0 : Fuel mass based average melt fraction is used.
			=1 : Area melt fraction is used.
	2	0	Flag to select routines for fuel ejection model.
			=0 : No fuel ejection model.
			=1 : Equilibrium pressure model.
			=2 : SAS model.
	3	0	Flag to select the fuel pin model.
			=0 : Standard fuel pin model.
			=1 : Block-type fuel compact model.

Variable	Dimension	Default	Description
RSTOPT	(100)		Code control option flags for the restart function.

Variable	Dimension	Default	Description
	1		Flag to specify whether the run is new or whether the run is restarting from a dump. =0 : Start a new run. >0 : The previous dump file sequential number to use for restarting the run from a dump.
	2	0	Option for restart calculation with neutronics from URANUS dump file. =0 : Nominal restart run. >0 : Only the fluid dynamics information is read from URANUS dump file. RSTOPT(2) is the previous dump file sequential number to use for the restart.

Variable	Dimension	Default	Description
ERROPT	(100)		Code control option flags for the error handling condition. The definition of the flags depends upon the computer being used. If HISTORIAN code option FACOM is ON: n =1 : Error number n is ignored (where n is defined in the FACOM system). =0 : The run stops if error number n is encountered. If HISTORIAN code option RS6000 is ON: 1 =1 : The run stops if the RS6000 system detects floating point exceptions. =0 : The run does not stop even if floating point exceptions are encountered. If HISTORIAN code option RS6000, SUN, HP9000, ALPHA, or ALPHANT is ON: 2 =1 : If wrong input variable names are specified, they are listed in the error information. 3 =0 : Continues program execution if a floating-point operation results in overflow, a division by zero, invalid data, or floating-point underflow (The SIMMER-III issues a information if ERROPT (3)=1 is set), if HISTORIAN code option RS6000 is ON.

3. XMSH

The fluid-dynamics mesh cell dimension variables.

Variable	Dimension	Default	Description
IGEOM		0	Flag to select the geometry. = 0 : Cylindrical geometry. = 1 : Cartesian geometry.
IB			Number of radial fluid-dynamics mesh cells.
JB			Number of axial fluid-dynamics mesh cells.
NPB			Number of radial nodes in the pellet. Used only for DPIN model.
NREG			Number of fluid-dynamics cell regions.
DRINP	(IB)		Radial fluid-dynamics mesh width.
DZINP	(JB)		Axial fluid-dynamics mesh height.
ICL			Left-most radial cell of the core containing fuel pins.
ICR			Right-most radial cell of the core containing fuel pins.
JCB			Bottom axial cell of the core containing fuel pins.
JCT			Top axial cell of the core containing fuel pins.
JLPB			Bottom axial cell of the lower fission gas plenum.
JLPT			Top axial cell of the lower fission gas plenum.
JUPB			Bottom axial cell of the upper fission gas plenum.
JUPT			Top axial cell of the upper fission gas plenum.

4. XTME

The real time and time-step control variables.

Variable	Dimension	Default	Description
TSTART		0.0 s	Real time to be used for the first time-step (s).
TWFIN		0.01 s	Last (largest) real time for the current run (s).
TCPU			Maximum CPU time for the run (s).
CYCFIN		10000000	Last (largest) cycle number for the current run.
DTSTRT		10^{-5} s	Initial fluid-dynamics time-step size (s).
DTMIN		10^{-6} s	Minimum fluid-dynamics time-step size (s).
DTMAX		10^{-3} s	Maximum fluid-dynamics time-step size (s).
DTINC		1.05	Maximum fractional change of the fluid-dynamics time-step size in one cycle. DTINC is used to reduce the source-term splitting error (see also control option ALGOPT(4) in NAMELIST /XCNTL/) as well as to restrict the increase in time step size (recommended value: 1.05).
NDT0		10	Number of fluid-dynamics time-steps for which the time-step size is kept less than or equal to DTSTRT.
DTHINI		10^{-1} s	Initial heat-transfer time-step size used in the fuel pin modeling (s). (DTHINI is also the initial reactivity time-step size used in the neutronics calculation.)
DTHMIN		10^{-5} s	Minimum heat-transfer time-step size used in the fuel pin modeling (s). (DTHMIN is also the minimum reactivity time-step size used in the neutronics calculation.)
DTHMAX		1.0 s	Maximum heat-transfer time-step size used in the fuel pin modeling (s). (DTHMAX is also the maximum reactivity time-step size used in the neutronics calculation.)
FEDT		0.5	Fractional fuel-pin structure energy change allowed per fuel-pin heat-transfer time step.
IDTH		10	Maximum number of fluid-dynamics time steps allowed per fuel-pin heat-transfer time step (>1). IDTH=1 : the heat-transfer time step is forced to be equal to the fluid-dynamics time step. IDTH≠0 : the heat-transfer time step is forced to be equal to the neutronics time step; Used only if URANUS-off.
DTMPF		1.0×10^{-5} s	Maximum time step after mechanical pin failure (s). Used only when HISTORIAN code option DPIN is on.

5. XRGN

The mesh cell input variables for each cell region.

Note: a. NAMELIST /XRGN/ must be entered for NREG times (NREG is specified in NAMELIST /XMSH/).

b. NAMELIST /XRGN/ can appear in any order.

c. The region boundaries can overlap and the later input overrides the former mesh cell variables.

d. The mesh-cell-wise input variables in NAMELIST /XCWD/ override the region-wise variables.

Variable	Dimension	Default	Description
LRGN			Fluid-dynamics mesh cell region number.
RGNAMB			Name of the mesh cell region (A80).
ILB			Left cell boundary for the region.
IUB			Right cell boundary for the region.
JLB			Lower cell boundary for the region.
JUB			Upper cell boundary for the region.
ILM	100		Left cell boundary for the each region in the LRGN.
IUM	100		Right cell boundary for the each region in the LRGN.
JLM	100		Lower cell boundary for the each region in the LRGN.
JUM	100		Upper cell boundary for the each region in the LRGN.
NST1B		0	Flag to exclude this region from the calculation. = 0 : Do not exclude. = 1 : Exclude.
ASMINB	(MCSRE)		Structure component volume fractions.
TSINB	(MCSRE)		Structure component temperatures (K).
ASMTB			Volume fraction of the pin fuel interior node.
TSINTB			Temperature of the pin fuel interior node (K).
ALMINB	(MCLRE)		Liquid component volume fractions.
TLMINB	(MCLRE)		Liquid component temperatures (K).
ANFIPB			No-flow volume fraction of the pin.
ANFILB			No-flow volume fraction of the left can wall.
ANFIRB			No-flow volume fraction of the right can wall.
PSAINB			Surface area per unit volume of the pin (m^{-1}). The surface area per unit volume of the pin is automatically calculated by the code. This can be replaced with a user-defined value by this input if necessary. Note: Although RPINIB is overwritten by PSAINB, non-zero RPINIB must be specified.
ALCWIB			Surface area per unit volume of the left can wall (m^{-1}).
ARCWIB			Surface area per unit volume of the right can wall (m^{-1}).

Variable	Dimension	Default	Description
RPINIB			Fuel pin outer radius when the control option FPNOPT(3)=0 (default) is specified (m). If APINTB is specified, this input variable is regarded as the intact fuel pin outer radius. Thickness of an elementary motif of the fuel matrix when the control option FPNOPT(3)=1 is specified (m).
RCOMPB			Total radius of an elementary motif of the fuel matrix when the control option FPNOPT(3)=1 is specified (m).
APINTB			Volume fraction of pin structure in intact geometry (m). This input variable is only needed when the user wants SIMMER to initialize the pin outer radius reflecting the change of pin volume fraction from the intact geometry
RFUEL	(NPB+1)		Fuel radius of each radial node NP with $1 \leq NP \leq NPB + 1$. Used only for DPIN model. RFUEL(1) corresponds to radius of central hole when an annular fuel pellet is adopted, while RFUEL(1) must be zero when a solid fuel pellet is adopted. RFUEL(NPB+1) corresponds to outer radius of a fuel pellet.
RBPB	(NPB)		Macroscopic density of pin fuel in the radial fuel node NP with $1 \leq NP < NPB + 1$. Used only for DPIN model.
TPB	(NPB)		Fuel temperature in the radial fuel node NP with $1 \leq NP < NPB + 1$. Used only for DPIN model.
EPSMIB	(NPB)		Porosity for pin component in radial fuel node NP with $1 \leq NP < NPB + 1$. Used only for DPIN model.
EPSFIB	(MFMAM1)		Porosity of the each fuel component (pin, left crust, right crust, liquid, particles and chunks).
XFINB			Fission gas to pin fuel mass ratio (for fission gas in pin fuel).
XFINB	(NPB)		Fission gas to pin fuel mass ratio in radial fuel node NP with $1 < NP < NPB + 1$. Used only for DPIN model.
XLINB			Fission gas to liquid fuel mass ratio (for fission gas in liquid fuel).
XPINB			Fission gas to particle fuel mass ratio (for fission gas in fuel particles).
XCNINB			Fission gas to chunk fuel mass ratio (for fission gas in fuel chunk).
XENRIB	(MFMAT)		Mass fraction of each fuel component (pin, left crust, right crust, liquid, particles, vapor and chunks).
PGMINB	(3)		Partial pressures of the condensable gases (fuel, steel and sodium vapor) (Pa). See also control option EOSOPT(1) in NAMELIST /XCNTL/.
PG4INB			Partial pressure of the non-condensable gas (Pa).
PSFINB			Pressure in single-phase cells (Pa). If PSFINB is assigned to two-phase cells and the two-phase

Variable	Dimension	Default	Description
			pressure of these cells is lower than PSFINB, the partial pressure of non-condensable gas is so adjusted that the two-phase pressure is equal to PSFINB.
VGMINB	(MCGM1)		Specific volume of the vapor component (fuel, steel, sodium vapor and non-condensable gas) (m^3/kg). See also control option EOSOPT(1) in NAMELIST /XCNTL/.
TGINB			Vapor mixture temperature (K).
UINB	(MMOM)		Radial velocity of each momentum field (m/s).
VINB	(MMOM)		Axial velocity of each momentum field (m/s).
RLMOIB	(MCLRE)	5.0×10^{-3} m	Initial radii of the liquid components (m).
RGBOIB		5.0×10^{-3} m	Initial radius of vapor bubbles (m).
RLMINB	(MCLRE)	5.0×10^{-5} m	Minimum radii allowed for droplets (m).
RLMAXB	(MCLRE)	0.01 m	Maximum radii allowed for droplets (m).
RGMINB		5.0×10^{-5} m	Minimum radius allowed for bubbles (m).
RGMAXB		0.01 m	Maximum radius allowed for bubbles (m).
TGLB			Lower fission gas plenum temperature (K).
PGLB			Lower fission gas plenum pressure (Pa).
TGUB			Upper fission gas plenum temperature (K).
PGUB			Upper fission gas plenum pressure (Pa).
RGB			Thermal resistance of the plenum fission gas ($\text{m}^2 \text{K/W}$). The thermal resistance of the plenum fission gas is automatically calculated by the code. This can be replaced with a user-defined value by this input if necessary.
ER0INB		0	Entrainment fraction of liquid components.
RCB			Initial cavity radius (m). Used only when HISTORIAN code option DPIN is on.
ACB			Initial volume fraction of cavity. Used only when HISTORIAN code option DPIN is on.
XCINB	(2)		Initial fission gas to fuel mass ratio in cavity. Used only when HISTORIAN code option DPIN is on.
TCB			Initial cavity temperature (K). Used only when HISTORIAN code option DPIN is on.
PCB			Initial cavity pressure (Pa). Used only when HISTORIAN code option DPIN is on.
DAXDRB			Relative power (heat source) which is applied to all components in the region. DAXDRB is multiplied with input variable FRTP in NAMELIST /XSOS/ to give the region-wise specific power density of each component, such that the total (global) power generated is normalized to input variable POW in /XSOS/. Used only when HISTORIAN code option URANUS is on.

Variable	Dimension	Default	Description
IDHB		2	<p>Input flag to control the definition of the hydraulic diameter in the cell in which only right- or left-side can wall exists.</p> <p>=0 : Hydraulic diameter is based on mesh-cell width:</p> $D_h = (1 - \alpha_s) \times \Delta R.$ <p>=1 : Input variable DHFB (defined below) is used.</p> <p>=2 : The former definition of the hydraulic diameter in SIMMER is used:</p> $D_h = 4 \times (1 - \alpha_s) / a_s,$ <p>where the terms used in the equations are:</p> <p>D_h: hydraulic diameter,</p> <p>α_s: structure component volume fraction,</p> <p>a_s: structure surface area per unit volume, and</p> <p>ΔR: radial width of the mesh-cell.</p>
DHFB			Cell hydraulic diameter (m), to be used if IDHB=1.
DHPOLB			Hydraulic diameter above which the flow is regarded as pool flow unconditionally (m). See also variable DHPOOL in NAMELIST /XIFA/.
ILSOIB		7	<p>Parameter which determines the fluid-structure contact mode. Fluid-structure heat transfer and momentum exchange are calculated only for structures defined below:</p> <p>= 1 : Pin.</p> <p>= 2 : Left can wall.</p> <p>= 3 : Right can wall.</p> <p>= 4 : Pin and left can wall.</p> <p>= 5 : Pin and right can wall.</p> <p>= 6 : Left can wall and right can wall.</p> <p>= 7 : All structure.</p>
CPVISB		5.0	Coefficient of the exponent in the particle viscosity formulation. CPVIS and CPVISI parameters in NAMELIST /XMXF/ take precedence over CPVISB.

6. XCWD

The mesh-cell-wise input variables for each mesh cell.

Note: a. /XCWD/ input data overrides /XRGN/ input only for those cells entered.

b. The radial node number must always be specified when the actual number of radial meshes is less than the maximum number allowed.

Variable	Dimension	Default	Description
NST1C	(0:IB+1, 0:JB+1)	0	Flag to exclude this cell from the calculation. = 0 : Do not exclude. = 1 : Exclude.
ASC	(0:IB+1, 0:JB+1, MCSRE)		Structure component volume fractions.
TSC	(0:IB+1, 0:JB+1, MCSRE)		Structure component temperatures (K).
ASIC	(0:IB+1, 0:JB+1)		Volume fraction of the pin fuel interior node.
TSIC	(0:IB+1, 0:JB+1)		Temperature of the pin fuel interior node (K).
ALC	(0:IB+1, 0:JB+1, MCLRE)		Liquid component volume fractions.
TLC	(0:IB+1, 0:JB+1, MCLRE)		Liquid component temperatures (K).
ANFC	(0:IB+1, 0:JB+1)		No-flow volume fraction of the pin.
ANLC	(0:IB+1, 0:JB+1)		No-flow volume fraction of the left can wall.
ANRC	(0:IB+1, 0:JB+1)		No-flow volume fraction of the right can wall.
SARC	(0:IB+1, 0:JB+1, 3)		Surface areas per unit volume of the pin, the left can wall and the right can wall (m^{-1}). The surface area per unit volume of the pin is automatically calculated by the code. This can be replaced with a user defined value by this input if necessary.
RPC	(0:IB+1, 0:JB+1)		Fuel pin outer radius when the control option FPNOPT(3)=0 (default) is specified (m). If APINTC is specified, this input variable is regarded as the intact fuel pin outer radius. Thickness of an elementary motif of the fuel matrix when the control option FPNOPT(3)=1 is specified (m).
RCOMPC	(0:IB+1,		Total radius of an elementary motif of the fuel matrix when

Variable	Dimension	Default	Description
	0:JB+1)		the control option FPNOPT(3)=1 is specified (m).
APINTC	(0:IB+1, 0:JB+1)		Volume fraction of pin structure in intact geometry (m). This input variable is only needed when the user wants SIMMER to initialize the pin outer radius reflecting the change of pin volume fraction from the intact geometry
RFUELC	(NPB+1, 0:IB+1, 0:JB+1)		Fuel radius of each radial node NP with $1 \leq NP \leq NPB + 1$. Used only for DPIN model. RFUELC(1,i,j) corresponds to radius of central hole when an annular fuel pellet is adopted, while RFUEL(1) must be zero when a solid fuel pellet is adopted. RFUELC(NPB+1,i,j) corresponds to outer radius of a fuel pellet.
RBPC	(NPB, 0:IB+1, 0:JB+1)		Macroscopic density of pin fuel in the radial fuel node NP with $1 \leq NP < NPB + 1$. Used only for DPIN model.
TPC	(NPB, 0:IB+1, 0:JB+1)		Fuel temperature in the radial fuel node NP with $1 \leq NP < NPB + 1$. Used only for DPIN model.
EPMSC	(NPB, 0:IB+1, 0:JB+1)		Porosity for pin component in radial fuel node NP with $1 \leq NP < NPB + 1$. Used only for DPIN model.
EPSC	(0:IB+1, 0:JB+1, MFMAM1)		Porosity of the each fuel component (pin, left crust, right crust, liquid, particles and chunks).
XFGC	(0:IB+1, 0:JB+1)		Fission gas to pin fuel mass ratio (for fission gas in pin fuel).
	(NPB+1, 0:IB+1, 0:JB+1)		Fission gas to pin fuel mass ratio in each node NP with $1 < NP < NPB + 1$ in the DPIN model (for fission gas in pin fuel).
XLFGC	(0:IB+1, 0:JB+1)		Fission gas to liquid fuel mass ratio (for fission gas in liquid fuel).
XPFGC	(0:IB+1, 0:JB+1)		Fission gas to particle fuel mass ratio (for fission gas in fuel particles).
XCNFGC	(0:IB+1, 0:JB+1)		Fission gas to chunk fuel mass ratio (for fission gas in fuel chunks).
ENRC	(0:IB+1, 0:JB+1, MFMAT)		Fissile fuel mass fraction of each fuel component (pin, left crust, right crust, liquid, particles, vapor and chunks).
PGMC	(0:IB+1, 0:JB+1, 3)		Partial pressures of the condensable gases (fuel, steel and sodium vapor) (Pa). See also control option EOSOPT(1) in NAMELIST /XCNTL/.
PG4C	(0:IB+1, 0:JB+1)		Partial pressure of the non-condensable gas (Pa).
PSFC	(0:IB+1, 0:JB+1)		Pressure in single-phase cells (Pa). If PSFC is assigned to a two-phase cell and the two-phase pressure of this cell is lower than PSFC, the partial pressure of non-condensable gas is so adjusted that the two-phase

Variable	Dimension	Default	Description
			pressure is equal to PSFC.
VGMC	(0:IB+1, 0:JB+1, MCGM1)		Specific volume of the vapor component (fuel, steel, sodium vapor and non-condensable gas) (m ³ /kg). See also control option EOSOPT(1) in NAMELIST /XCNTL/.
TGC	(0:IB+1, 0:JB+1)		Vapor mixture temperature (K).
UC	(0:IB+1, 0:JB+1, MMOM)		Radial velocity of each momentum field (m/s).
VC	(0:IB+1, 0:JB+1, MMOM)		Axial velocity of each momentum field (m/s).
RLMOC	(0:IB+1, 0:JB+1, MCLRE)	5.0×10 ⁻³ m	Initial radii of the liquid components (m).
RGBOC	(0:IB+1, 0:JB+1)	5.0×10 ⁻³ m	Initial radius of vapor bubbles (m).
RLMINC	(0:IB+1, 0:JB+1, MCLRE)	5.0×10 ⁻⁵ m	Minimum radii allowed for droplets (m).
RLMAXC	(0:IB+1, 0:JB+1, MCLRE)	0.01 m	Maximum radii allowed for droplets (m).
RGMINC	(0:IB+1, 0:JB+1)	5.0×10 ⁻⁵ m	Minimum radius allowed for bubbles (m).
RGMAXC	(0:IB+1, 0:JB+1)	0.01 m	Maximum radius allowed for bubbles (m).
EROC	(0:IB+1, 0:JB+1)	0.0	Entrainment fraction of liquid components.
RCC	(0:IB+1, 0:JB+1)		Initial cavity radius (m). Used only when HISTORIAN code option DPIN is on.
ACC	(0:IB+1, 0:JB+1)		Initial volume fraction of cavity. Used only when HISTORIAN code option DPIN is on.
XCFGC	(0:IB+1, 0:JB+1, 2)		Initial fission gas to fuel mass ratio in cavity. Used only when HISTORIAN code option DPIN is on.
TCC	(0:IB+1, 0:JB+1)		Initial cavity temperature (K). Used only when HISTORIAN code option DPIN is on.
PCC	(0:IB+1, 0:JB+1)		Initial cavity pressure (Pa). Used only when HISTORIAN code option DPIN is on.
DAXDRC	(0:IB+1, 0:JB+1)		Relative power (heat source) which is applied to all components in the cell. DAXDRC is multiplied with input variable FRTP in NAMELIST /XSOS/ to give the cell-wise specific power density of each component, such that the total

Variable	Dimension	Default	Description
			(global) power generated is normalized to input variable POW in /XSOS/. Used only when HISTORIAN code option URANUS is on.
IDHC	(0:IB+1, 0:JB+1)	2	<p>Input flag to control the definition of the hydraulic diameter in the cell in which only right- or left-side can wall exists.</p> <p>=0 : Hydraulic diameter is based on mesh-cell width:</p> $D_h = (1 - \alpha_s) \times \Delta R.$ <p>=1 : Input variable DHFC (defined below) is used.</p> <p>=2 : The former definition of the hydraulic diameter in SIMMER is used:</p> $D_h = 4 \times (1 - \alpha_s) / a_s,$ <p>where the terms used in the equations are:</p> <p>D_h: hydraulic diameter,</p> <p>α_s: structure component volume fraction,</p> <p>a_s: structure surface area per unit volume, and</p> <p>ΔR: radial width of the mesh-cell.</p>
DHFC	(0:IB+1, 0:JB+1)		Cell hydraulic diameter (m), to be used if IDHC(IB, JB)=1.
DHPOLC	(0:IB+1, 0:JB+1)		Hydraulic diameter above which the flow is regarded as pool flow unconditionally (m). See also variable DHPOOL in NAMELIST /XIFA/.
ILSOC	(0:IB+1, 0:JB+1)	7	<p>Parameter which determines the fluid-structure contact mode. Fluid-structure heat transfer and momentum exchange are calculated only for structures defined below:</p> <p>= 1 : Pin.</p> <p>= 2 : Left can wall.</p> <p>= 3 : Right can wall.</p> <p>= 4 : Pin and left can wall.</p> <p>= 5 : Pin and right can wall.</p> <p>= 6 : Left can wall and right can wall.</p> <p>= 7 : All structure.</p>
CPVISC	(0:IB+1, 0:JB+1)	5.0	Coefficient of the exponent in the particle viscosity formulation. See also variables CPVIS and CPVISI in NAMELIST /XMXF/.
ISPC	(0:IB+1, 0:JB+1)	0	Flag to specify the single-phase cell. If ISPC(I,J) = 1, the cell will be filled with the real liquid component which has the maximum volume fraction such that the cell becomes single phase.

7. XEDT

The output control variables. A complete description of the variables PCGRP, PPGRP, PRCEL, and LPRGN are given in Attachment 2.

Variable	Dimension	Default	Description
PRTC		50	Number of cycles between prints.
PPFC		25	Number of cycles between postprocessor dumps.
BSFC		10	Number of cycles between base file (SIMBF) dumps.
DMPC		100	Number of cycles between restart dumps. See also control option EDTOPT(20).
DTPRT	(10)	1.0×10^{10} s	Time intervals between "long prints" (s), i.e. listings of cell-wise and global variables. DTPRT(n) is the print interval from time TCPRT(n-1) to TCPRT(n).
DTPPF	(10)	1.0×10^{10} s	Time intervals between postprocessor dumps from time TCPPF(n-1) to TCPPF(n) (s).
DTBSF	(10)	1.0×10^{10} s	Time intervals between base file (SIMBF) dumps from time TCBSF(n-1) to TCBSF(n) (s).
DTDMP	(10)	1.0×10^{10} s	Time intervals between restart dumps from time TCDMP(n-1) to TCDMP(n) (s).
TCPRT	(10)	1.0×10^{20} s	Times at which to change to DTPRT(n+1) as the time interval between prints (s).
TCPPF	(10)	1.0×10^{20} s	Times at which to change to DTPPF(n+1) as the time interval between postprocessor dumps (s).
TCBSF	(10)	1.0×10^{20} s	Times at which to change to DTBSF(n+1) as the time interval between base file (SIMBF) dumps (s).
TCDMP	(10)	1.0×10^{20} s	Times at which to change to DTDMP(n+1) as the time interval between restart dumps (s).
PCGRP	(50)		Control flag of cell-wise variables to be printed. See Attachment 2.
PPGRP	(50)		Control flag of cell-wise and global variables to be dumped to the postprocessor file. See Attachment 2.
SN	(200)		Short names of variables to be sent to the base file (SIMBF). See Table G-1.
SF	(200)		Name of fuel variables to be dumped in SIMFF. Used only for DPIN model.
NSN			Number of variables to be sent to the base file (SIMBF). This input variable is needed only for the CRAY system.
NSF			Number of variables to be dumped in SIMFF. Used only for DPIN model.
IVBF		0	Flag to determine whether the velocities in the boundary cells are written to the base file (SIMBF). =1 : Base file (SIMBF) dumps contain boundary cell velocities.

Variable	Dimension	Default	Description
			=0 : Base files (SIMBF) do not contain boundary cell velocities.
PRCEL	(5, 50)		Print the requested cells. See Attachment 2.
LPRGN	(270)		Print the requested cell variables for the entire mesh. See Attachment 2.
NPAGE			In the global variable listing, NPAGE variables are printed on each page.
DTEOS	(3, MNMAT)		Minimum, incremental, and maximum values of temperature to be printed in the EOS tables (K). See also control option EDTOPT(6) in NAMELIST /XCNTL/.
DTTPP	(3, MNMAT)		Minimum, incremental, and maximum values of temperature to be printed in the TPP tables (K). See also control option EDTOPT(7) in NAMELIST /XCNTL/.
NPRINT	(MNMAT)		Sub-material number printed in the EOS and TPP tables.

8. XEOS

The equation of state (EOS) input variables.

Variable	Dimension	Default	Description
ALPHA0		10^{-2}	$\alpha_{ge} = \max [\alpha_o(1 - \alpha_s), 1 - \alpha_s - (1 - \alpha_o)\alpha_L]$, where α_L is the total liquid volume fraction, α_s is the total structure volume fraction, and $\alpha_o(1 - \alpha_s)$ is the minimum effective vapor-volume fraction.
EPSTG		10^{-6}	Convergence criterion for the vapor temperature iteration, ϵ_{ig} .
EPSEN		10^{-6}	Convergence criterion for the energy iteration, ϵ_{en} .
EPSSV		10^{-6}	Convergence criterion for the specific volume iteration, ϵ_{sv} .
TGMIN		273.15 K	Minimum temperature allowed in the iteration schemes to evaluate the vapor temperature, $T_{G,min}$ (K). See also control option ALGOPT(33) in NAMELIST /XCNTL/.
PTS	(MNMATN, MNMAT)		Percentage of the melting temperature used to calculate the internal energy of absent material components M, PTS_M .
ESOLUS	(MNMATN, MNMAT)		Solidus internal energy of material M, $e_{Sol,M}$ (J/kg).
ELIQUUS	(MNMATN, MNMAT)		Liquidus internal energy of material M, $e_{Liq,M}$ (J/kg).
ECRT	(MNMATN, MNMAT)		Critical internal energy of material M, $e_{Cr,M}$ (J/kg).
ELIQG	(MNMATN, MNMAT)		Internal energy of the saturated vapor of material M at its liquidus temperature (J/kg).
TSOLUS	(MNMATN, MNMAT)		Solidus temperature of material M, $T_{Sol,M}$ (K).
TLIQUUS	(MNMATN, MNMAT)		Liquidus temperature of material M, $T_{Liq,M}$ (K).
TCRT	(MNMATN, MNMAT)		Critical temperature of material M, $T_{Cr,M}$ (K).
VSOLUS	(MNMATN, MNMAT)		Solidus specific volume of material M, $v_{Sol,M}$ (m ³ /kg).
VLIQUUS	(MNMATN, MNMAT)		Liquidus specific volume of material M, $v_{Liq,M}$ (m ³ /kg).
ROCRT	(MNMATN, MNMAT)		Critical density of material M, $\rho_{Cr,M}$ (kg/m ³).
PCRT	(MNMATN, MNMAT)		Critical pressure of material M, $p_{Cr,M}$ (Pa).
WM	(MNMATN,		Molecular weight of material M, W_M (g/mol).

Variable	Dimension	Default	Description
			MNMAT)
AS	(3, MNMATN, MNMAT)		Coefficients to calculate the solid temperature of material M, $a_{S1,M} \sim a_{S3,M}$.
BS	(3, MNMATN, MNMAT)		Coefficients to calculate the solid specific volume of material M, $b_{S1,M} \sim b_{S3,M}$.
DTDPS	(MNMATN, MNMAT)		Derivative of the solid particle temperature of material M with respect to the pressure, $\left(\frac{\partial T_{Lm}}{\partial p}\right)_M^o$ (K/Pa).
DVDPS	(MNMATN, MNMAT)		Derivative of the solid particle specific volume of material M with respect to the pressure, $\left(\frac{\partial v_{Lm}}{\partial p}\right)_M^o$ (m ³ /kg-Pa).
AL	(6, MNMATN, MNMAT)		Coefficients to calculate the saturated-liquid temperature of material M, $a_{L1,M} \sim a_{L6,M}$.
BL	(4, MNMATN, MNMAT)		Coefficients to calculate the saturated-liquid vapor pressure of material M, $b_{L1,M} \sim b_{L4,M}$.
CL	(4, MNMATN, MNMAT)		Coefficients to calculate the liquid-temperature derivative of material M, $c_{L1,M} \sim c_{L4,M}$.
DL	(6, MNMATN, MNMAT)		Coefficients to calculate the saturated-liquid specific volume of material M, $d_{L1,M} \sim d_{L6,M}$.
FL	(6, MNMATN, MNMAT)		Coefficients to calculate the liquid specific volume derivative of material M, $f_{L1,M} \sim f_{L6,M}$.
BETA	(MNMATN, MNMAT)		Coefficients to calculate the liquid specific volume of material M, β_M .
DTDPC	(MNMATN, MNMAT)		Derivative of the temperature of material M with respect to the pressure at the critical internal energy, $\left(\frac{\partial T_{Lm}}{\partial p}\right)_{e_{Cr,M}}$ (K/Pa).
AG	(4, MNMATN, MNMAT)		Coefficients to calculate the vapor pressure of material M, $a_{G1,M} \sim a_{G4,M}$.
BG	(6, MNMATN, MNMAT)		Coefficients to calculate the saturation vapor density of material M, $b_{G1,M} \sim b_{G6,M}$.
CG	(6,		Coefficients to calculate the saturation vapor energy of

Variable	Dimension	Default	Description
	MNMATN, MNMAT)		material M, $c_{G1,M} \sim c_{G6,M}$.
DG	(2, MNMATN, MNMAT)		Coefficients to calculate the equilibrium constant of material M, $d_{G1,M} \sim d_{G2,M}$. The equilibrium constant is used to calculate the dimer fraction for a reacting system.
FG	(4, MNMATN, MNMAT)		Coefficients to calculate the vapor spinodal volume of material M, $f_{G1,M} \sim f_{G4,M}$.
RUGM	(MNMATN, MCGR)		Gas constant of material M, R_M (J/kg-K).
CVG	(MNMATN, MNMAT)		Heat capacity of vapor, to calculate the vapor internal energy of material M, $c_{vG,M}$ (J/kg-K).
ELIQGD	(MNMATN, MNMAT)		Internal energy of the infinitely dilute vapor at the liquidus temperature in the equation of the vapor internal energy of material M, $e_{Liq,Gm}^D$ (J/kg).
ASAT	(4, MNMATN, MNMAT)		Coefficients to calculate the saturation temperature of material M, $a_{Sat1,M} \sim a_{Sat4,M}$.
BSAT	(6, MNMATN, MNMAT)		Coefficients to calculate the condensate density of material M, $b_{Sat1,M} \sim b_{Sat6,M}$.
CSAT	(6, MNMATN, MNMAT)		Coefficients to calculate the condensate energy of material M, $c_{Sat1,M} \sim c_{Sat6,M}$.
PSMIN	(MNMATN, MNMAT)		Lowest saturation pressure allowed for the calculation of the saturation temperature of material M, $p_{Smin,M}$ (Pa).
BSL	(2, MNMATN, MNMAT)		Coefficients to calculate the liquid adiabatic compressibility of material M, $b_{SL1,M}$ and $b_{SL2,M}$ for the FFEOS model. See also IFREE parameter in NAMELIST /XEOS/.
TLBND	(MNMATN, MNMAT)		Upper limit temperature to extrapolate the liquid density equation of material M, $T_{Lbnd,M}$ for the FFEOS model. See also IFREE parameter in NAMELIST /XEOS/.
ISAE	(MNMATN, MNMAT)		Flag to select the type of analytic EOS model for material M. =0 : Standard analytic EOS model. =1 : Simplified analytic EOS model.
IMRK	(MNMATN, MNMAT)		Flag to select the type of Modified Redlich-Kwong (MRK) EOS for vapor of material M. =0 : Standard MRK EOS. =1 : Extended MRK EOS, for a reacting system.
ISPN	(MNMATN,		Flag to determine the vapor spinodal volume calculation of

Variable	Dimension	Default	Description
	MNMAT)		material M. =0 : Spinodal volume is not calculated. =1 : Spinodal volume is iteratively calculated. =2 : Spinodal volume is calculated by an analytical function, in subroutine XVSPN.
IFREE	(MNMATN, MNMAT)		Flag to select the type of EOS models for material M. =0 : Standard EOS functions are used. =1 : Fitting-Free EOS (FFEOS) model is used. The coefficient $a_{G^4, M}$ for the MRK equation is calculated by a built-in preprocessor for the FFEOS model. =2 : FFEOS model is used. The coefficient $a_{G^4, M}$ should be specified as the EOS parameter.

9. XMXF

The momentum exchange input variables.

Variable	Dimension	Default	Description
ALPDM		1.0	
ALPMP		0.62	Maximum packing fraction for defining the particle viscosity, α_{MP} (recommended value: 0.62).
ALPMP2		0.9	Maximum packing fraction for defining the particle viscosity based on melt fraction, α_{MP2} (recommended value: 0.9).
ALPSID		0.9	Structure volume fraction above which the structure prevents fluid motion, α_{SID} (recommended value: 0.9).
CTC		1.0	Multiplier of the drag coefficient between continuous components and structure, C_{Tc} .
CTD		1.0	Multiplier of the drag coefficient between dispersed components and structure, C_{Td} .
CDD		1.0	Multiplier of the drag coefficient among dispersed components, C_{dd} .
CCD		1.0	Multiplier of the drag coefficient between dispersed and continuous components, C_{CD} .
CCPG		1.0	Multiplier of the drag coefficient between continuous liquid and vapor, $C_{CP,G}$.
CQS	(MMOM)	1.0	Multiplier of momentum exchange functions between fluids and structure, $C_{qm,s}$.
CT1		0.0791	Fluid-structure drag coefficient, C_{T1} .
CT2		-0.25	Fluid-structure drag coefficient, C_{T2} .
APJ		0.7	Maximum packing fraction used in the particle jamming model.
BPJ		0.95	Fraction of APJ above which the particle jamming model is applied.
CPJ		-10.0	Exponent in the particle jamming model which is used to calculate the momentum exchange function increment.
CFRS1		2.3	Coefficient for the correlation of superficial liquid velocity in Ueda's model, for evaluating the two-phase pressure drop in the bubbly flow region, C_4 . See also control option MXFOPT(1) in NAMELIST /XCNTL/.
CFRS2		0.3	Coefficient for the correlation of superficial liquid velocity in Ueda's model, for evaluating the two-phase pressure drop in the bubbly flow region, C_5 . See also control option MXFOPT(1) in NAMELIST /XCNTL/.
CFRS3		1.8	Coefficient for the correlation of superficial liquid velocity in Ueda's model, for evaluating the two-phase pressure drop in

Variable	Dimension	Default	Description
			the bubbly flow region, C_6 . See also control option MXFOPT(1) in NAMELIST /XCNTL/.
CANUL1		0.75	Coefficient for the correlation of superficial liquid velocity in Ueda's model, for evaluating the two-phase pressure drop in the annular flow region, C_1 . See also control option MXFOPT(1) in NAMELIST /XCNTL/.
CANUL2		-0.25	Coefficient for the correlation of superficial liquid velocity in Ueda's model, for evaluating the two-phase pressure drop in the annular flow region, C_2 . See also control option MXFOPT(1) in NAMELIST /XCNTL/.
CANUL3		-12.0	Coefficient for the correlation of superficial liquid velocity in Ueda's model, for evaluating the two-phase pressure drop in the annular flow region, C_3 . See also control option MXFOPT(1) in NAMELIST /XCNTL/.
FCOUPG		-10^{-10}	Void fraction below which the vapor velocity is set to the velocity field containing continuous phase liquid. If the void fraction is less than FCOUPG, the momentum exchange function between the vapor field and the relevant liquid velocity field is set to $10^{10} \times (1 - \alpha_s) / \Delta t$, where α_s is the structure volume fraction. This prevents unphysical bubble velocities by small fractions of vapor. If the numerical instability is encountered due to the non-physically large velocity of a small amount of vapor mixture, a small positive value such as 10^{-10} is typically recommended.
FCOUPL		10^{-10}	Volume fraction of liquid below which the liquid velocity is forced to a very small value. If the volume fraction of material components in velocity fields 1 or 2 is less than FCOUPL, the momentum exchange function between the structure and the relevant liquid velocity fields is set to $10^7 \times (1 - \alpha_s) / \Delta t$, where α_s is the structure volume fraction, even if there is no structure component in the cell. This prevents unphysical velocities by small fractions of liquids or particles. If the numerical instability is encountered due to the non-physically large velocity of a small amount of liquid or particles, a small positive value such as 10^{-10} is typically recommended.
CPVIS		5.0	Coefficient of the exponent in the particle viscosity formulation.
CPVISI	(0:IB+1, 0:JB+1)	5.0	Coefficient of the exponent in the particle viscosity formulation. CPVISI takes precedence over CPVIS.
CORFRN	(0:IB+1, 0:JB+1)	0.0	Orifice coefficient at the right boundary of the cell.
CORFZN	(0:IB+1,	0.0	Orifice coefficient at the top boundary of the cell.

Variable	Dimension	Default	Description
	0:JB+1)		<p>Orifice coefficient is defined by</p> $\Delta p = -C_{ORF} \times \bar{\rho}_q \times v_q ^2,$ <p>where</p> <p>Δp is the pressure drop across the orifice,</p> <p>C_{ORF} is the orifice coefficient,</p> <p>$\bar{\rho}_q$ is the macroscopic density of liquid components in velocity field q, and</p> <p>v_q is the velocity of field q at the orifice.</p>
PVS1		0.2×10^{20}	Ratio of particle diameter to the characteristic length of momentum exchange process above which the particle viscosity begins to decrease.
PVS2		0.4×10^{20}	Ratio of particle diameter to the characteristic length of momentum exchange process above which the particle viscosity is not applied. To switch off the particle viscosity dependency on the particle size, set $1.0 < PVS1 < PVS2$.
PVSCL		2.5×10^{-3} m	Characteristic length compared with a particle diameter. The ratio of particle diameter to the characteristic length is used to estimate the particle viscosity (MXFOPT(4)=1).
DHINP		3.33×10^{-2} m	Hydraulic diameter specified by user only when MXFOPT(95)=1.
AN		-1.75	Index of the viscosity multiplier for multi-particle system (MXFOPT(5)=1).
CDFBL0		8.49×10^{-1}	Coefficient for the droplet-laminar liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBL1		2.05×10^{-3}	Coefficient for the droplet-laminar liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBL2		3.47	Coefficient for the droplet-laminar liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBL3		4.24×10^{-2}	Coefficient for the droplet-laminar liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBL4		-2.18	Coefficient for the droplet-laminar liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBT0		6.5×10^{-3}	Coefficient for the droplet-turbulent liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBT1		6.89×10^{-2}	Coefficient for the droplet-turbulent liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBT2		1.15×10^{-2}	Coefficient for the droplet-turbulent liquid coupling under film boiling condition (MXFOPT(5)=1).
CDFBT3		5.11	Coefficient for the droplet-turbulent liquid coupling under film boiling condition (MXFOPT(5)=1).

Variable	Dimension	Default	Description
ICRGT	(IB)	0	Active only if MXFOPT(7)=1. The particle viscosity is determined only by the effective volume fraction of particles $\frac{\alpha_p}{1-\alpha_s}$ in I-th radial column, if ICRGT(I)=1 and both the left and right can walls exist. In addition, if the left and/or right can walls do not exist in a cell in the I-th radial column, and the left and/or right can wall exist in the neighboring cells respectively, the surface area of the can walls in the neighboring cells are used to calculate the momentum coupling in the referring cell.
CWST			Pitch for arrays of cylinder in radial direction (m). Used only when MXFOPT(8)=2.
CWSL			Pitch of arrays of cylinder in axial direction (m). Used only when MXFOPT(8)=2.
DTUBE			Hydraulic diameter of tube in cylinder array (m). Used only when MXFOPT(8)=2.
CWMXF	4		Flag to specify the momentum coupling area for a rod bundle. (I1, J1, I2, J2). Used only when MXFOPT(8)=2.

The following input variables are provided for a simple model to take account of the turbulence-diffusion effect on the viscous-drag term in the momentum equations and required only when MXFOPT(3)=1 is specified.

FACGOM		0.125	Geometrical factor for the boundary layer region.
ALMNTU		1.0×10^{-3}	Liquid volume fraction to calculate the height of the pool.
AGMNTU		1.0×10^{-3}	Void fraction to determine the limit between liquid and two-phase regions.
AGLIMT		0.3	Limit value of void fraction under which the viscous effects in two-phase regions is taken into account.
CMU		0.9	The k- ϵ model classical constant.
RATIOL		0.1	Ratio between fluctuations and averaged turbulent velocities in the liquid continuous phase.
RATIOD		0.1	Ratio between fluctuations and averaged turbulent velocities in the two-phase region.
XLARG		0.2 m	Horizontal dimension of the tank in rectangular cases (IGEOM=1) and the radius of the tank in cylindrical case (IGEOM=0) (m).
XBULLE		0.01 m	Typical length for the bubbly region. This can be the diameter of bubbles, or the radial expansion of the bubbly region depending on the case (m).
RPMXLB		1.0×10^6	Maximum value of the ratio between molecular and turbulent viscosity in the liquid phase region.
RPMAXD		1.0×10^4	Maximum value of the ratio between molecular and turbulent viscosity in two phase and in the boundary layer region. In

the gas region, liquid turbulent viscosity is zero.

10. XIFA

The interfacial area (IFA) input variables.

Variable	Dimension	Default	Description
ALPBUB		0.3	
ALPDSP		0.7	Minimum void fraction in the liquid components above which the dispersed flow regime can exist, α_D (recommended value: 0.7).
ALPB1		0.3	Maximum relative volume fraction of the second continuous phase (CP2) for which only the first continuous phase (CP1) is continuous (i.e. the boundary of the CP-continuous regime), α_{B1} (recommended value: 0.3).
ALPB2		0.7	Minimum relative volume fraction of the second continuous phase (CP2) for which CP2 is the continuous flow regime, α_{B2} (recommended value: 0.7).
RLMIN	(MCLRE)	5.0×10^{-5} m	Minimum droplets' radii allowed, $r_{Lm, min}$ (m). (Recommended value: 5.0×10^{-5} m.)
RLMAX	(MCLRE)	0.01 m	Maximum droplets' radii allowed, $r_{Lm, max}$ (m). (Recommended value: 0.01 m.)
RGBMIN		5.0×10^{-5} m	Minimum bubble radius allowed, $r_{G,B, min}$ (m). (Recommended value: 5.0×10^{-5} m.)
RGBMAX		0.01 m	Maximum bubble radius allowed, $r_{G,B, max}$ (m). (Recommended value: 0.01 m.)
RLINI	(MCLRE)	5.0×10^{-3} m	Initial droplets' radii (m).
RGINI		5.0×10^{-3} m	Initial bubble radius (m).
RPCNTL		5.0×10^{-4} m	Radius of a control particle (m).
RLSBK	(MCLRE)	5.0×10^{-4} m	Radii of the liquid components newly born by structure breakup (m).
RGSBK		5.0×10^{-4} m	Radii of bubbles for gas newly born by structure breakup (m).
RLHMT	(MCLRE)	5.0×10^{-4} m	Radii of liquid components newly born by mass transfer (m).
CHYS		1.0	User-defined constant less than or equal to unity which controls a hysteresis in the change of continuous phase, C_{HYS} (suggested value: 1.0).
CBD		1.0	Multiplier for the interfacial area between bubbly and dispersed regions, $C_{B,D}$ (recommended value: 1.0).
CPSR		5.0×10^{-2}	Fraction of particle contact area to the structure surface at the maximum packing fraction. See also ALPMP parameter in NAMELIST /XMXF/. (Recommended value: 5.0×10^{-2} .)
CLDS	(MCLRE)	1.0	Binary contact area multipliers for droplet-structure contacts, $C_{Lm,D,S}$ (recommended values: 1.0).
CLCS	(MCLRE)	1.0	Binary contact area multipliers for continuous liquid-structure

Variable	Dimension	Default	Description
			contacts, $C_{Lm,C,S}$ (recommended values: 1.0).
CGBS		1.0	Binary contact area multiplier for bubble-structure contact, $C_{G,B,S}$ (recommended value: 1.0).
CGCS		1.0	Binary contact area multiplier for continuous vapor-structure contact, $C_{G,C,S}$ (recommended value: 1.0).
CLL	(MCLRE, MCLRE)	1.0	Binary contact area multipliers for liquid-liquid contacts, $C_{Lm,Lk}$ (recommended values: 1.0).
CLG	(MCLRE)	1.0	Binary contact area multipliers for liquid-vapor contacts, $C_{Lm,G}$ (recommended values: 1.0).
ALPNT		10^{-2}	Minimum volume fraction at which bubble nucleation is allowed, α_N^t (recommended value: 10^{-2}).
MMIN		10^5 m^{-3}	Minimum nucleation site density, M_{min} (m^{-3}). (Recommended value: 10^4 m^{-3} .)
MMAX		10^{11} m^{-3}	Maximum nucleation site density, M_{max} (m^{-3}). (Recommended value: 10^7 m^{-3} .)
THETA0		2.0×10^{-3}	Minimum dimensionless superheat to participate in bubble nucleation, θ_0 (recommended value: 2.0×10^{-3}).
TAUNUC		10^{-4} s	Nucleation time constant, τ_{NUC} (s). (Recommended value: 10^{-4} s .)
ALPNC		0.7	Void fraction in the liquid component above which bubble nucleation cannot occur, α_{NC} (it is recommended to use the same value as input variable ALPDSP: 0.7).
CNC		1.0	Coefficient in the exponent of nucleation time equation, C_{NC} (recommended value: 1.0).
CTHETA		10^5	Coefficient in the exponent of nucleation site density equation, C_θ (recommended value: 10^5).
WEB		10.0	Critical Weber number for bubbles, We_B (recommended value: 10.0).
CFV		10^{-4}	Multiplier of the viscous term in the Weber breakup criterion equation for bubbles, C_{FV} (recommended value: 10^{-4}).
CFT		1.0	Time constant multiplier for the Weber breakup of bubbles, C_{FT} (recommended value: 1.0).
WED		12.0	Critical Weber number for droplets, We_D (recommended value: 12.0).
DVRT		0.2 m/s	User-defined velocity difference to accelerate droplet disintegration by Weber number breakup at high velocity difference, Δv_{RT} (m/s). (Recommended value: 0.2 m/s.)
CFDB		1.0	Equilibrium radius multiplier for the Weber breakup of droplets in the bubbly region, C_{FDB} (recommended value: 1.0).

Variable	Dimension	Default	Description
CFSB		1.0	Time constant multiplier for the Weber breakup of droplets in the bubbly region, C_{FSB} (recommended value: 1.0).
CFCB		0.245	Empirical constant in the Taylor-type correlation for the Weber breakup of droplets in the bubbly region (recommended value: 0.245).
CTWB		13.7	Empirical constant in the correlation of time constant for the Weber breakup of droplets in the bubbly region (recommended value: 13.7). See also control option IFAOPT(21) in NAMELIST /XCNTL/.
CFDD		1.0	Equilibrium radius multiplier for the Weber breakup of droplets in the dispersed region, C_{FDD} (recommended value: 1.0).
CFSD		1.0	Time constant multiplier for the Weber breakup of droplets in the dispersed region, C_{FSD} (recommended value: 1.0).
CFCD		0.245	Empirical constant in the Taylor-type correlation for the Weber breakup of droplets in the dispersed region (recommended value: 0.245).
CTWD		32.5	Empirical constant in the correlation of time constant for the Weber breakup of droplets in the dispersed region (recommended value: 32.5). See also control option IFAOPT(21) in NAMELIST /XCNTL/.
OMEGAB		1.0	Coalescence probability per each collision for bubbles, ω_B (recommended value: 1.0).
OMEGAD		1.0	Coalescence probability per each collision for droplets, ω_D (recommended value: 1.0).
CFL		1.0	Time constant multiplier for the flashing of droplets, C_{FL} (recommended value: 1.0).
CTTB		1.0	Time constant multiplier for the turbulent breakup of bubbles, C_{TTB} (recommended value: 1.0).
CPTB		1.0	Multiplier of the square of the bubble velocity fluctuation in Prandtl's mixing length hypothesis, C_{PTB} (recommended value: 1.0).
CRGB		1.0	Multiplier of the square of the bubble velocity fluctuation due to turbulence from buoyancy, C_{RGB} (recommended value: 1.0).
CTTL		1.0	The time constant multiplier for the turbulent breakup of droplets, C_{TTL} (recommended value: 1.0).
CPTL		1.0	The multiplier of the square of the droplet velocity fluctuation in Prandtl's mixing length hypothesis, C_{PTL} (recommended value: 1.0).
CRGL		1.0	The multiplier of the square of the droplet velocity fluctuation due to turbulence from buoyancy, C_{RGL} (recommended

Variable	Dimension	Default	Description
			value: 1.0).
CSFL		1.0	The multiplier of the IFA of the interface between the bubbly and dispersed regions, C_{SFL} , in the annular-dispersed flow regime.
CSSX		1.0	The multiplier of the IFAs between fluids and lower/upper structures, C_{SSX} . Active only when control option HMTOPT(76)=1 in NAMELIST /XCNTL/.
DLB		0.03 m	The length of Taylor bubble in the slug flow regime (m).
CE1		7.0×10^{-7}	Constant used to calculate the equilibrium fraction entrainment in the entrainment model, C_{E1} .
CE2		1.25	Constant used to calculate the entrainment fraction in the entrainment model, C_{E2} .
CE3		1.0	Constant used to calculate the entrainment fraction in the entrainment model, C_{E3} .
CE4		45.0	Constant used to calculate the equilibrium entrainment time constant in the entrainment model, C_{E4} .
CSF		1.0	An exponent used to calculate the wetted surface fraction in the annular-dispersed flow regime.
DHPOOL		1.0 m	Hydraulic diameter above which the flow is regarded as pool flow unconditionally (m).
JBEGIN		1.2	Dimensionless vapor superficial velocity at which the flooding (entrainment) begins.
JSTOP		0.4	Dimensionless vapor superficial velocity at which the flooding (entrainment) stops.
FTHMIN		5.0×10^{-4} m	Minimum liquid film thickness (m).
FRTHKP		10^{-2}	Fraction of minimum liquid film thickness on the solid particle to the particle radius.
CANG		50 degrees	Contact angle used in a correlation of bubble departure diameter (degree). See also control option IFAOPT(25) in NAMELIST /XCNTL/.
ISRCBB	(10)	0, 0, 0, 0	Flags to suppress the IFA source terms of bubbles in the bubbly flow region (0 : activate, 1 : suppress). The mechanisms are: (1) : nucleation. (2) : fluid dynamics breakup, (3) : turbulence, and (4) : coalescence.
ISRCDB	(10)	0, 0, 0	Flags to suppress the IFA source terms of droplets in the bubbly flow region (0 : activate, 1 : suppress). The mechanisms are: (1) : fluid dynamic breakup,

Variable	Dimension	Default	Description
ISRCDD	(10)	0, 0, 0	(2) : turbulence, and (3) : coalescence. Flags to suppress the IFA source terms of droplets in the dispersed flow region (0: activate, 1: suppress). The mechanisms are: (1) fluid dynamic breakup, (2) flashing, and (3) coalescence.

11. XHTC

The heat transfer coefficients (HTC) input variables.

Variable	Dimension	Default	Description
HCDP	(MCLRE + MCGRE)	10	Steady-state conduction internal Nusselt numbers for particles, droplets and bubbles (recommended values: 10).
HCDLP	(MCLRE - 4)	2	Steady-state conduction Nusselt numbers for continuous phase liquids around particles, droplets and bubbles (recommended values: 2).
HCDGP		2	Steady-state conduction Nusselt number for gas in dispersed flow around particles and droplets (recommended value: 2).
HCDLBS	(MCLRE - 4)	5	Steady-state conduction Nusselt numbers for continuous phase liquid in bubbly flow which is exchanging heat with structure (recommended values: 5).
HCDLAS	(MCLRE - 4)	2	Steady-state conduction Nusselt numbers for continuous phase liquid in annular flow which is exchanging heat with structure (recommended values: 2).
HCDGS		5	Steady-state conduction Nusselt number for continuous phase gas which is exchanging heat with either structure or a liquid film on structure (recommended value : 5).
HFCLP	(5, MCLRE - 3)		Coefficients in the correlations which calculate steady-state forced convection HTCs between continuous phase liquids and rigid particles, droplets and bubbles. Recommended and default values are: Fuel: (1,1) = 0.542, 0.5, 0.45, 0.012, 0.333 Steel: (1,2) = 0.646, 0.5, 0.5, 0.008, 0.333 Sodium: (1,3) = 0.68, 0.5, 0.5, 0.0, 0.0
HFCGP	(5)		Coefficients in the correlation which calculates steady-state forced convection HTCs between gas in dispersed flow and rigid particles, droplets and bubbles (recommended and default values: 0.542, 0.5, 0.45, 0.012, 0.333).
HNCLP	(3, MCLRE - 4)		Coefficients in the correlations which calculate steady-state natural convection HTCs between continuous phase liquids and particles, droplets and bubbles. See also control option HTCOPT(3) in NAMELIST /XCNTL/. Recommended and default values are: Fuel: (1,1) = 0.474, 0.25, 1.44 Steel: (1,2) = 0.530, 0.25, 1.74 Sodium: (1,3) = 0.620, 0.25, 1.91
HNCGP	(3)		Coefficients in the correlation which calculates steady-state natural convection HTCs between gas in dispersed flow and particles, droplets and bubbles. See also control option HTCOPT(3) in NAMELIST /XCNTL/. (Recommended and default values: 0.474, 0.25, 1.44.)

Variable	Dimension	Default	Description
HFCLS	(3, MCLRE - 4)		Coefficients in the correlations which calculate steady-state forced convection HTC's between continuous phase liquids and structure. Recommended and default values are: Fuel: (1,1) = 0.023, 0.8, 0.3 Steel: (1,2) = 0.025, 0.8, 0.8 Sodium: (1,3) = 0.025, 0.8, 0.8
HFCGS	(3)		Coefficients in the correlation which calculates steady-state forced convection HTC's between gas in dispersed flow and structure. (Recommended and default values: 0.023, 0.8, 0.3.)
HREIC		50	Minimum Reynolds number for internal circulation of droplets and bubbles. See also control option HTC OPT(7) in NAMELIST /XCNTL/.
HREOS		300	Minimum Reynolds number for oscillation of droplets and bubbles. See also control option HTC OPT(7) in NAMELIST /XCNTL/.
HICLCP	(6, MCLRE - 4)		Coefficients in the correlations which calculate external steady-state forced convection HTC's between continuous phase liquids and droplets and bubbles, when the droplets and bubbles are circulating. See also control option HTC OPT(7) in NAMELIST /XCNTL/. (Recommended and default values: 1.13, 0.5, 2.89, 2.15, 0.64, 0.5.)
HICLDP	(3, MCLRE - 4)		Coefficients in the correlations which calculate HTC's for droplets when the droplets are circulating. See also control option HTC OPT(7) in NAMELIST /XCNTL/. (Recommended and default values: 0.842, 1.025, 200.)
HOSLDP	(3)		Coefficients to enhance HTC's for droplets when the droplets are oscillating. See also control option HTC OPT(7) in NAMELIST /XCNTL/. (Recommended and default values: 2.7.)
HOSGBU		2.7	Coefficient to enhance HTC's for bubbles when the bubbles are oscillating. See also control option HTC OPT(7) in NAMELIST /XCNTL/. (Recommended and value: 2.7.)
HGSMUL		1.0	Multipliers of the HTC's between gas and structure.
HRSMUL	(11)	1.0	Multipliers of the HTC's between all liquid energy components (including solid particles) and structure surfaces.
HGLMUL	(MCLRE)	1.0	Multipliers of the HTC's between gas and all liquid energy components (including solid particles).
HLGMUL	(MCLRE - 4)	1.0	Multipliers of the HTC's between liquid energy components and gas/vapor.
HRTMUL	(18)	1.0	Multipliers of the HTC's between all liquid energy components (including solid particles) and all other liquid energy components.

Variable	Dimension	Default	Description
HPTMUL	(4)	1.0	Multipliers of the HTCs between particle and all liquid energy components (fuel particle, steel particle, control particle and fuel chunk).
FFB		1.0	Fractional area of a droplet for which heat transfer takes place during film boiling (see also control option HTCOPT(14) in NAMELIST /XCNTL/). (Recommended value: 1.0.)
CMFB		0.55	Coefficient used to calculate the minimum film boiling temperature (recommended value: 0.55).
CDNB		0.1	Constant used to calculate the departure from nucleate boiling temperature (recommended value: 0.1)
BESLIP		3.0	Vapor-liquid slip parameter used in the natural convection film boiling model (recommended value: 3.0).
BESLP2		3.0	Vapor-liquid slip parameter used in the forced convection film boiling model (recommended value: 3.0).
FILMIN		1.4×10^{-4} m	Minimum thickness of a vapor film surrounding droplets (m). (Recommended value: 1.4×10^{-4} m.)
EHTCFB		5.0×10^{-2}	Convergence criterion in the film boiling iteration.
HAFMUL		1.0	Multiplier of the convection HTC between a liquid film and structure.
HCDMXS		5.0	Steady-state conduction Nusselt number for a bubbly flow mixture exchanging heat with structure.
HKEXP		-0.2	Exponent used to calculate the thermal conductivity of a multi-component, multi-phase mixture.
HFCXS	(3, MCLRE - 3)		Coefficients in the correlations which calculate steady-state forced convection HTCs between continuous phase liquid and lower/upper structures. Active only when control option HMTOPT(76)=1 in NAMELIST /XCNTL/. Recommended and default values are: Fuel: (1,1) = 0.023, 0.8, 0.3 Steel: (1,2) = 0.025, 0.8, 0.8 Sodium: (1,3) = 0.025, 0.8, 0.8 Vapor: (1,4) = 0.023, 0.8, 0.3

12. XBND

The boundary conditions input variables.

With the current method for specifying boundary conditions, NAMELIST /XBND/ usually appears several times in an input data file. /XBND/ should be used once to specify the locations of the N types of boundary condition, and then /XBND/ should be used a further N times to set each type of boundary condition required. This method gives the user the flexibility to specify various boundary conditions on different surfaces.

Note that the initial boundary-cell variables can be directly specified by the input variables in NAMELIST /XRGN/ or NAMELIST /XCWD/, otherwise the variables of real cells adjacent to the boundaries are reflected into the boundary cells.

Variable	Dimension	Default	Description
NBC			<p>Number of the boundary condition set. This entry must always be specified in each /XBND/ NAMELIST using the current method. The entry should be either zero or an integer value.</p> <p>=0 : Input variables LBCSET, LWASET and LWATME should be specified in the NAMELIST containing NBC=0. These variables set the locations of each type of boundary condition, and the locations and times of the virtual walls.</p> <p>=n : n is the flag identifying the boundary condition. The boundary condition is applied to the surface specified by LBCSET.</p>

The following three variables should be entered only for the NAMELIST /XBND/ containing NBC=0.

LBCSET	(IJBP2)	0	<p>Boundary specification flag. LBCSET(ij) is the boundary specification flag for boundary cell (ij). Boundary cell (ij) is identified by counting along each row of radial cells before moving to a new axial cell:</p> $ij = (IB+2) \times j + i + 1 \quad \begin{array}{l} i : 0, IB+1 \\ j : 0, JB+1, \end{array}$ <p>where:</p> <p>i=0 refers to the left-side boundary cells, i=IB+1 refers to the right-side boundary cells, j=0 refers to the bottom boundary cells, and j=JB+1 refers to the top boundary cells.</p> <p>The entries specified to LBCSET(ij) have the following definitions:</p> <p>=0 : The boundary cell (ij) is assigned a free slip rigid wall boundary condition.</p> <p>=n : The boundary cell (ij) is assigned the boundary condition specified in the NAMELIST /XBND/ containing the</p>
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identification flag NBC=n.

If LBCSET(ij) is not explicitly defined, the boundary cell (ij) is regarded as having a free slip rigid wall condition (i.e. default value: LBCSET(ij)=0). Note that the function of LBCSET in this method differs from its role in the former method.

LWASET	(IB, JB)	Flag to assign "virtual wall". The entry for each cell (I,J) should be a four digit number, with each decimal place referring to one of the four cell boundaries: Left, Right, Bottom, and Top (LRBT). A non-zero digit denotes the existence of a virtual wall at the specified boundary. This wall prevents all thermal and fluid dynamic interactions between the two cells adjacent to it. If a negative value is assigned, the cell is omitted from the normal calculational procedure and is instead treated as an unerodible structure which has no interaction with adjacent cells.
LWATME	(10, IB, JB)	Time table to control the periods for which the virtual walls exist. The walls specified for each cell are active between the first and second time entries in LWATME, inactive between the second and third entries, active again between the third and fourth entries, etc.
MCR	0	Number of computational cells, in which the inner boundary condition is used to simulate the water leakage. Used only when ALGOPT(49)>0. =0 : Do not used the inner boundary condition. >1 : Specify number of cells.
ICRC	MCR	Radial mesh cell, in which the inner boundary condition is used to simulate the water leakage. Used only when ALGOPT(49)>0.
JCRC	MCR	Axial mesh cell, in which the inner boundary condition is used to simulate the water leakage. Used only when ALGOPT(49)>0.
UCR	MCR,3	Radial velocity of each momentum field at (ICRC, JCRC), in which the inner boundary condition is used to simulate the water leakage. Used only when ALGOPT(49)>0.
VCR	MCR,3	Axial velocity of each momentum field at (ICRC, JCRC), in which the inner boundary condition is used to simulate the water leakage. Used only when ALGOPT(49)>0.

The following variables should be entered only for the NAMELIST /XBND/ containing NBC>0.

LBCS	0	Flow boundary condition flag. = 0 : Free slip at the boundary wall surface. = 1 : No-slip at the boundary wall surface. = 2 : Continuous inflow/outflow (boundary cells have the same contents as the adjacent real cells). = 3 : Flow is kept constant at the initial value.
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Note: if LBCS is set to 2 or 3 without specifying LBCP explicitly, the input variable LBCP is automatically set to 0 or 1, respectively.

LBCP		Pressure boundary condition flag. = -1 : Pressure is extrapolated from the adjacent real cell using the pressure gradient in that cell. = 0 : Pressure is set to the adjacent real cell pressure. = 1 : Pressure is kept constant at the initial value. ≥ 2 : Time-dependent pressure boundary condition. LBCP is the number of entries in the table of pressure vs. time. See variables PTME and PTAB below.
PTME	(k)	Time in the pressure vs. time table (k is defined below).
PTAB	(k)	Pressure in the pressure vs. time table (k is defined below).
LBCV	(MMOM)	Velocity boundary condition flag. There are three flags, one for each velocity field. = 0 : Velocity is set equal to the adjacent real cell velocity. = 1 : Velocity is kept constant at the initial value. ≥ 2 : Time-dependent velocity boundary condition. LBCV(q) gives the number of entries in the table of velocity vs. time for the (q)th velocity field. See variables VTME and VTAB below.
VTME	(k, q)	Times in the velocity vs. time table (k and q are defined below).
VTAB	(k, q)	Velocities in the velocity vs. time table (k and q are defined below).
LBCT	(MCLRE)	Temperature boundary condition flag. There is one flag for each liquid energy component. = 0 : The temperature is set equal to the adjacent real cell temperature. = 1 : The temperature is kept constant at its initial value. ≥ 2 : Time-dependent temperature boundary condition. LBCT(m) gives the number of entries in the table of temperature vs. time for the (m)th component. See variables TTME and TTAB below.
TTME	(k, m)	Times in the temperature vs. time table (k and m are defined below).
TTAB	(k, m)	Temperatures in the temperature vs. time table (k and m are defined below).
LBCG	0	Vapor boundary condition flag. < 0 : No adjustment of vapor properties. = 0 : Vapor densities are adjusted to be consistent with the given boundary pressure and gas temperature. The

adjustment maintains the ratios of the partial pressures at the same value.

= 1 : The vapor pressure is calculated from the liquid temperature using the saturation curve. The resulting total pressure is kept to the specified boundary pressure by either adding fission gas (to raise the pressure) or by reducing all partial pressures by the same proportion (to lower the pressure).

= 2 : A three-step calculation is performed. Firstly the condensable vapor partial pressures are calculated from the liquid temperatures, whilst the fission gas partial pressure is calculated from the current thermophysical condition. Secondly all partial pressures are adjusted by the same factor so that the total pressure becomes equal to the specified boundary pressure. Finally the temperatures of the liquid components are set to the saturation temperatures which correspond to the respective vapor partial pressures.

Definitions of the indices in the time-dependent tables:

k : Data number (maximum allowed is 15).

q : Velocity field number.

= 1 : Velocity field 1 (q1).

= 2 : Velocity field 2 (q2).

= 3 : Velocity field 3 (q3).

m : Material component number.

= 1 : Liquid fuel.

= 2 : Liquid steel.

= 3 : Liquid sodium.

= 4 : Fuel particle.

= 5 : Steel particle.

= 6 : Control particle.

= 7 : Fuel chunk.

= 8 : Vapor.

13. XTPP

The thermophysical properties input variables.

Variable	Dimension	Default	Description
KPOPT	(MNMATN, MNMAT)		Flag to select the method for calculating the thermal conductivity of material M. = 0 : Simple analytical function (liquid) : Theoretical evaluation (vapor) = 1 : Simple analytical function (liquid) : Simple analytical function (vapor) = 2 : Extended analytical function (liquid) : Extended analytical function (vapor)
MUOPT	(MNMATN, MNMAT)		Flag to select the method for calculating the viscosity of material M. = 0 : Simple analytical function (liquid) : Theoretical evaluation (vapor) = 1 : Simple analytical function (liquid) : Simple analytical function (vapor) = 2 : Extended analytical function (liquid) : Extended analytical function (vapor)
AKPS	(5, MNMATN, MNMAT)		Coefficients to calculate the solid thermal conductivity of material M, $a_{KS1,M} \sim a_{KS5,M}$.
AKPL	(6, MNMATN, MNMAT)		Coefficients to calculate the liquid thermal conductivity of material M, $a_{KL1,M} \sim a_{KL6,M}$.
AKPG	(5, MNMATN, MNMAT)		Coefficients to calculate the vapor thermal conductivity of material M, $a_{KG1,M} \sim a_{KG5,M}$.
BMUL	(5, MNMATN, MNMAT)		Coefficients to calculate the liquid viscosity of material M, $b_{ML1,M} \sim b_{ML5,M}$.
BMUG	(3, MNMATN, MNMAT)		Coefficients to calculate the vapor viscosity of material M, $b_{MG1,M} \sim b_{MG3,M}$.
CSGL	(3, MNMATN, MNMAT)		Coefficients to calculate the surface tension of material M, $c_{SL1,M} \sim c_{SL3,M}$.
DCPL	(6, MNMATN, MNMAT)		Coefficients to calculate the liquid heat capacity at constant pressure of material M, $d_{CL1,M} \sim d_{CL6,M}$.
CPLMAX	(MNMATN,		Maximum liquid heat capacity at constant pressure of

Variable	Dimension	Default	Description
	MNMAT)		material M, $c_{pL,max,M}$.
CPGMAX	(MNMATN, MNMAT)		Maximum vapor heat capacity at constant pressure of material M, $c_{pG,max,M}$.
MULMP	(MNMATN, MNMAT)		Particle viscosity of material M, $\mu_{p,M}$ (Pa s).
KPCRT	(MNMATN, MNMAT)		Thermal conductivity at the critical point of material M, $\kappa_{Cr,M}$ (used for extended analytical functions) (W/m/s).
MUCRT	(MNMATN, MNMAT)		Viscosity at the critical point of material M, $\mu_{Cr,M}$ (used for extended analytical functions) (Pa s).
NF	(MNMATN, MNMAT)		Coefficient to calculate the thermal conductivity and viscosity of material M, $n_{f,M}$ (used for extended analytical functions).
TLMAX	(MNMATN, MNMAT)		Maximum liquid temperature for the calculation of the liquid thermal conductivity and viscosity of material M, $T_{L,max,M}$ (used for simple analytical functions) (K).
TGMAX	(MNMATN, MNMAT)		Maximum vapor temperature for the calculation of the vapor thermal conductivity and viscosity of material M, $T_{G,max,M}$ (used for simple analytical functions) (K).
EPSM	(MNMATN, MNMAT)		Maximum energy of attraction of material M divided by the Boltzmann constant, used in the Lenard-Jones model, ϵ_M/k_B (K).
SIGM	(MNMATN, MNMAT)		Collision diameter of material M, used in the Lenard-Jones model, σ_M (Å).
NATOM	(MNMATN, MNMAT)		Number of atoms per molecule of material M, N_M .
EMSVS	(MNMATN, MNMAT)		Values of emissivity for the solid material M. (Recommended values: Fuel: 0.84; Steel: 0.3.)
EMSVL	(MNMATN, MNMAT)		Values of emissivity for the liquid material M. (Recommended values: Fuel: 0.9; Steel: 0.37, Sodium: 0.2; Water: 0.95.)

14. XSOS

The heat source input variables. This set of variables is used only when the HISTORIAN code option URANUS is ON.

Variable	Dimension	Default	Description
DAX	(JB)		Axial distribution of relative power, which is applied to all components. DAX is multiplied with input variables DRAD and FRTP (specified below) to give the space-dependent specific power density of each component, such that the total (global) power generated is normalized to input variable POW. Note that DAX and DRAD are overwritten by region-wise or cell-wise relative powers specified using input variables DAXDRB in NAMELIST /XRGN/ or DAXDRC in NAMELIST /XCWD/.
DRAD	(IB)		Radial distribution of relative power, which is applied to all components. DRAD is multiplied with input variables DAX and FRTP to give the space-dependent specific power density of each component, such that the total (global) power generated is normalized to input variable POW. Note that DRAD and DAX are overwritten by region-wise or cell-wise relative powers specified using input variables DAXDRB in NAMELIST /XRGN/ or DAXDRC in NAMELIST /XCWD/.
DPEL	(NPB, IB)		Radial power shape in fuel $1 \leq NP \leq NPB + 1$. Used only for DPIN model.
FRTP	(MHSO)	0, 1, 0, 0, 0	Component-wise fractions of specific power generation.
POW		0.0	Total initial power of the system (W).
IPOW		0	Flag to control the power profile. = 0 : The power profile is normalized only in the initialization. The total power changes according to the change of mass distribution. = 1 : The power profile is normalized in every step to keep the total power exactly to POW.
AMPTAB	(15)	1.0, 1.0	Normalized amplitude of power in the table of power vs. time (the initial value must be 1.0).
TIMAMP	(15)	0.0, 1.0	Times of normalized powers in the table of power vs. time.

15. XHMT

The melting/freezing (M/F) and vaporization/condensation (V/C) model input variables.

Variable	Dimension	Default	Description
PHI		0.01	Constant, ϕ , used in the calculation of non-equilibrium M/F to control the decrease in the macroscopic densities. The interfacial areas are adjusted in order to restrict the fractional decrease in densities to $(1 - \phi)$.
MIVC		150	Maximum number of iterations for the V/C iteration.
DVCRG		10^{-6}	Convergence criterion for the mass-transfer rate of vapor component in the V/C iteration, $\Delta_{VC, RG}$.
DVCE3		10^{-6}	Convergence criterion for the energy-transfer rate of coolant in the V/C iteration, $\Delta_{VC, E3}$.
DVCTG		10^{-6}	Convergence criterion for the energy-transfer rate of vapor in the V/C iteration, $\Delta_{VC, TG}$.
EVCRG		10^{-6}	Relative convergence criterion for the mass conservation of vapor component in the V/C iteration, $\epsilon_{VC, RG}$.
EVCE3		10^{-6}	Relative convergence criterion for the energy conservation of coolant in the V/C iteration, $\epsilon_{VC, E3}$.
EVCTG		10^{-6}	Relative convergence criterion for the energy conservation of vapor in the V/C iteration, $\epsilon_{VC, TG}$.
FVCRG		10^{-6} kg/m^3	Absolute convergence criterion for the mass conservation of vapor component in the V/C iteration, $f_{VC, RG}$ (kg/m^3).
FVCE3		10^{-6} J/m^3	Absolute convergence criterion for the energy conservation of coolant in the V/C iteration, $f_{VC, E3}$ (J/m^3).
FVCTG		10^{-6} J/m^3	Absolute convergence criterion for the energy conservation of vapor in the V/C iteration, $f_{VC, TG}$ (J/m^3).
FMTLG		0.0	Constant to restrict the heat and mass transfer for a small amount of liquid. A liquid component is forced to be vapor component if the liquid to vapor mass ratio is less than $f_{MT, LG}$. See also control option HMTOPT(13) in NAMELIST /XCNTL/.
FUND	(4)	0.4, 0.6, 0.8, 1.0	Under-relaxation constants, which multiply the matrix elements $C(m)$ in the V/C iteration, f_{UND} .
FRG		0.5	Maximum fraction of vapor mass that can condense in one V/C iteration, f_{RG} .
FEL		1.1	Maximum fractional change of coolant energy in one V/C iteration, f_{EL} .
FTG		0.5	Maximum fractional change of vapor temperature in one V/C iteration, f_{TG} .
FTSTL		0.6	The multiplier for the lower limiter of saturation temperature,

Variable	Dimension	Default	Description
			$f_{st,1}$.
FTSTH		0.95	The multiplier for the higher limiter of saturation temperature, $f_{st,h}$.
FPG4L		1.0	Fractional effect of fission gas partial pressure in reducing the vapor/liquid contact area for heat and mass transfer $f_{G4,L}$.
FPG4K		1.0	Fractional effect of fission gas partial pressure in reducing the vapor/solid contact area for heat and mass transfer $f_{G4,K}$.
FDTGMX		2.0	Fractional change of vapor temperature allowed in one time step due to V/C calculation, $f_{DTG,max}$.
RGLMAX		1.0	Maximum fraction of vapor/liquid contact area for condensation process, $R_{GL,max}$.
HLGMIN	(6)	$10^6, 10^5, 10^4, 10^3, 10^2, 10^8$ J/kg	Minimum values of effective heat of vaporization allowed in the V/C iteration, $h_{lg,min}$ (J/kg). The first four values of HLGMIN are applied over the first four V/C iterations. The fifth value is applied for $5 < IVC \leq IVCHLG$, where IVC is the number of iterations and IVCHLG is defined below. The last value is applied for $IVC \geq IVCHLG$.
IVCHLG		101	V/C iteration number after which the last value of HLGMIN is applied to the minimum value of effective heat of vaporization. This application is active only when IVCHLG is less than the maximum number of V/C iterations, MIVC.
TSUP	(MNMATN, MNMAT)	6*0.0 K	Superheat temperature of material M (K). During vaporization the interface temperature between a liquid and its vapor is set to the saturation temperature plus TSUP.
DTLMAX		10^3 K	Maximum liquid-temperature change allowed in one V/C iteration (K).
RBGMIN	MCGM1-1	1.0×10^{-10} kg/m ³	Minimum macroscopic densities allowed to condense during V/C iteration, $\bar{\rho}_{Gm,min}$ (kg/m ³).
CNP1		3.0×10^7 m ⁻²	Variable used to calculate the contact points density (m ⁻²).
CNP2		2.5×10^6 m ⁻²	Variable, which denotes a velocity dependence, used to calculate the contact points density (m ⁻²).
RAOB		0.1	Contact length to separation length ratio for contact points.
WCRST		0.5	Crust thickness criterion, used in the fuel caps freezing model (HMTOPT(81)=3).
HCRGAP		10^{12} W/m ² /K	Constant gap conductance HTC between crust and underlying steel wall (W/m ² /K). (HMTOPT(85)=2.)
TFNUCL		2700 K	Liquid fuel nucleation temperature, used in the interface resistance model (K). (HMTOPT(81)=2.)
TILFW		3002 K	Constant liquid fuel-structure interface temperature (K).
TILSW		1713 K	Constant liquid steel-structure interface temperature (K).
TILFC		3002 K	Constant liquid fuel-crust interface temperature (K).

Variable	Dimension	Default	Description
CHGL	(3)	0.9	Multipliers of limiters for vapor-side HTC's at vapor/liquid contact, $c_{G,Lm}$.
CHLG	(3)	0.9	Multipliers of limiters for liquid-side HTC's at vapor/liquid contact, $c_{Lm,G}$.
CHGK	(7)	0.9	Multipliers of limiters for vapor-side HTC's at vapor/solid contact, $c_{G,K(k)}$.
CHK	(7)	0.9	Multipliers of limiters for solid-side HTC's at vapor/solid contact, $c_{K(k)}$.
CHLL	(3, 3)	0.9	Multipliers of limiters for HTC's at liquid/liquid contact, $c_{Lm,Lm'}$ ($m' \neq m$).
CASC	1	0.091	Coefficient to calculate the super-cooling temperature in the fuel caps freezing model (HMTOPT(81)=3).
PSC1		0.292	Coefficient to calculate the super-cooling temperature in the fuel caps freezing model (HMTOPT(81)=3).
PSC2		1.169	Coefficient to calculate the super-cooling temperature in the fuel caps freezing model (HMTOPT(81)=3).
NGAMMF	(10)	10*0	Flags to suppress the non-equilibrium M/F occurring at liquid-solid contact interfaces (0 : activate, 1 : suppress). The interfaces are (1) : liquid fuel-fuel particles, (2) : liquid fuel-steel particles, (3) : liquid steel-steel particles, (4) : liquid fuel-pin structure, (5) : liquid steel-pin structure, (6) : liquid fuel-left wall structure, (7) : liquid fuel-right wall structure, (8) : liquid steel-left wall structure, (9) : liquid steel-right wall structure, and (10) : liquid fuel-fuel chunk. Note that NGAMMF=1 precedes control options HMTOPT(86)-(88) in NAMELIST /XCNTL/.
NGAMVC	(9)	9*0	Flags to suppress the non-equilibrium V/C occurring at vapor-liquid and liquid-liquid contact interfaces (0 : activate, 1 : suppress). The mass transfers are (1) : Fuel V/C at vapor-liquid fuel interface, (2) : Steel V/C at vapor-liquid steel interface, (3) : Sodium V/C at vapor-liquid sodium interface, (4) : Fuel condensation at vapor-liquid steel interface, (5) : Fuel condensation at vapor-liquid sodium interface,

Variable	Dimension	Default	Description
			(6) : Steel condensation at vapor-liquid sodium interface, (7) : Steel vaporization at liquid fuel-liquid steel interface, (8) : Sodium vaporization at liquid fuel-liquid sodium interface, and (9) : Sodium vaporization at liquid steel-liquid sodium interface.
NGAMIK	(7)	7*0	Flags to suppress the non-equilibrium vapor condensation occurring at vapor-solid contact interfaces (0 : activate, 1 : suppress). The interfaces are (1) : vapor-fuel particles, (2) : vapor-steel particles, (3) : vapor-control particles, (4) : vapor-fuel chunk, (5) : vapor-pin structure, (6) : vapor-left wall structure, and (7) : vapor-right wall structure.

16. XSTR

The structure (fuel-pin and can-wall structures) model input variables.

Variable	Dimension	Default	Description
FMELT		0.5	Pin fuel melt fraction for breakup (SPIN model). Fraction of solidus fuel region included in cavity (DPIN model).
FAFAIL		0.0	Mass based melt fraction or area melt fraction threshold for pin failure (DPIN model). See also FPNOPT(1) in NAMELIST /XCNTL/.
FAFAIL	(3)	0.0, 0.8, 0.5	Mass based melt fraction or area melt fraction threshold for pin failure. Used only when HISTORIAN code option DPIN is on. See also FPNOPT(1) in NAMELIST /XCNTL/.
PMELT	(2)	0.0, 1.0	Minimum fuel melt fraction in cavity and solid fuel, respectively. Used only when HISTORIAN code option DPIN is on.
CMELT		0.0	Cladding melt fraction for thermal breakup.
XCSTR		1.0	Fraction of the solid material that is left as a cladding when the thermal breakup of the cladding is predicted (see also CMELT parameter in NAMELIST /XSTR/). (1.0-XCSTR) becomes the fraction of the solid material that is transferred to solid particles.
WMELT		0.0	Can wall melt fraction of interior node for thermal breakup.
XWSTR		1.0	Fraction of the solid material that is left as a can wall when the thermal breakup of the can wall is predicted (see also WMELT parameter in NAMELIST /XSTR/). (1.0-XWSTR) becomes the fraction of the solid material that is transferred to solid particles.
DWFAL		2.0×10^{-3} m	Can-wall mechanical failure thickness (m). The can wall is presumed to fail mechanically allowing radial fluid motion when its thickness is less than DWFAL. Active only if control option HMTOPT(64)=1 in NAMELIST /XCNTL/.
TWFAL		1541 K	Can-wall mechanical failure temperature (K). The can wall is presumed to fail mechanically when its temperature exceeds TWFAL. Active only if control option HMTOPT(64)=1 in NAMELIST /XCNTL/.
BETACW		0.1	Fractional area of the can-wall surface allowing radial fluid motion due to the mechanical failure. The orifice coefficient at the right boundary of the cell is calculated by $C_{ORF} = 1.35(1 - \beta)(1 - \beta^2) \frac{1}{\beta^2}.$
ACRMIN		1.0×10^{-5}	Minimum volume fraction of fuel crust which is allowed to exist on can wall structure.
TCRMIN		3.0×10^{-4} m	Minimum fuel-crust thickness for the stable crust. The crust

Variable	Dimension	Default	Description
			which is thinner than this variable breaks when the underlying wall melts. Active only if control option HMTOPT(65)=1 in NAMELIST /XCNTL/.
HKMUL	(3)	1.0	Multipliers of the structure-side HTC's (pin, left can wall and right can wall).
OHEMF		0.9	Emissivity of fuel. Active only when HTCOP(22)=1.
OHEMC		0.18	Emissivity of cladding. Active only when HTCOP(22)=1.
TL11G5		10^{-3} s	Time constant for fission gas release from liquid fuel to the vapor field (s).
FL11G5		1.0	Multiplier for the mass transfer rate of fission gas release from liquid fuel to the vapor field.
TL12G5		10^{-2} s	Time constant for fission gas release from particulate fuel to the vapor field (s).
FL12G5		1.0	Multiplier for the mass transfer rate of fission gas release from particulate fuel to the vapor field.
TL13G5		10^{-2} s	Time constant for fission gas release from fuel chunk to the vapor field (s).
FL13G5		1.0	Multiplier for the mass transfer rate of fission gas release from fuel chunk to the vapor field.
FP34			Fraction of fission gas to dissolve. Used only for DPIN model.
FC34			Fraction of dissolved fission gas transferred to free. Used only for DPIN model.
TC34			Time constant for transfer from dissolved to free gas. Used only for DPIN model.
SGUTS0		7.66×10^8 Pa	Ultimate tensile stress at the minimum fuel specific energy (Pa). Used only when HISTORIAN code option DPIN is on.
FCT		-5.06×10^5 Pa/K	Slope of ultimate tensile stress versus fuel temperature (Pa/K). Used only when HISTORIAN code option DPIN is on.
ES4ST		7.82354×10^5 J	Maximum clad energy with mechanical strength (J). Used only when HISTORIAN code option DPIN is on.
FEJ		0.5	Maximum fraction of ejected mass per fluid dynamics time-step. Used only when HISTORIAN code option DPIN is on.
FRICT		1.0	Friction for calculating the fuel axial velocity in the in-pin fuel motion model. Used only when HISTORIAN code option DPIN is on.
TAUST	(MNMAT)	10^{-3} s	Heat-transfer time constant of material M to determine thermal penetration lengths, $\tau_{Sr,M}$ (s).
AHGAP		5678.26	Gap conductance of the pin ($W/m^2/K$). (Recommended

Variable	Dimension	Default	Description
		W/m ² /K	value: 1000 Btu/ft ² /F = 5678.26 W/m ² /K.) See also control option HTCLOPT(20) in NAMELIST /XCNTL/.
AKGAP		0.511043 W/m/K	Thermal conductivity of the gas in the gap (W/m/K). See also control option HTCLOPT(20) in NAMELIST /XCNTL/.
AHGMIN		100 W/m ² /K	Minimum gap conductance of the pin (W/m ² /K). See also control option HTCLOPT(20) in NAMELIST /XCNTL/.
AHGMAX		40000 W/m ² /K	Maximum gap conductance of the pin (W/m ² /K). See also control option HTCLOPT(20) in NAMELIST /XCNTL/.
EPSSPN		10 ⁻⁴	Convergence criterion for the energy iteration in the fuel-pin heat-transfer calculation.
MSIT		20	Maximum number of iterations for the energy iteration in the fuel-pin heat-transfer calculation.
JGPL1	(IB)		Lower cell location for the lower gas plenum. Used only when HISTORIAN code option BLOW is on.
JGPL2	(IB)		Upper cell location for the lower gas plenum. Used only when HISTORIAN code option BLOW is on.
JGPU1	(IB)		Lower cell location for the upper gas plenum. Used only when HISTORIAN code option BLOW is on.
JGPU2	(IB)		Upper cell location for the upper gas plenum. Used only when HISTORIAN code option BLOW is on.
PGPL	(IB)	1.0×10 ⁷ Pa	Pressure in the lower gas plenum (Pa). Used only when HISTORIAN code option BLOW is on.
PGPU	(IB)	1.0×10 ⁷ Pa	Pressure in the upper gas plenum (Pa). Used only when HISTORIAN code option BLOW is on.
TGPL	(IB)	1.0×10 ³ K	Temperature in the lower gas plenum (K). Used only when HISTORIAN code option BLOW is on.
TGPU	(IB)	1.0×10 ³ K	Temperature in the upper gas plenum (Pa). Used only when HISTORIAN code option BLOW is on.
DHGB		1.0×10 ⁻⁴ m	Hydraulic diameter of the gas leakage path (m). Used only when HISTORIAN code option BLOW is on.
AGLS		2.0×10 ⁻⁶ m ²	The cross section of the gas leakage path in a pin (m ²). Used only when HISTORIAN code option BLOW is on.
TMFAIL		150.0 K	The gas blowout starts when the cladding temperature reaches (T _{melt, steel} - TMFAIL) (K). Used only when HISTORIAN code option BLOW is on.
RJGB		6.332930×10 ⁵ ergs / g / K	Gas constant (ergs / g / K). Used only when HISTORIAN code option BLOW is on.
GAMGB		1.5	Heat capacity ratio. Used only when HISTORIAN code option BLOW is on.
U0GB		6.25×10 ⁻⁴ poise	Reference viscosity at T0GB (poise). Used only when HISTORIAN code option BLOW is on.
T0GB		726.85 deg. C	Reference temperature for U0GB (deg. C). Used only when

Variable	Dimension	Default	Description
			HISTORIAN code option BLOW is on.
AFRGB		7.915×10^{-2}	Coefficient used to calculate the gas friction. Used only when HISTORIAN code option BLOW is on.
BFRGB		-0.25	Coefficient used to calculate the gas friction. Used only when HISTORIAN code option BLOW is on.

17. XMSC

The miscellaneous input variables and convergence precisions.

Variable	Dimension	Default	Description
G		-9.80665 m/s ²	Gravitational acceleration in the axial direction (m/s ²).
GANG		0.0 degree	Angle at which the z axis is inclined in the clockwise direction to the vertical (degree). This applies only to an X-Z coordinate.
COURTN		0.4	Velocity Courant condition.
OPTPIT		8	Optimum number of pressure iterations.
MPIT		25	Maximum number of pressure iterations.
MAXITC		25	Maximum number of velocity iterations.
EPSVEL		10 ⁻⁴	Convergence criterion for the velocity iterations.
EPSP		10.0 Pa	Convergence criterion for the pressure convergence in the pressure iteration (Pa).
EPSRO		10 ⁻⁴ kg/m ³	Convergence criterion for the density convergence in the pressure iteration (kg/m ³).
EPST		1000 W/m ³	Convergence criterion for the vapor-energy convergence in the pressure iteration (W/m ³).
EPSPCV		10 ⁻⁴	Convergence criterion for the pressure iteration. See also control option ALGOPT(6) in NAMELIST /XCNTL/.
NITRF		100	Maximum number of iterations for the pressure equation PCG solver. See also control option ALGOPT(1) in NAMELIST /XCNTL/.
EITRF		10 ⁻⁶	Convergence criterion for the pressure equation PCG solver. See also control option ALGOPT(1) in NAMELIST /XCNTL/.
FXR	(6)	0.5, 4*0.999999, 0.5	Maximum reduction fraction of the independent variables during the pressure iteration.
FXE	(6)	5*10 ¹⁰ , 2.0	Maximum enlargement factor of the independent variables during the pressure iteration.
DPMK1		1.0	Maximum relative pressure difference allowed between STEP1 and STEP2. See also control option ALGOPT(4) in NAMELIST /XCNTL/.
DPMK4		1.0	Maximum relative pressure difference allowed between STEP2 and STEP4. See also control option ALGOPT(4) in NAMELIST /XCNTL/.
DTGMK1		1.0	Maximum relative vapor temperature difference allowed between STEP1 and STEP2. See also control option ALGOPT(4) in NAMELIST /XCNTL/.
DTGMK4		1.0	Maximum relative vapor temperature difference allowed between STEP2 and STEP4. See also control option

Variable	Dimension	Default	Description
			ALGOPT(4) in NAMELIST /XCNTL/.
ALPEXC		10 ⁻¹⁰	Constant used to prevent overfilling of a mesh-cell.
FVCCF1		1.0	Multiplier for the compression term, which is used in the source-term decoupling relaxation Method-1. The term is calculated in subroutine DIVRGV. See also control option ALGOPT(3) in NAMELIST /XCNTL/.
EXPPR1		1.0	Multiplier used in the source-term decoupling relaxation Method-1B. See also control option ALGOPT(3) in NAMELIST /XCNTL/.
ONLIQ	(3)		<p>Flag to specify which material components are present in the run. ONLIQ(I) is used in the source-term decoupling relaxation Method-1. The three material components (I) are:</p> <p>I=1 : Fuel (fertile and fissile).</p> <p>I=2 : Steel.</p> <p>I=3 : Sodium.</p> <p>ONLIQ(I) should be set to either zero or one:</p> <p>ONLIQ(I)=1 : Component I is present.</p> <p>ONLIQ(I)=0 : Component I is absent.</p> <p>See also control option ALGOPT(3) in NAMELIST /XCNTL/.</p>
FRAND			Fraction of randomness to define the random time-step size. It is recommended that the value be between about 0.1 and 0.5. See also control option ALGOPT(41) in NAMELIST /XCNTL/.
SEED			Initiator of the uniform random number generator, used to define the random time-step size. This initiator is currently only operational for the random number generator on an RS6000 machine, in which case SEED can be any positive integer. See also control option ALGOPT(41) in NAMELIST /XCNTL/.
IVDL	(MCLRE + MCGRE)	1, 2, 2, 1, 1, 2, 2, 3	Table to assign fluid energy components to the three velocity fields.
NSTEF		3	<p>Flag to control Steffensen's method for the pressure iteration.</p> <p>=0 : No Steffensen's method is applied to the pressure iteration.</p> <p>≠1 : Steffensen's method is applied to the pressure iteration. NSTEF is the number of tables for applying Steffensen's method to the pressure iteration. See variable ISTEFE below.</p>
ISTEF	(6, 10)	ISTEF(m,1)= 0, 0, 0, 0, 0, 0 ISTEF(m, 2) = 1, 1, 1, 1, 1, 0	Tables for Steffensen's method applied to the pressure iteration. If ISTEFE (m, *)=1, Steffensen's method is applied to the residual of the m-th independent variable in the pressure iteration. The first table, ISTEFE(*, 1), is used for the normal operation of Steffensen's method. If the pressure

Variable	Dimension	Default	Description
		ISTEF(m, 3) = 1, 1, 1, 1, 1, 1	<p>iteration fails under the normal operation, Steffensen's method using the other tables, ISTE(*, 2) ~ ISTE(*, NSTEF), are tried to obtain the convergence. The independent variables are:</p> <p>m=1: $\mathcal{E} = p_{cell} - p_{EOS}$, the difference between the cell pressure and the EOS pressure,</p> <p>m=2: $\bar{\rho}_{q1}$, the sum of the macroscopic density components in a liquid velocity field which does not include the liquid energy component L2,</p> <p>m=3: $\bar{\rho}_{L2}$, macroscopic density of the liquid energy component L2,</p> <p>m=4: $\bar{\rho}_{LL}$, (the sum of the macroscopic density components in a liquid velocity field which includes the liquid energy component L2) - $\bar{\rho}_{L2}$,</p> <p>m=5: $\bar{\rho}_G$, vapor mixture density, and</p> <p>m=6: e_G, vapor internal energy.</p>

18. XERG

The EOS region input variables.

Variable	Dimension	Default	Description
REGN			Number of EOS regions.
REGC	(4, REGN)		<p>Location of each EOS region. The EOS region is bounded by a rectangle which is specified by its bottom left and top right corners.</p> <p>Cell (IBL, JBL) in the bottom left of the EOS region is identified by:</p> <p style="padding-left: 40px;">REGC(1, *)=IBL, and</p> <p style="padding-left: 40px;">REGC(2, *)=JBL.</p> <p>Cell (ITR, JTR) in the top right of the EOS region is identified by:</p> <p style="padding-left: 40px;">REGC(3, *)=ITR, and</p> <p style="padding-left: 40px;">REGC(4, *)=JTR.</p>
MATEOS	(MNMAT, REGN)		Sub-material number to be assigned to each EOS region. The default assignment of sub-material number is listed in Attachment 1.
ENGEOS	(MNSV, REGN)	0	<p>Sub-material number to be assigned to each energy component. ENGEOS overwrites MATEOS.</p> <p>ENGEOS(1,*) : The pin fuel</p> <p>ENGEOS(2,*) : The left crust</p> <p>ENGEOS(3,*) : The right crust</p> <p>ENGEOS(4,*) : The cladding</p> <p>ENGEOS(5,*) : The left can wall boundary node</p> <p>ENGEOS(6,*) : The left can wall interior node</p> <p>ENGEOS(7,*) : The right can wall boundary node</p> <p>ENGEOS(8,*) : The right can wall interior node</p> <p>ENGEOS(9,*) : The control</p> <p>ENGEOS(10,*) : The liquid fuel</p> <p>ENGEOS(11,*) : The liquid steel</p> <p>ENGEOS(12,*) : The liquid coolant</p> <p>ENGEOS(13,*) : The fuel particle</p> <p>ENGEOS(14,*) : The steel particle</p> <p>ENGEOS(15,*) : The control particle</p> <p>ENGEOS(16,*) : The fuel chunk</p> <p>ENGEOS(17,*) : The fuel vapor</p> <p>ENGEOS(18,*) : The steel vapor</p>

Variable	Dimension	Default	Description
			ENGEOS(19,*) : The sodium vapor
			ENGEOS(20,*) : The fission gas
			MNSV = MCSRE+MELRE+MCGM1

19. XSWC

The Sodium-Water reaction input variables for a chemical reaction model. The set of variables is used only when the HISTRIAN code option SW is ON.

Variable	Dimension	Default	Description
FMOL		0.75	Conversion ratio of water into hydrogen in the chemical reactions. Used only when ALGOPT(50)>0.
FKCR		0.1	Constant of hydrogen generation reaction ($0.1 \cdot \text{m}^4/\text{mol/s}$). Used only when ALGOPT(50)>0.
FLIMITER	4	10^{-3} , 10^{-3} , 10^{-6} , 10^{-6} ,	Minimum values of masses allowed in the chemical reaction. The chemical reaction model is not applied if the mass of each component generated is less than FLIMITER in a calculation cell. Used only when ALGOPT(50)>0. The components generated in the sodium-water chemical reaction are (1) = liquid sodium (2) = liquid water (3) = sodium vapor (4) = steam
WMNA		23.0	Molecular weight of sodium (g/mol). Used only when ALGOPT(50)>0.
WMH		1.0	Molecular weight of hydrogen (g/mol). Used only when ALGOPT(50)>0.
WMO		16.0	Molecular weight of oxygen (g/mol). Used only when ALGOPT(50)>0.
MAXITR		30	Maximum number of iterations for energy of the generated components. Used only when ALGOPT(50)>0.
EPSTR		1.0×10^{-4}	The convergence criterion for energy iterations of the generated components. Used only when ALGOPT(50)>0.
QNAOH		189000	Heat of sodium hydroxide generated by the chemical reaction (J/mol). Used only when ALGOPT(50)>0.
QNA2O		176000	Heat of sodium oxide generated by the chemical reaction (J/mol). Used only when ALGOPT(50)>0.
HEATOPT	10	0	Flag for allocation of the energy generation by the chemical reaction. =0 : Allocate to all components in the fraction each of the component heat capacity. =1 : Allocate only to NAOH(P), NA2O(P), H2(G) in the fraction each of the component heat capacity. =2 : Allocate only to NAOH(P), NA2O(P), H2(G)+NAOH(L) in the fraction each of the component heat capacity.

20. NCNTL

The neutronics option flag input variables.

Variable	Dimension	Default	Description
NIOPT	(200)		Code control flags for the neutronics.
	1-3		Not currently used.
	4	1	Neutronics edit control flag for reactivity time step summary information. The summary is printed at every NIOPT(4) reactivity steps.
	5	0	Option flag for time step control at TWFIN (last real time for the current run) in NAMELIST /XTME/. =0 : conventional time step control is used. =1 : Current run terminates precisely at TWFIN by adjusting neutronics shape time step.
	6-31		Not currently used.
	32	1	Option flag to select the approximate treatment for anisotropic (P1) scattering based on the Bell-Hansen-Sandmeir prescription. =0 : Do not consider the P1 scattering. Total cross section is calculated from each cross section of capture, fission and scattering. =1 : Consider the P1 scattering (approximate treatment). Transport cross section is calculated from each cross section of capture, fission and scattering. =2 : Do not consider the P1 scattering. Total cross section is derived from the cross-section library. =3 : Consider the P1 scattering (approximate treatment). Transport cross section is derived from the cross-section library.
	33	0	Option flag to select the treatment of the flux shape derivative during outer iterations. <0: Approximate treatment of the flux shape derivative (with respect to time) during shape recalculations (the angular part is taken into account for an additional inner iteration sweep the last outer iteration only), original SIMMER approach. >=0: Rigorous treatment (i.e. taking into account the angular part) of the flux shape derivative during all outer iterations.
	34-35		Not currently used.
	36	0	Option flag for external neutron source case. =0: Critical reactor at t=0. =1: Source-driven reactor, k-eff-adjoint weighting function. =2: Source-driven reactor, alpha-adjoint weighting function.
	37	0	Option flag to select the initial guess for steady-state flux calculations with external source.

Variable	Dimension	Default	Description
			<0: Do not perform a direct k-eff calculation at t=0 (to provide an initial guess for steady-state flux calculations with external source) if NIOPT(36)>0.
			>=0: Perform a direct k-eff calculation at t=0 (to provide an initial guess for steady-state flux calculations with external source) if NIOPT(36)>0.
38			Not currently used.
39		0	Option to select whether the external reactivity is given as reactivity or ramp rate; Used only when IRAMPT > 0. =0: RCRATE is reactivity. =1: RCRATE is ramp rate.
40		0	Option flag to select the unit of input external reactivities (NIOPT(39) = 0) or ramp rates (NIOPT(39) = 1) ; Used only when IRAMPT > 0. Related input variables are RCRATE and RAMPT. =0: RCRATE are input in $\Delta k/kk'$ or $\Delta k/kk'/s$. =1: RCRATE are input in \$ or \$/s, which are internally converted to $\Delta k/kk'$ or $\Delta k/kk'/s$ using the initial effective delayed neutron fraction, respectively. =2: RCRATE are input in \$ or \$/s, which are internally converted to $\Delta k/kk'$ or $\Delta k/kk'/s$ using the transient effective delayed neutron fraction, respectively.
41-44			Not currently used.
45		0	Option flag to control fission amplitude profile. =0: Fission amplitude is calculated in every time step. =1: Fission amplitude keeps constant.
46		0	Option flag to control decay amplitude profile. =0: Decay amplitude is calculated in every time step. =1: Decay amplitude keeps constant.
47-48			Not currently used.
49		0	Option flag to select the format of BRKOXS file. =0: New format based on cccc version IV. =1: Conventional format based on cccc version III.
50		0	Option flag to select the neutron up-scattering treatment. =0: Neutron up-scattering is not considered. =1: Neutron up-scattering is considered. ISOTXS file must contain up-scattering data.
51			Not currently used.
52		0	Option flag to select the approximate treatment of heterogeneity effect based on a fuel pin geometry. This flag

Variable	Dimension	Default	Description
			is currently active only when the code option ISOTOPE is ON. =0: Heterogeneity effect is not considered. =1: Heterogeneity effect is considered. The variables, IHETE, INUCF, RPEL and RCOOL, must be specified in NAMELIST /NHET/.
53		0	Option flag to skip transient recalculations of self-shielded macroscopic cross-sections. This option can be used to eliminating unnecessary self-shielding calculations for the cells at constant temperature and composition. =0: The self-shielding calculations are performed for all the neutronics cells during transient. =1: No recalculation is performed during transient for the neutronics cells specified by NOXSCL in NAMELIST /NSHL/. The initial self-shielded cross sections are used throughout the transient.
54-89			Not currently used.
90		0	Option flag to dump the input data for some standard neutronics codes. =0: Do not dump input data. =1: Dump input data of TWODANT for the real flux calculation. =2: Dump input data of TWODANT for the adjoint calculation. =3: Dump input data and macroscopic cross-section for TWOTRAN calculation.
91-99			Not currently used.
100		0	Option flag to dump neutronics time step summary on SIMPK. =0: Do not dump time step summary on SIMPK. ≠0: Dump time step summary on SIMPK
101-109			Dump option for neutronics post-processing file, SIMNP. The dump control can be specified by each record type separately.
101		1	Record type 1 of SIMNP (neutronics time step summary). =0: No data are dumped. =1: Data are dumped at each reactivity time step. =2: Data are dumped at each shape time step.
102		0	Record type 2 of SIMNP (cell-wise number densities). =0: No data are dumped. ≠0: Data are dumped.

Variable	Dimension	Default	Description
103	0	0	Record type 3 of SIMNP (cell-wise data of effective macroscopic cross-sections). =0: No data are dumped. ≠0: Data are dumped.
104	1	1	Record type 4 of SIMNP (geometries and isotopes). =0: No data are dumped. ≠0: Data are dumped.
105	0	0	Record type 5 of SIMNP (cell-wise data of reactivity components). =0: No data are dumped. =1: Data are dumped at each reactivity time step. =2: Data are dumped at each shape time step.
106	0	0	Record type 6 of SIMNP (cell-wise data of material density and temperature). =0: No data are dumped. =1: Data are dumped at each reactivity time step. =2: Data are dumped at each shape time step.
107	0	0	Record type 7 of SIMNP (adjoint flux distribution). =0: No data are dumped. ≠0: Data are dumped.
108	0	0	Record type 8 of SIMNP (real flux distribution). =0: No data are dumped. ≠0: Data are dumped.
109	0	0	Record type 9 of SIMNP (reactivity components). =0: No data are dumped. =1: Data are dumped at each reactivity time step. =2: Data are dumped at each shape time step.
110-200			Not currently used.

21. NPAR

The neutronics integer control input variables.

Variable	Dimension	Default	Description
NREGB	(4)		Fluid-dynamics mesh cell boundaries that correspond to the neutronics mesh cells (left, right, bottom, top).
NCRAD	(IB)		Number of neutronics mesh cells per fluid dynamics cell in the radial direction (NREGB(2) - NREGB(1) data).
NCAXI	(JB)		Number of neutronics mesh cells per fluid dynamics cell in the axial direction (input NREGB(4) - NREGB(3) data).
NFRAD	(NCRAD, IB)	0	Input to specify neutronics mesh divisions in the radial direction. The i-th radial mesh cell for fluid dynamics is subdivided into neutronics meshes in the ratio of NFRAD(1,I) : NFRAD(2,I) : ... : NFRAD(NCRAD(I), I). The variables must be specified by integers.
NFAXI	(NCAXI, JB)	0	Input to specify neutronics mesh divisions in the axial direction. The j-th axial mesh cell for fluid dynamics is subdivided into neutronics meshes in the ratio of NFAXI(1,J) : NFAXI(2,J) : ... : NFAXI(NCAXI(J), J). The variables must be specified by integers.
IDIVR		1	Option for radial mesh sub-division. This option is valid only for the cells for which NFRAD(1,I) = NFRAD(2,I) = ... = NFRAD(NCRAD(I), I) = 0 is specified. =0: Equal volume sub-division. =1: Equal mesh width sub-division.
IT			Total number of neutronics radial mesh cells (the total of NCRAD).
JT			Total number of neutronics axial mesh cells (the total of NCAXI).
ISNT		4	Sn order. If negative, quadrature coefficients are taken from interface file SNCONS. Otherwise (for ISNT = 2 through 16), built-in constants are used.
IGM		18	Number of neutron energy groups. If IGM < 0, the detailed information from TWODANT-SOLVER module is printed in SIMMER output file, SIM06.
IGD		6	Number of delayed neutron precursor groups.
NDKGRP		6	Number of decay heating groups (input if using decay heat model).
MT		5	Number of component materials.
LNISIP		5	Number of isotopes (ISOTOPE-ON) or materials (ISOTOPE-OFF) to be read from ISOTXS and BRKOXS.
NRXS		1	Number of input cross-section regions.
IXSREG	(4, NRXS)		Cross-section region boundaries (left, right, bottom, top).

Variable	Dimension	Default	Description
ITR		0	Transient neutronics initialization flag. =0: Start from a steady state. =1: Start from a transient state.
ICOS		0	Initial flux guess flag. =0: Unity for both adjoint and real fluxes. =1: Cosine shape for adjoint flux, adjoint solution for real flux. =2: Input data for adjoint flux, adjoint solution for real flux. =3: Unity for adjoint flux, input data for real flux. =4: Input data for both adjoint and real fluxes.
NEZFLG	(IB,JB)	0	Input to specify the fluid dynamics mesh cells over which the density and temperature are averaged only for neutronics calculation.

22. NEDT

The neutronics edit control input variables.

Variable	Dimension	Default	Description
NEUPRI		1	Neutronics summary output option. = 0: No print on SIM06. > 0: Print summary on SIM06.
LCELPT	(IT, JT)	0	Mesh cell locations for which detailed information of cross sections and shielding factors are dumped on SIM06. Used only if IEDXST = 2 or IEDSFT = 2. =0: No print. =1: Print cell-wise cross-sections. =2: Print cell-wise shielding factors. =3: Print both cross-sections and shielding factors.
IEDXST		0	Cross section print option. =0: No print. =1: Print input cross sections. =2: Print cell-wise cross sections.
IEDSFT		0	Shielding factor print option. =0: No print. =1: Print input shielding factors. =2: Print cell-wise shielding factors.
INVPRT		0	Print option flag for region-wise number density inventories. =0: No print. =1: Initial state only. =2: Transient state only. =3: Both initial and transient states.
INVREG		0	Total number of inventory regions to print isotopic number densities; Not printed if INVREG \leq 0. This input is merely a print option flag and does not affect the calculation.
IRGBND	(4, INVREG)		Region boundaries for isotopic inventory to be printed (left, right, bottom, top).

23. NINI

The neutronics initialization input variables.

Variable	Dimension	Default	Description
POWER			Initial reactor power (W).
RHOIN			Initial reactivity (-); Used only if ITR=1.
GENTIN			Initial neutron generation time (s); Used only if ITR=1.
IRAMPT		0	The number of points for the external reactivity-vs.-time table (≤ 9).
RAMPT	(10)		Time points (s) for the external reactivity-vs.-time table (≤ 9).
RCRATE	(10)		External reactivities for the external reactivity-vs.-time table (≤ 9). The unit of reactivities is in $\Delta k/kk'$ when NIOPT(40) = 0, or in \$ when NIOPT(40) = 1 or 2. External reactivities (NIOPT(39) = 0) or ramp rates (NIOPT(39) = 1) for the external reactivity-vs.-time table (≤ 9). If NIOPT(39) = 0, the unit is in $\Delta k/kk'$ when NIOPT(40) = 0, and in \$ when NIOPT(40) = 1 or 2. If NIOPT(39) = 1, the unit is in $\Delta k/kk'/s$ when NIOPT(40) = 0, and in $\$/s$ when NIOPT(40) = 1 or 2.
OM			Initial inverse period (1/s); Used only if ITR=1.
DECAY	(IGD)	Default data built in.	Delayed neutron precursor decay constants (1/s).
BETAD	(IGD)	Default data built in.	Delayed neutron fission yields.
DSPECT	(IGD, IGM)	Not available.	Delayed neutron fission spectra.
ETAINP	(IGD)		Initial weighted precursor concentrations divided by the prompt fission power amplitude; Used only if ITR=1.
BETINP	(IGD)		Initial effective delayed neutron fractions; Used only if ITR=1.
DKYLDS		0.0	Initial fraction of decay heat in total power (= fission power + decay heat); Used only if NDKGRP>0.
DKYLD	(NDKGRP)	Default data built in.	Initial decay heat fraction for each decay group, which is normalized internally using DKYLDS. Used only if NDKGRP>0.
DKLAM	(NDKGRP)	Default data built in.	Decay constant for each decay heating group (1/s); Used only if NDKGRP>0.
DKHETI	(NDKGRP)	0.0	Initial value of decay heat source for each decay heating group. This is an alternative way to specify initial decay heat contribution. The values of DKYLDS and DKYLD are ignored if DKHETI>0.0.

24. NQUS

The neutronics quasi-static method control input variables.

Variable	Dimension	Default	Description
LIPSTP		7	Maximum number of reactivity steps allowed per shape step.
ITGAMM		5	Maximum number of gamma iterations permitted.
IWTF		0	Option for a weighting function used in the quasi-static method. =0: The stationary-state adjoint flux is used. =1: The unity (uniform distribution) is used.
IQUASI		0	Flag to override the quasi-static time step controls. =0: No effect. =1: The flux shape step is always set to DTSMAX. =2: The reactivity step is always set to DTHMAX. =3: The above two time steps are always set to DTSMAX and DTHMAX.
IFXUDL		0	The model selection for either the flux-shape extrapolation method or the flux-shape update method. =0: The flux-shape extrapolation method is used. >0: The flux shape update method is used. IFXUDL represents the maximum number of outer iterations permitted for flux shape updates per reactivity step (suggested value: 6).
DTSH		0.0001 s	Initial flux shape time step (s).
DTSMAX		0.01 s	Maximum allowed shape step (s).
EPSG		10^{-5}	Convergence precision for the gamma equation.
EPSPHY		10^{-5}	Convergence precision for the amplitude iteration.
EPS4		0.02	Quasi-static method time step reduction factor parameter; Used together with EPS17.
EPS5		5.0 \$	Maximum permissible reactivity change per reactivity step (\$).
EPS6		1.0	Maximum allowed relative change in the weighted current inner product (representing leakage) per shape step.
EPS7		1.0	Minimum number of reactivity steps per amplitude decade.
EPS8		10^6 s^{-1}	Maximum allowed inverse period change per reactivity step (s^{-1}).
EPS9		0.5	Maximum allowed spatial tilt in the total flux per shape step.
EPS10		0.01	Maximum allowed deviation from unity for the quasi-static constraint before taking a shape step. This depends on the input flag IFXUDL as follows. IFXUDL=0: The EPS10 control is inactive, and EPS18, EPS6 and EPS9 function as described.

Variable	Dimension	Default	Description
			IFXUDL>0 : The EPS10 control replaces the EPS18, EPS6 and EPS9 controls.
EPS11		0.5	Maximum allowed relative change in the total internal energy of fuel per reactivity step.
EPS12		0.5	Maximum allowed relative change in the total internal energy of steel per reactivity step.
EPS13		0.5	Maximum allowed relative change in the total internal energy of sodium per reactivity step.
EPS14		0.25	Maximum allowed relative change in the total mass of fuel per reactivity step.
EPS15		0.25	Maximum allowed relative change in the total mass of steel per reactivity step.
EPS16		0.25	Maximum permissible relative change in the total mass of sodium per reactivity step.
EPS17		0.08516	Quasi-static method time step reduction factor parameter; used together with EPS4.
EPS18		10.0 \$	Maximum permissible reactivity change per shape step (\$).

25. NCNV

The neutron flux shape convergence control input variables.

Variable	Dimension	Default	Description
ITLMOU		200	Maximum number of outer iterations permitted.
ITLMIN		50	Maximum number of inner iterations per group permitted per outer iteration.
EPSO		1.0×10^{-5}	Convergence precision for the total fission source.
EPSPT		1.0×10^{-5}	Convergence precision for the point-wise fission source.
EPSFAC		15.0	Factor relating the inner iteration to the outer iteration convergence precision.
EPSMIN		1.0×10^{-6}	Minimum convergence precision for inner iteration.
ERRFXU		1.0×10^{-6}	Convergence precision in the total fission source for the outer iteration flux shape updates at reactivity steps; Use only if IFXUDL>0.

26. NSHL

The shielding factor related input variables.

Variable	Dimension	Default	Description
ISHLD		0	Flag to defeat cross section shielding. =0: Shield input cross sections normally. =1: No shielding.
ITLMBG		10	Maximum number of iterations over background cross sections.
ITEMIP		0	Flag to alter selection of the interpolation function for the temperature dependence of the cross section self-shielding factors; Used only if ISOTOPE-off. =0: No change. =1: The B-spline interpolation is converted to the parabolic interpolation.
EPSBKG		1.0×10^{-3}	Maximum fractional change in background cross section permitted for each isotope.
ISIGOD		2	Number of background points used for interpolation of shielding factors; Used only if ISOTOPE-on.
ITEMOD		2	Number of temperature points used for interpolation of shielding factor; Used only if ISOTOPE-on.
NOXSCL	(IT, JT)	0	Flag not to recalculate shielded macroscopic cross sections during transient. This option, active only when NIOPT (53) = 1, can be used to eliminate those cells which do not need to recalculate cross sections. =0: The macroscopic cross sections are re-calculated during transient. =1: The macroscopic cross sections are not re-calculated during transient. The constant cross sections calculated in steady state are used. Do not flag cells where the material mass and/or temperature may change with time.

27. NISO

The isotope and cross-section related input variables.

Variable	Dimension	Default	Description
ISOTOP	(LNISIP+1)		Names of isotopes or materials for which cross sections and shielding factors are to be read. The last name denotes the cross section input set from which the prompt fission spectrum is taken.
NCMIX	(NC, NRXS)		Component cross section identification numbers. These numbers assign a set of component mixtures to each cross section block.
THDENS	(MT)		Theoretical densities for each component assigned previously (kg/m^3). The unit can be arbitrary but made consistent with AVDEN, since the specific number densities, defined as AVDENS divided by THDENS, are actually used.
LNMN	(MT)		Number of isotopes in the input materials.
LMC	(LNMN(MT), MT)		Numbers specifying the composition of component mixtures in terms of input isotopes or materials (isotope ID).
AVDENS	(LNMN(MT), MT)		Atomic number densities of the isotopes or materials specified in LMC (1/barn-m). The unit can be arbitrary but made consistent with THDENS, since the specific number densities, defined as AVDENS divided by THDENS, are actually used.

28. NHET

The additional neutronics input variables for special treatment such as the heterogeneity effect.

Variable	Dimension	Default	Description
IHETE	(IT*JT)	0	Cell-wise flag to calculate the heterogeneity effects for the thermal neutron group. Active only when NIOPT (52) = 1. =0: No heterogeneity effect considered. =1: Calculate macroscopic cross sections using an inhomogeneous model assuming a fuel-pin geometry.
INUCF	(LNSIP)	0	Flag to specify isotopes included or excluded in the fuel pellet. Active only when NIOPT (52) = 1. =0: The isotopes are excluded from the fuel pellet. The background cross sections outside the fuel pellet are calculated for the specified isotopes. =1: The isotopes are included in the fuel pellet. The background cross sections inside the fuel pellet are calculated for the specified isotopes.
RPEL		0.0 m	Effective fuel pellet radius used in the inhomogeneous model (m). Active only when NIOPT (52) = 1.
RCOOL		0.0 m	Effective unit cell radius used in the inhomogeneous model (m). The pellet volume fraction used in the model is calculated by $(RPEL)/(RCOOL)^2$. Active only when NIOPT (52) = 1.

29. NSOU

The neutronics input variables for source-driven reactors.

Variable	Dimension	Default	Description
NSOUTM		0	Number of entries in the amplitude.vs.time tables SOUTM/SOUAM, this number has to be less than 100, 0 means a time-independent source. Used only when NIOPT(36)>0.
IITLAD		1	Maximum number of inner iterations at first outer iteration for adjoint alpha-search. Used only when NIOPT(36)>0.
GAMMAZ		1.0	Neutron production cross-section normalization constant. Used only when NIOPT(36)>0.
EVAD		0.0	Initial eigenvalue estimation for adjoint alpha-search. Used only when NIOPT(36)>0.
EVMAD		100.0	Initial search parameter increment for adjoint alpha-search. Used only when NIOPT(36)>0.
XLALAD		0.01	Lambda lower limit for adjoint alpha-search. Used only when NIOPT(36)>0.
XLAHAD		0.5	Lambda upper limit for adjoint alpha-search. Used only when NIOPT(36)>0.
XLAXAD		0.001	Lambda convergence criterion for second and subsequent adjoint alpha-search steps (default=0.001, recommended 0.0001). Used only when NIOPT(36)>0.
PODAD		1.0	Damping parameter of SIMDANT for adjoint alpha-search. Used only when NIOPT(36)>0.
SOUSPE	(IGM)	0.0	Source energy spectrum. Used only when NIOPT(36)>0.
SOURCF	(IT, JT)	0.0	Source spatial distribution. Used only when NIOPT(36)>0.
SOUPR	10	0.0	SOUPR(1)=Shape step restriction after the time points at which the source amplitudes are given (see SOUTM); by default (SOUPR(1)=0.) the time step restriction is 10^{-4} ; if SOUPR(1)<0., there is no restriction. SOUPR(2)=Maximum source amplitude variation restriction per shape step; by default (SOUPR(2)=0.) the amplitude may vary by a factor of 3; if SOUPR(2)<0. There is no restriction, this restriction cannot make a step smaller than 10^{-7} Used only when NIOPT(36)>0.
SOUTM	100	-	Time points for which neutron source amplitudes are given. Used only when NIOPT(36)>0.
SOUAM	100	-	The corresponding amplitude values. Used only when NIOPT(36)>0.

Attachment 1: Definition of Dimension Indexes.

Fluid Mesh Cell Region boundary:

IB	The number of real radial mesh cells
JB	The number of real axial mesh cells
NPB	The number of radial nodes in the fuel pin (only used in the detailed pin model)
IBP2	=IB+2
JBP2	=JB+2
IJBP2	=IBP2*JBP2

MCSR: The number of structure-field density components.

1	fertile pin fuel
2	fissile pin fuel
3	left fertile crust fuel
4	left fissile crust fuel
5	right fertile crust fuel
6	right fissile crust fuel
7	cladding
8	left can wall boundary node
9	left can wall interior node
10	right can wall boundary node
11	right can wall interior node
12	control

MCLR: The number of liquid-field density components.

1	liquid fertile fuel
2	liquid fissile fuel
3	liquid steel
4	liquid sodium
5	fertile fuel particles
6	fissile fuel particles
7	steel particles
8	control particles
9	fertile fuel chunks
10	fissile fuel chunks
11	fission gas in liquid fuel
12	fission gas in fuel particles
13	fission gas in fuel chunks

MCGR: The number of vapor-field density components.

- 1 fertile fuel vapor
- 2 fissile fuel vapor
- 3 steel vapor
- 4 sodium vapor
- 5 fission gas

MCSRE: The number of structure-field energy components.

- 1 pin fuel
- 2 left crust fuel
- 3 right crust fuel
- 4 cladding
- 5 left can wall boundary node
- 6 left can wall interior node
- 7 right can wall boundary node
- 8 right can wall interior node
- 9 control

MCLRE: The number of liquid-field energy components.

- 1 liquid fuel
- 2 liquid steel
- 3 liquid coolant
- 4 fuel particles
- 5 steel particles
- 6 control particles
- 7 fuel chunks

MCGRE: The number of vapor-field energy components.

- 1 vapor mixture

MCGM1: The number of vapor-field material components.

- 1 fuel vapor
- 2 steel vapor
- 3 sodium vapor
- 4 fission gas

MFMAT: The number of fuel energy components.

- 1 pin fuel
- 2 left crust fuel
- 3 right crust fuel
- 4 liquid fuel
- 5 fuel particles
- 6 fuel vapor

7 fuel chunks

MFAM1: The number of fuel energy components.

1 pin fuel
 2 left crust fuel
 3 right crust fuel
 4 liquid fuel
 5 fuel particles
 6 fuel chunks

MMOM: The number of momentum fields. The default values are:

1 velocity component 1 (liquid fuel, fuel particles and steel particles)
 2 velocity component 2 (liquid steel, sodium, control particles and fuel chunks)
 3 velocity component 3 (vapor mixture)

MNMAT: The number of EOS material components.

1 fuel
 2 steel
 3 sodium
 4 control
 5 fission gas

MHSO: The number of heat-source material components.

1 fertile fuel
 2 fissile fuel
 3 steel
 4 sodium
 5 control

MNMATN: The number of sub-materials (default: 1). The default assignment of sub-material number is as follows:

Material Number	Sub-material Number	
	1	2
1 (fuel)	MOX (20% Pu)	UO ₂
2 (steel)	Type 316 SS	Type 316 SS
3 (sodium)	Sodium	Water
4 (control)	B ₄ C	B ₄ C
5 (fission gas)	Xe	Air

Attachment 2: Description of Output Control Variables.

A complete description of the variables PCGRP, PPGRP, PRCEL, and LPRGN in NAMELIST XEDT is given here.

PCGRP	(50)	The cell-wise variables to print. =1 : Print the variables. =0 : Do not print the variables.
	1 :	Structure component volume fractions,
	2 :	Structure component macroscopic densities,
	3 :	Structure component temperatures,
	4 :	Structure component specific internal volumes,
	5 :	Structure component specific internal energies,
	6 :	Liquid component volume fractions,
	7 :	Liquid component macroscopic densities,
	8 :	Liquid component temperatures,
	9 :	Liquid component specific internal volumes,
	10 :	Liquid component specific internal energies,
	11 :	Void fraction, vapor temperature, vapor component specific internal energies,
	12 :	Vapor component macroscopic densities,
	13 :	Vapor component specific internal volumes,
	14 :	Convectible interfacial areas in the bubbly flow region,
	15 :	Convectible interfacial areas in the dispersed flow region,
	16 :	Convectible interfacial area of bubbles and the interface between the bubbly and dispersed flow region,
	17 :	Pressure, hydraulic diameter, virtual mass,
	18 :	Radial velocities,
	19 :	Axial velocities,
	20 :	Pin internal node macroscopic densities,
	21 :	Pin internal node specific internal energies and temperature, and
	22 :	Pin internal node specific volume fraction and volume fraction.
PRCEL	(5, 50)	Print the requested cells.
	(1, *)	Flag to control the way of cell specification. =1 : Print the variables in the cell (I, J) specified by: PRCEL(2, *)=I, and PRCEL(3, *)=J. =2 : Print the variables in the cells bounded by a rectangle with its bottom left cell (IBL,JBL) and its top right cell (ITR,JTR) specified by:

		PRCEL(2, *)=IBL, PRCEL(3, *)=JBL, PRCEL(4, *)=ITR, and PRCEL(5, *)=JTR.
PPGRP	(50)	The variable groups to send to the postprocessor dump flag. The variable groups are described in Appendix F.
LPRGN	(220)	Print the requested cell variables for the entire mesh. See Table G-1 for the list of variables LPRGN(n) to be printed.

Table G-1. List of variables to be printed for the entire mesh.

<u>ALPSK</u>	<u>MCSRE</u>			<u>N = 1, 9</u>
'ALPSK1'	'ALPSK2'	'ALPSK3'	'ALPSK4'	'ALPSK5'
'ALPSK6'	'ALPSK7'	'ALPSK8'	'ALPSK9'	
<u>ALPLK</u>	<u>MCLRE</u>			<u>N = 10, 16</u>
'ALPLK1'	'ALPLK2'	'ALPLK3'	'ALPLK4'	'ALPLK5'
'ALPLK6'	'ALPLK7'			
<u>ALPGK</u>				<u>N = 17</u>
'ALPGK'				
<u>PK</u>				<u>N = 18</u>
'PK'				
<u>RBSK</u>	<u>MCSR</u>			<u>N = 19, 30</u>
'RBSK1'	'RBSK2'	'RBSK3'	'RBSK4'	'RBSK5'
'RBSK6'	'RBSK7'	'RBSK8'	'RBSK9'	'RBSK10'
'RBSK11'	'RBSK12'			
<u>RBLK</u>	<u>MCLR</u>			<u>N = 31, 43</u>
'RBLK1'	'RBLK2'	'RBLK3'	'RBLK4'	'RBLK5'
'RBLK6'	'RBLK7'	'RBLK8'	'RBLK9'	'RBLK10'
'RBLK11'	'RBLK12'	'RBLK13'		
<u>RBGK</u>	<u>MCGR</u>			<u>N = 44, 48</u>
'RBGK1'	'RBGK2'	'RBGK3'	'RBGK4'	'RBGK5'
<u>SIESK</u>	<u>MCSRE</u>			<u>N = 49, 57</u>
'SIESK1'	'SIESK2'	'SIESK3'	'SIESK4'	'SIESK5'
'SIESK6'	'SIESK7'	'SIESK8'	'SIESK9'	
<u>SIELK</u>	<u>MCLRE</u>			<u>N = 58, 64</u>
'SIELK1'	'SIELK2'	'SIELK3'	'SIELK4'	'SIELK5'
'SIELK6'	'SIELK7'			
<u>SIEGK</u>				<u>N = 65</u>
'SIEGK'				
<u>TSK</u>	<u>MCSRE</u>			<u>N = 66, 74</u>
'TSK1'	'TSK2'	'TSK3'	'TSK4'	'TSK5'
'TSK6'	'TSK7'	'TSK8'	'TSK9'	
<u>TLK</u>	<u>MCLRE</u>			<u>N = 75, 81</u>
'TLK1'	'TLK2'	'TLK3'	'TLK4'	'TLK5'
'TLK6'	'TLK7'			
<u>TGK</u>				<u>N = 82</u>
'TGK'				

<u>SVSK</u>	<u>MCSRE</u>			<u>N = 83, 91</u>
'SVSK1'	'SVSK2'	'SVSK3'	'SVSK4'	'SVSK5'
'SVSK6'	'SVSK7'	'SVSK8'	'SVSK9'	
<u>SVLK</u>	<u>MCLRE</u>			<u>N = 92, 98</u>
'SVLK1'	'SVLK2'	'SVLK3'	'SVLK4'	'SVLK5'
'SVLK6'	'SVLK7'			
<u>SVGK</u>	<u>MCGM1</u>			<u>N = 99, 102</u>
'SVGK1'	'SVGK2'	'SVGK3'	'SVGK4'	
<u>VK</u>	<u>MMOM</u>			<u>N = 103, 105</u>
'VK1'	'VK2'	'VK3'		
<u>UK</u>	<u>MMOM</u>			<u>N = 106, 108</u>
'UK1'	'UK2'	'UK3'		
<u>EPSFK</u>	<u>MFMAM1</u>			<u>N = 109, 114</u>
'EPSFK1'	'EPSFK2'	'EPSFK3'	'EPSFK4'	'EPSFK5'
'EPSFK6'				
<u>RBIK</u>	<u>2</u>			<u>N = 115, 116</u>
'RBIK1'	'RBIK2'			
<u>EIPINK</u>				<u>N = 117</u>
'EIPINK'				
<u>TIPINK</u>				<u>N = 118</u>
'TIPINK'				
<u>SVIPK</u>				<u>N = 119</u>
'SVIPK'				
<u>ALPINK</u>				<u>N = 120</u>
'ALPINK'				
<u>KGAP</u>				<u>N = 121</u>
'KGAP'				
<u>ALPNFK</u>	<u>3</u>			<u>N = 122, 124</u>
'ALPNFK1'	'ALPNFK2'	'ALPNFK3'		
<u>RPINK</u>				<u>N = 125</u>
'RPINK'				
<u>DHK</u>				<u>N = 126</u>
'DHK'				
<u>AQQLK</u>	<u>MMOM</u>			<u>N = 127, 129</u>
'AQQLK1'	'AQQLK2'	'AQQLK3'		
<u>BQQLK</u>	<u>MMOM</u>			<u>N = 130, 132</u>

'BQQLK1'	'BQQLK2'	'BQQLK3'			
<u>AQOTK</u>	<u>MMOM</u>				<u>N = 133, 135</u>
'AQQTK1'	'AQQTK2'	'AQQTK3'			
<u>BQOTK</u>	<u>MMOM</u>				<u>N = 136, 138</u>
'BQQTK1'	'BQQTK2'	'BQQTK3'			
<u>AQSLK</u>	<u>MMOM</u>				<u>N = 139, 141</u>
'AQSLK1'	'AQSLK2'	'AQSLK3'			
<u>BQSLK</u>	<u>MMOM</u>				<u>N = 142, 144</u>
'BQSLK1'	'BQSLK2'	'BQSLK3'			
<u>AQSTK</u>	<u>MMOM</u>				<u>N = 145, 147</u>
'AQSTK1'	'AQSTK2'	'AQSTK3'			
<u>BQSTK</u>	<u>MMOM</u>				<u>N = 148, 150</u>
'BQSTK1'	'BQSTK2'	'BQSTK3'			
<u>VMK</u>					<u>N = 151</u>
'VMK'					
<u>SARK</u>	<u>5</u>				<u>N = 152, 156</u>
'SARK1'	'SARK2'	'SARK3'	'SARK4'	'SARK5'	
<u>SALMBK</u>	<u>MARL</u>				<u>N = 157, 163</u>
'SALMBK1'	'SALMBK2'	'SALMBK3'	'SALMBK4'	'SALMBK5'	
'SALMBK6'	'SALMBK7'				
<u>SALMDK</u>	<u>MARL</u>				<u>N = 164, 170</u>
'SALMDK1'	'SALMDK2'	'SALMDK3'	'SALMDK4'	'SALMDK5'	
'SALMDK6'	'SALMDK7'				
<u>SALMK</u>	<u>MARL</u>				<u>N = 171, 177</u>
'SALMK1'	'SALMK2'	'SALMK3'	'SALMK4'	'SALMK5'	
'SALMK6'	'SALMK7'				
<u>SABDK</u>					<u>N = 178</u>
'SABDK'					
<u>XBK</u>					<u>N = 179</u>
'XBK'					
<u>ALPGB</u>					<u>N = 180</u>
'ALPGB'					
<u>ERK</u>					<u>N = 181</u>
'ERK'					
<u>QN</u>	<u>MHSO</u>				<u>N = 182, 186</u>
'QN1'	'QN2'	'QN3'	'QN4'	'QN5'	

<u>RGBK</u>					<u>N = 187</u>
'RGBK'					
<u>RLMBK</u>	<u>MCLRE</u>				<u>N = 188, 194</u>
'RLMBK1'	'RLMBK2'	'RLMBK3'	'RLMBK4'	'RLMBK5'	
'RLMBK6'	'RLMBK7'				
<u>RLMDK</u>	<u>MCLRE</u>				<u>N = 195, 201</u>
'RLMDK1'	'RLMDK2'	'RLMDK3'	'RLMDK4'	'RLMDK5'	
'RLMDK6'	'RLMDK7'				
<u>QNNK</u>	<u>MHSO</u>				<u>N = 202, 206</u>
'QNNK1'	'QNNK2'	'QNNK3'	'QNNK4'	'QNNK5'	
<u>ALPGEK</u>					<u>N = 207</u>
'ALPGEK'					
<u>ASMZ</u>					<u>N = 208</u>
'ASMZ'					
<u>DLIQK</u>					<u>N = 251</u>
'DLIQK'					
<u>CPK</u>					<u>N = 252</u>
'CPK'					
<u>CP2K</u>					<u>N = 253</u>
'CP2K'					
<u>DPK</u>					<u>N = 254</u>
'DPK'					
<u>ILSK</u>					<u>N = 255</u>
'ILSK'					
<u>IRGMK</u>					<u>N = 256</u>
'IRGMK'					
<u>WALLK</u>					<u>N = 257</u>
'WALLK'					
<u>NSEXK</u>	<u>7</u>				<u>N = 258, 264</u>
'NSEXK1'	'NSEXK2'	'NSEXK3'	'NSEXK4'	'NSEXK5'	
'NSEXK6'	'NSEXK7'				
<u>PHK</u>	<u>3</u>				<u>N = 265, 267</u>
'PHK1'	'PHK2'	'PHK3'			
<u>ILWBRK</u>					<u>N = 268</u>
'ILWBRK'					
<u>IRWBRK</u>					<u>N = 269</u>

'IRWBRK'

Attachment 3: Index of Input Variables.

<u>Variable</u>	<u>Page</u>	<u>Variable</u>	<u>Page</u>	<u>Variable</u>	<u>Page</u>	<u>Variable</u>	<u>Page</u>
ACB	33	ARCWIB	31	CE2	53	CPVIS	46
ACC	37	AS	42	CE3	53	CPVISB	34
ACRMIN	69	ASAT	43	CE4	53	CPVISC	38
AFRGB	72	ASC	35	CFCB	52	CPVISI	46
AG	42	ASIC	35	CFCD	52	CQS	45
AGLIMT	48	ASMINB	31	CFDB	52	CRGB	52
AGLS	71	ASMTB	31	CFDD	52	CRGL	53
AGMNTU	48	AVDENS	91	CFL	52	CSAT	43
AHGAP	70	BESLIP	57	CFRS1	45	CSF	53
AHGMAX	71	BESLP2	57	CFRS2	45	CSFL	53
AHGMIN	71	BETA	42	CFRS3	45	CSSL	62
AKGAP	71	BETACW	69	CFSB	52	CSSX	53
AKPG	62	BETAD	86	CFSD	52	CT1	45
AKPL	62	BETINP	86	CFT	51	CT2	45
AKPS	62	BFRGB	72	CFV	51	CTC	45
AL	42	BG	42	CG	43	CTD	45
ALC	35	BL	42	CGBS	51	CTHETA	51
ALCWIB	31	BMUG	62	CGCS	51	CTTB	52
ALGOPT	4	BMUL	62	CHGK	67	CTTL	52
ALMINB	31	BPJ	45	CHGL	67	CTWB	52
ALMNTU	48	BS	42	CHK	67	CTWD	52
ALPB1	50	BSAT	43	CHLG	67	CVG	43
ALPB2	50	BSFC	39	CHLL	67	CWMXF	48
ALPBUB	50	BSL	43	CHYS	50	CWSL	48
ALPDM	45	CANG	53	CL	42	CWST	48
ALPDSP	50	CANUL1	46	CLCS	51	CYCFIN	30
ALPEXC	74	CANUL2	46	CLDS	50	DAX	64
ALPHA0	41	CANUL3	46	CLG	51	DAXDRB	33
ALPMP	45	CASC	67	CLL	51	DAXDRC	37
ALPMP2	45	CBD	50	CMELT	69	DCPL	62
ALPNC	51	CCD	45	CMFB	57	DECAY	86
ALPNT	51	CCPG	45	CMU	48	DG	43
ALPSID	45	CDD	45	CNC	51	DHFB	34
AMPTAB	64	CDFBL0	47	CNP1	66	DHFC	38
AN	47	CDFBL1	47	CNP2	66	DHGB	71
ANFC	35	CDFBL2	47	CORFRN	46	DHINP	47
ANFILB	31	CDFBL3	47	CORFZN	47	DHPOLB	34
ANFIPB	31	CDFBL4	47	COURTN	73	DHPOLC	38
ANFIRB	31	CDFBT0	47	CPGMAX	63	DHPOOL	53
ANLC	35	CDFBT1	47	CPJ	45	DKHETI	86
ANRC	35	CDFBT2	47	CPLMAX	62	DKLAM	86
APINTB	32	CDFBT3	47	CPSR	50	DKYLD	86
APINTC	36	CDNB	57	CPTB	52	DKYLDS	86
APJ	45	CE1	53	CPTL	52	DL	42

DLB	53	EPMSC	36	EXPPR1	74	HCDGP	55
DMPC	39	EPS10	87	FACGOM	48	HCDGS	55
DPEL	64	EPS11	88	FAFAIL	69	HCDLAS	55
DPMK1	73	EPS12	88	FC34	70	HCDLBS	55
DPMK4	73	EPS13	88	FCOUPG	46	HCDLP	55
DRAD	64	EPS14	88	FCOUPL	46	HCDMXS	57
DRINP	29	EPS15	88	FCT	70	HCDP	55
DSPECT	86	EPS16	88	FDTGMX	66	HCRGAP	66
DTBSF	39	EPS17	88	FEDT	30	HEATOPT	78
DTDMP	39	EPS18	88	FEJ	70	HFCGP	55
DTDPC	42	EPS4	87	FEL	65	HFCGS	56
DTDPS	42	EPS5	87	FFB	57	HFCLP	55
DTEOS	40	EPS6	87	FG	43	HFCLS	56
DTGMK1	73	EPS7	87	FILMIN	57	HFCXS	57
DTGMK4	73	EPS8	87	FKCR	78	HGLMUL	56
DTHINI	30	EPS9	87	FL	42	HGSMUL	56
DTHMAX	30	EPSBKG	90	FL11G5	70	HICLCP	56
DTHMIN	30	EPSC	36	FL12G5	70	HICLDP	56
DTINC	30	EPSEN	41	FL13G5	70	HKEXP	57
DTLMAX	66	EPSFAC	89	FLIMITER	78	HKMUL	70
DTMAX	30	EPSFIB	32	FMELT	69	HLGMIN	66
DTMIN	30	EPSG	87	FMOL	78	HLGMUL	56
DTMPF	30	EPSM	63	FMTLG	65	HMTOPT	15
DTPPF	39	EPSMIB	32	FP34	70	HNCGP	55
DTPRT	39	EPSMIN	89	FPG4K	66	HNCLP	55
DTSH	87	EPSO	89	FPG4L	66	HOSGBU	56
DTSMAX	87	EPSP	73	FPNOPT	27	HOSLDP	56
DTSTRT	30	EPSPCV	73	FRAND	74	HREIC	56
DTTPP	40	EPSPHY	87	FRG	65	HREOS	56
DTUBE	48	EPSPT	89	FRICT	70	HRSMUL	56
DVCE3	65	EPSRO	73	FRTHKP	53	HRTMUL	56, 57
DVCRG	65	EPSSPN	71	FRTP	64	HTCOPT	10
DVCTG	65	EPSSV	41	FTG	65	IB	29
DVDPS	42	EPST	73	FTHMIN	53	ICL	29
DVRT	51	EPSTG	41	FTSTH	66	ICOS	84
DWFAL	69	EPSTR	78	FTSTL	65	ICR	29
DZINP	29	EPSVEL	73	FUND	65	ICRC	59
ECRT	41	ER0C	37	FVCCF1	74	ICRGT	48
EDTOPT	22	ER0INB	33	FVCE3	65	IDHB	34
EHTCFB	57	ERRFXU	89	FVCRG	65	IDHC	38
EITRF	73	ERROPT	28	FVCTG	65	IDIVR	83
ELIQG	41	ES4ST	70	FXE	73	IDTH	30
ELIQGD	43	ESOLUS	41	FXR	73	IEDSFT	85
ELIQUS	41	ETAINP	86	G	73	IEDXST	85
EMSVL	63	EVAD	93	GAMGB	71	IFAOPT	13
EMSVS	63	EVCE3	65	GAMMAZ	93	IFREE	44
ENGEOS	76	EVCRG	65	GANG	73	IFXUDL	87
ENRC	36	EVCTG	65	GENTIN	86	IGD	83
EOSOPT	8	EVMAD	93	HAFMUL	57	IGEOM	29

IGM	83	JGPU2	71	NEUPRI	85	PRTC	39
IHETE	92	JLB	31	NEZFLG	84	PSAINB	31
IITLAD	93	JLM	31	NF	63	PSC1	67
ILB	31	JLPB	29	NFAXI	83	PSC2	67
ILM	31	JLPT	29	NFRAD	83	PSFC	36
ILS0C	38	JSTOP	53	NGAMMF	67	PSFINB	32
ILS0IB	34	JT	83	NGAMVC	67, 68	PSMIN	43
IMRK	43	JUB	31	NIOPT	79	PTAB	60
INUCF	92	JUM	31	NITRF	73	PTME	60
INVPRT	85	JUPB	29	NOXSCL	90	PTS	41
INVREG	85	JUPT	29	NPAGE	40	PVS1	47
IPOW	64	KPCRT	63	NPB	29	PVS2	47
IQUASI	87	KPOPT	62	NPRINT	40	PVSCL	47
IRAMPT	86	LBCG	60	NREG	29	QNA2O	78
IRGBND	85	LBCP	60	NREGB	83	QNAOH	78
ISAE	43	LBCS	59	NRXS	83	RAMPT	86
ISHLD	90	LBCSET	58	NSF	39	RAOB	66
ISIGOD	90	LBCT	60	NSN	39	RATIOD	48
ISNT	83	LBCV	60	NSOUTM	93	RATIOL	48
ISOTOP	91	LCELPT	85	NST1B	31	RBGMIN	66
ISPC	38	LIPSTP	87	NST1C	35	RBPB	32
ISPN	44	LMC	91	NSTEF	74	RBPC	36
ISRCBB	53	LNISIP	83	OHMC	70	RCB	33
ISRCDB	54	LNMN	91	OHMF	70	RCC	37
ISRCDD	54	LPRGN	40, 98	OM	86	RCOMPB	32
ISTEF	74	LRGN	31	OMEGAB	52	RCOMPC	35
IT	83	LWASET	59	OMEGAD	52	RCOOL	92
ITEMIP	90	LWATME	59	ONLIQ	74	RCRATE	86
ITEMOD	90	MATEOS	76	OPTPIT	73	REGC	76
ITGAMM	87	MAXITC	73	PCB	33	REGN	76
ITLMBG	90	MAXITR	78	PCC	37	RFUEL	32
ITLMIN	89	MCR	59	PCGRP	39, 97	RFUELC	36
ITLMOU	89	MIVC	65	PCRT	41	RGB	33
ITR	84	MMAX	51	PG4C	36	RGB0C	37
IUB	31	MMIN	51	PG4INB	32	RGB0IB	33
IUM	31	MPIT	73	PGLB	33	RGBMAX	50
IVBF	39	MSIT	71	PGMC	36	RGBMIN	50
IVCHLG	66	MT	83	PGMINB	32	RGINI	50
IVDL	74	MUCRT	63	PGPL	71	RGLMAX	66
IWTF	87	MULMP	63	PGPU	71	RGMAXB	33
IXSREG	83	MUOPT	62	PGUB	33	RGMAXC	37
JB	29	MXFOPT	25	PHI	65	RGMINB	33
JBEGIN	53	NATOM	63	PMELT	69	RGMINC	37
JCB	29	NBC	58	PODAD	93	RGNAMB	31
JCRC	59	NCAXI	83	POW	64	RGSBK	50
JCT	29	NCMIX	91	POWER	86	RHOIN	86
JGPL1	71	NCRAD	83	PPFC	39	RJGB	71
JGPL2	71	NDKGRP	83	PPGRP	39, 98	RLHMT	50
JGPU1	71	NDT0	30	PRCEL	40, 97	RLINI	50

RLM0C	37	TAUNUC	51	TLBND	43	VTAB	60
RLM0IB	33	TAUST	70	TLC	35	VTME	60
RLMAX	50	TC34	70	TLIQUS	41	WCRST	66
RLMAXB	33	TCB	33	TLMINB	31	WEB	51
RLMAXC	37	TCBSF	39	TMFAIL	71	WED	51
RLMIN	50	TCC	37	TPB	32	WM	42
RLMINB	33	TCDMP	39	TPC	36	WMELT	69
RLMINC	37	TCPPF	39	TPPOPT	10	WMH	78
RLSBK	50	TCPRT	39	TSC	35	WMNA	78
ROCRT	41	TCPU	30	TSIC	35	WMO	78
RPC	35	TCRMIN	69	TSINB	31	XBUFIN	48
RPCNTL	50	TCRT	41	TSINTB	31	XCFGC	37
RPEL	92	TFNUCL	66	TSOLUS	41	XCINB	33
RPINIB	32	TGC	37	TSTART	30	XCNFGC	36
RPMAXD	48	TGINB	33	TSUP	66	XCINIB	32
RPMXLB	48	TGLB	33	TTAB	60	XCSTR	69
RSTOPT	27	TGMAX	63	TTME	60	XENRIB	32
RUGM	43	TGMIN	41	TWFAL	69	XFGC	36
SARC	35	TGPL	71	TWFIN	30	XFINB	32
SEED	74	TGPU	71	U0GB	71	XLAHAD	93
SF	39	TGUB	33	UC	37	XLALAD	93
SGUTS0	70	THDENS	91	UCR	59	XLARG	48
SIGM	63	THETA0	51	UINB	33	XLAXAD	93
SN	39	TILFC	66	VC	37	XLFGC	36
SOUAM	93	TILFW	66	VCR	59	XLINB	32
SOUPR	93	TILSW	66	VGMC	37	XPFGC	36
SOURCF	93	TIMAMP	64	VGMINB	33	XPINB	32
SOUSPE	93	TL11G5	70	VINB	33	XWSTR	69
SOUTM	93	TL12G5	70	VLIQUS	41		
T0GB	71	TL13G5	70	VSOLUS	41		

APPENDIX H

SAMPLE INPUT LISTING

In this appendix, input data listings are given for the four sample problems described in **Section 3.3**. These are:

1. Little Work Energy (LWE) problem (Table H-1),
2. Little Boiling Pool (LBP) problem (Table H-2),
3. Fuel-Coolant Interaction (FCI) problem (Table H-3), and
4. Space-Time Neutronics (STN) problem (Table H-4).

Table H-1. Input data for LWE problem.

START : LITTLE WORK ENERGY PROBLEM EURO-PNC FOR S-III VER.3.A

&XCNTL

```

HMTOPT(71)=1,2,1,1,0,1,
HMTOPT(80)=1,3,1,
ERROPT(3) =11,
/

```

&XMSH

```

IB=3,JB=12,
DRINP(1)=3*0.935,
DZINP(1)=12*0.9144,
NREG= 8,
/

```

&XTME

```

TWFIN=0.30,DTSTRT=1.0D-6,DTMIN=5.0D-07,DTMAX=2.0D-4,
NDT0=1,TCPU=100000.0,
/

```

&XRGN

```

RGNAMB=' SHIELD AND BLANKET ',
LRGN=1, IILB=1,IUB=1,JLB=1,JUB=1,
ALMINB(3) = 0.099291,
TLMINB(3) = 661.0, TGINB = 661.0,
PSFINB = 2.35277D5,
ASMINB(8) = 0.92054, ARCWIB= 34.4,
TSINB(7) = 661.0, TSINB(8) = 661.0,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' CORE ',
LRGN=2, IILB=1,IUB=1,JLB=2,JUB=2,
ALMINB(1) = 0.626771, ALMINB(2) = 0.18243,
TLMINB(1) = 5966.0, TLMINB(2) = 1754.0, TGINB = 5966.0,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' FISSION GAS PLENUM ',
LRGN=3, IILB=1,IUB=1,JLB=3,JUB=4,
ALMINB(3) = 0.4539,
TLMINB(3) = 1200.0, TGINB = 1200.,
ASMINB(4) = 0.11229, ASMINB(8) = 0.1077, ARCWIB = 34.4,
TSINB(4) = 1200.0, TSINB(7) = 1200.0, TSINB(8) = 1200.0,
PSAINB = 359.3,
RPINIB = 0.003,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' RADIAL STRUCTURE ',
LRGN=4, IILB=2,IUB=3,JLB=1,JUB=4,
ALMINB(3) = 0.099291,
TLMINB(3) = 661.0, TGINB = 661.0,
ASMINB(8) = 0.92054, ARCWIB= 34.4,
TSINB(7) = 661.0, TSINB(8) = 661.0,
PSFINB = 2.35277D5,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' FLOW GUIDE TUBES ',
LRGN=5, ILB=1,IUB=1,JLB=5,JUB=7,
ALMINB(3) = 0.31206,
TLMINB(3) = 1200.0, TGINB = 1200.,
ASMINB(4)=0.013514, ASMINB(8) = 0.16554, ARCWIB= 5.359,
TSINB(4) = 1000.0, TSINB(7) = 1000.0,TSINB(8) = 1000.0,
PSAINB = 359.3,
RPINIB = 0.003,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' SODIUM POOL 1 ',
LRGN=6, ILB=2,IUB=3,JLB=5,JUB=7,
ALMINB(3) = 1.0000,
TLMINB(3) = 1200.0, TGINB = 1200.0,
PSFINB = 2.0598D5,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' SODIUM POOL 2 ',
LRGN=7, ILB=1,IUB=3,JLB=8,JUB=11,
ALMINB(3) = 1.0000,
TLMINB(3) = 1200.0, TGINB = 1200.0,
PSFINB = 2.0598D5,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XRGN

```

RGNAMB=' COVER GAS ',
LRGN=8, ILB=1,IUB=3,JLB=12,JUB=12,
ALMINB(3) = 0.0,
TLMINB(3) = 1200.0, TGINB = 1200.0,
XENRIB(1) = 6*1.,
RLM0IB(1) = 6*0.001, RGB0IB = 0.001,
/

```

&XEDT

```

PRTC=50,PPFC=9999999,DMPC=9999999,
DTPPF(1)=0.0015,
DTPRT(1)=0.100,
PPGRP(19)=1,
PPGRP(20)=1,
PPGRP(21)=1,
PPGRP(24)=1,
PPGRP(29)=1,
PPGRP(30)=1,1,
NPAGE= 8,
LPRGN(10)=1,1,1,1,1,0,
LPRGN(16)=1,
LPRGN(17)=1,
LPRGN(30)=0,1,1,1,
LPRGN(70)=1,1,1,1,1,0,
LPRGN(76)=1,
LPRGN(96)=6*1,
SN='ALPSK1','ALPSK2','ALPSK3','ALPSK4','ALPSK5','ALPSK6',
'ALPSK7','ALPSK8','ALPSK9','ALPLK1','ALPLK2','ALPLK3',
'ALPLK4','ALPLK5','ALPLK6','ALPGK','ALPINK',
'ALPNFK1','ALPNFK2','ALPNFK3','DHK',
'PK','PGMK1','PGMK2','PGMK3','PGMK4',
'RBSK1','RBSK2','RBSK3','RBSK4','RBSK5','RBSK6',
'RBSK7','RBSK8','RBSK9','RBSK10','RBSK11','RBSK12',
'RBLK1','RBLK2','RBLK3','RBLK4','RBLK5','RBLK6',
'RBLK7','RBLK8','RBLK9','RBLK10','RBIK1','RBIK2',
'RBGK1','RBGK2','RBGK3','RBGK4','RBGK5',
'TSK1','TSK2','TSK3','TSK4','TSK5','TSK6',
'TSK7','TSK8','TSK9','TIPINK',

```

'TLK1', 'TLK2', 'TLK3', 'TLK4', 'TLK5', 'TLK6', 'TGK',
'VK1', 'VK2', 'VK3', 'UK1', 'UK2', 'UK3',
/

Table H-2. Input data for LBP problem.

START : LITTLE BOILING POOL PROBLEM EURO-PNC FOR S-III VER.3.A

```

&XCNTL
  HMTOPT(71)=1,2,1,1,0,1,
  HMTOPT(80)=1,3,1,
/

&XMSH
  IB=5,JB=7,
  DRINP(1)=5*0.2,
  DZINP(1)=6*0.2, 0.3,
  NREG=23,
  ICL = 4, ICR = 4,
  JCB = 1, JCT = 4,
  JLPB= 1, JLPT= 1,
  JUPB= 4, JUPT= 4,
/

&XTME
  TWFIN=5.00,DTSTRT=1.0D-6,DTMIN=1.0D-07,DTMAX=5.0D-4,
  NDT0=1,TCPU=100000.0,
  IDTH=1,
/

&XMSC
  COURTN=0.5,
/

&XRGN
  RGNAMB = 'POOL 1',
  LRGN=1, IILB=1,IUB=1,JLB=1,JUB=1,
  ALMINB(1) = 0.3300, ALMINB(2) = 0.2200,
  TLMINB(1) = 3300.0, TLMINB(2) = 3300.0, TGINB = 3300.0,
  RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

&XRGN
  RGNAMB = 'POOL 2',
  LRGN=2, IILB=2,IUB=2,JLB=1,JUB=1,
  ALMINB(1) = 0.4200, ALMINB(2) = 0.28200,
  TLMINB(1) = 3275.0, TLMINB(2) = 3275.0, TGINB = 3275.0,
  RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

&XRGN
  RGNAMB = 'POOL 3',
  LRGN=3, IILB=3,IUB=3,JLB=1,JUB=1,
  ALMINB(1) = 0.5100, ALMINB(2) = 0.3400,
  TLMINB(1) = 3250.0, TLMINB(2) = 3250.0, TGINB = 3250.0,
  RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

&XRGN
  RGNAMB = 'LOWER PLENUM',
  LRGN=4, IILB=4,IUB=4,JLB=1,JUB=1,
  ALMINB(1) = 0.2890, ALMINB(2) = 0.1920,
  TLMINB(1) = 3225.0, TLMINB(2) = 3225.0, TGINB = 3225.0,
  ASMINB(4) = 0.2856, ANFIPB = 0.1344, RPINIB= 0.0079,
  ASMINB(6) = 0.0494, ASMINB(8) = 0.0494, ALCWIB= 9.75, ARCWIB= 9.75,
  TSINB(4) = 1000.0, TGLB = 1000.0,
  TSINB(6) = 1000.0, TSINB(8) = 1000.0,
  PSFINB = 2.0488D5,
  PGLB = 1.5000D+5,
  RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

&XRGN
  RGNAMB = 'POOL 5',

```

```

LRGN=5, ILB=5,IUB=5,JLB=1,JUB=1,
ALMINB(1) = 0.3600, ALMINB(2) = 0.2400,
TLMINB(1) = 3200.0, TLMINB(2) = 3200.0, TGINB = 3200.0,
ASMINB(1) = 7*0.D0, ASMINB(8) = 0.4000, ARCWIB= 30.,
TSINB(7) = 1000.0, TSINB(8) = 1000.0,
PSFINB = 1.8400D5,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 6',
LRGN=6, ILB=1,IUB=1,JLB=2,JUB=2,
ALMINB(1) = 0.2400, ALMINB(2) = 0.1600,
TLMINB(1) = 3275.0, TLMINB(2) = 3275.0, TGINB = 3275.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 7',
LRGN=7, ILB=2,IUB=2,JLB=2,JUB=2,
ALMINB(1) = 0.3300, ALMINB(2) = 0.2200,
TLMINB(1) = 3250.0, TLMINB(2) = 3250.0, TGINB = 3250.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 8',
LRGN=8, ILB=3,IUB=3,JLB=2,JUB=2,
ALMINB(1) = 0.4200, ALMINB(2) = 0.2800,
TLMINB(1) = 3225.0, TLMINB(2) = 3225.0, TGINB = 3225.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'FUEL PIN',
LRGN=9, ILB=4,IUB=4,JLB=2,JUB=2,
ALMINB(1) = 0.1840, ALMINB(2) = 0.1230,
TLMINB(1) = 3200.0, TLMINB(2) = 3200.0, TGINB = 3200.0,
ASMINB(1) = 0.1224, ASMINB(4) = 0.2856, ANFIPB= 0.0120, RPINIB= 0.0079,
ASMINB(6) = 0.0494, ASMINB(8) = 0.0494, ALCWIB= 9.75, ARCWIB= 9.75,
TSINB(1) = 1000.0, TSINB(4) = 1000.0,
TSINB(6) = 1000.0, TSINB(8) = 1000.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 10',
LRGN=10, ILB=5,IUB=5,JLB=2,JUB=2,
ALMINB(1) = 0.3600, ALMINB(2) = 0.2400,
TLMINB(1) = 3175.0, TLMINB(2) = 3175.0, TGINB = 3175.0,
ASMINB(1) = 7*0.D0, ASMINB(8) = 0.4000, ARCWIB= 30.,
TSINB(7) = 1000.0, TSINB(8) = 1000.0,
PSFINB = 1.6499D5,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 11',
LRGN=11, ILB=1,IUB=1,JLB=3,JUB=3,
ALMINB(1) = 0.1500, ALMINB(2) = 0.1000,
TLMINB(1) = 3250.0, TLMINB(2) = 3250.0, TGINB = 3250.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 12',
LRGN=12, ILB=2,IUB=2,JLB=3,JUB=3,
ALMINB(1) = 0.2400, ALMINB(2) = 0.1600,
TLMINB(1) = 3225.0, TLMINB(2) = 3225.0, TGINB = 3225.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 13',
LRGN=13, ILB=3,IUB=3,JLB=3,JUB=3,
ALMINB(1) = 0.3300, ALMINB(2) = 0.2200,
TLMINB(1) = 3200.0, TLMINB(2) = 3200.0, TGINB = 3200.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'CONTROL',
LRGN=14, ILB=4,IUB=4,JLB=3,JUB=3,
ALMINB(1) = 0.1415, ALMINB(2) = 0.0943,
TLMINB(1) = 3175.0, TLMINB(2) = 3175.0, TGINB = 3175.0,
ASMINB(4) = 0.2856, ASMINB(9) = 0.1224, ANFIPB= 0.0120, RPINIB= 0.0079,
ASMINB(6) = 0.0494, ASMINB(8) = 0.0494, ALCWIB= 9.75, ARCWIB= 9.75,
TSINB(4) = 1000.0,
TSINB(6) = 1000.0, TSINB(8) = 1000.0,
TSINB(9) = 1000.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 15',
LRGN=15, ILB=5,IUB=5,JLB=3,JUB=3,
ALMINB(1) = 0.3060, ALMINB(2) = 0.2040,
TLMINB(1) = 3150.0, TLMINB(2) = 3150.0, TGINB = 3150.0,
ASMINB(1) = 7*0.D0, ASMINB(8) = 0.4000, ARCWIB= 30.,
TSINB(7) = 1000.0, TSINB(8) = 1000.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 16',
LRGN=16, ILB=1,IUB=1,JLB=4,JUB=4,
ALMINB(1) = 0.0600, ALMINB(2) = 0.0400,
TLMINB(1) = 3225.0, TLMINB(2) = 3225.0, TGINB = 3225.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 17',
LRGN=17, ILB=2,IUB=2,JLB=4,JUB=4,
ALMINB(1) = 0.1500, ALMINB(2) = 0.1000,
TLMINB(1) = 3200.0, TLMINB(2) = 3200.0, TGINB = 3200.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 18',
LRGN=18, ILB=3,IUB=3,JLB=4,JUB=4,
ALMINB(1) = 0.2400, ALMINB(2) = 0.1600,
TLMINB(1) = 3175.0, TLMINB(2) = 3175.0, TGINB = 3175.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'UPPER PLENUM',
LRGN=19, ILB=4,IUB=4,JLB=4,JUB=4,
ALMINB(1) = 0.0715, ALMINB(2) = 0.0476,
TLMINB(1) = 3150.0, TLMINB(2) = 3150.0, TGINB = 3150.0,
ASMINB(4) = 0.2856, ANFIPB = 0.1344, RPINIB= 0.0079,
ASMINB(6) = 0.0494, ASMINB(8) = 0.0494, ALCWIB= 9.75, ARCWIB= 9.75,
TSINB(4) = 1000.0, TGUB = 1000.0,
TSINB(6) = 1000.0, TSINB(8) = 1000.0,
PGUB = 1.5000D+5,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

&XRGN

```

RGNAMB = 'POOL 20',
LRGN=20, ILB=5,IUB=5,JLB=4,JUB=4,
ALMINB(1) = 0.2520, ALMINB(2) = 0.1680,
TLMINB(1) = 3125.0, TLMINB(2) = 3125.0, TGINB = 3125.0,
ASMINB(1) = 7*0.D0, ASMINB(8) = 0.4000, ARCWIB= 30.,
TSINB(7) = 1000.0, TSINB(8) = 1000.0,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

```
&XRGN
```

```

RGNAMB = 'NONCONDENSIBLE GAS WITHOUT STRUCTURE',
LRGN=21, ILB=1,IUB=4,JLB=5,JUB=6,
TGINB=3100,
TLMINB(1) = 3100.0, TLMINB(2) = 3100.0,
TGINB=3100.0,
PSFINB = 1.32D+5,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

```
&XRGN
```

```

RGNAMB = 'NONCONDENSIBLE GAS WITH RADIAL STRUCTURE',
LRGN=22, ILB=5,IUB=5,JLB=5,JUB=6,
ASMINB(1) = 7*0.D0, ASMINB(8) = 0.4000, ARCWIB= 30.,
TSINB(7) = 1000.0, TSINB(8) = 1000.0,
TLMINB(1) = 3100.0, TLMINB(2) = 3100.0,
TGINB=3100.0,
PSFINB = 1.32D+5,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

```
&XRGN
```

```

RGNAMB = 'UPPER CORE STRUCTURE WITH NONCONDENSIBLE GAS',
LRGN=23, ILB=1,IUB=5,JLB=7,JUB=7,
ASMINB(1) = 7*0.D0, ASMINB(8) = 0.4000, ARCWIB= 30.,
TSINB(7) = 1000.0, TSINB(8) = 1000.0,
TLMINB(1) = 3100.0, TLMINB(2) = 3100.0,
TGINB=3100.0,
PSFINB = 1.32D+5,
RLM0IB(1) =6*0.001, RGB0IB=0.001, XENRIB(1)=6*1.0,
/

```

```
&XEDT
```

```

PRTC=99999,PPFC=50,DMPC=99999999,
DTPRT(1)=0.50,
DTPPF(1)=0.01,
PCGRP(1)= 5*1,
PCGRP(6)=17*1,
PPGRP(14)=1,
PPGRP(16)=1,
PPGRP(19)=1,
PPGRP(21)=1,
PPGRP(24)=1,
PPGRP(29)=1,
PPGRP(33)=1,
LPRGN(1) =1,1,1,1,1,1,1,1,1,1,
LPRGN(10)=1,1,0,1,1,1,
LPRGN(16)=1,
LPRGN(17)=1,
LPRGN(61)=1,1,1,1,1,1,1,1,1,1,
LPRGN(70)=1,1,0,1,1,1,
LPRGN(76)=1,
LPRGN(110)=1,
LPRGN(112)=1,
LPRGN(96)=6*1,
SN='ALPSK1','ALPSK2','ALPSK3','ALPSK4','ALPSK5','ALPSK6',
'ALPSK7','ALPSK8','ALPSK9','ALPLK1','ALPLK2','ALPLK3',
'ALPLK4','ALPLK5','ALPLK6','ALPGK','ALPINK',
'ALPNFK1','ALPNFK2','ALPNFK3','DHK',
'PK','PGMK1','PGMK2','PGMK3','PGMK4',
'RBSK1','RBSK2','RBSK3','RBSK4','RBSK5','RBSK6',
'RBSK7','RBSK8','RBSK9','RBSK10','RBSK11','RBSK12',

```

```
'RBLK1','RBLK2','RBLK3','RBLK4','RBLK5','RBLK6',  
'RBLK7','RBLK8','RBLK9','RBLK10','RBIK1','RBIK2',  
'RBGK1','RBGK2','RBGK3','RBGK4','RBGK5',  
'TSK1','TSK2','TSK3','TSK4','TSK5','TSK6',  
'TSK7','TSK8','TSK9','TIPINK',  
'TLK1','TLK2','TLK3','TLK4','TLK5','TLK6','TGK',  
'VK1','VK2','VK3','UK1','UK2','UK3',  
/  

```

```
&XSTR  
ACRMIN=0.0D+0,  
/  

```

```
&XSOS  
POW = 1.D8,  
DAX(1) = 7*1.0,  
DRAD(1)= 5*1.0,  
FRTP(1)= 0., 1., 0., 0., 0.,  
TIMAMP(1) = -1., 10.,  
AMPTAB(1) = 1., 1.,  
/  

```

Table H-3. Input data for FCI problem.

START : PROBLEM SIMPLE FCI TEST PROBLEM FOR S-III VER.3.A

```

&XCNTL
  HMTOPT(71)=1,2,1,1,0,1,
  HMTOPT(80)=1,3,1,
/

&XMSH
  IB=1,JB=3,
  DRINP(1)=0.05,
  DZINP(1)=0.05,0.20,0.10,
  NREG=3,
/

&XTME
  TWFIN=0.10,DTSTRT=1.0D-5,DTMIN=1.0D-8,DTMAX=2.0D-4,
  NDT0=1,TCPU=100000.0,
/

&XRGN
  LRGN=1,IIB=1,IUB=1,JLB=1,JUB=1,
  ALMINB(1)=0.200,TLMINB(1)=3500.0,
  ALMINB(3)=0.800,TLMINB(3)=1150.0,
  PSFINB=1.2D+05,
  RLM0IB(1)=0.001,RLM0IB(3)=0.001,RLM0IB(4)=0.0005,RGB0IB=0.002,
/

&XRGN
  LRGN=2,IIB=1,IUB=1,JLB=2,JUB=2,
  ALMINB(3)=1.000,TLMINB(3)=1000.0,
  PSFINB=1.2D+05,TGINB=1000.0,
  RLM0IB(1)=0.001,RLM0IB(3)=0.001,RLM0IB(4)=0.0005,RGB0IB=0.002,
/

&XRGN
  LRGN=3,IIB=1,IUB=1,JLB=3,JUB=3,
  ALMINB(3)=0.200,TLMINB(3)=1000.0,
  PG4INB=1.0D+05,TGINB=1000.0,
  RLM0IB(1)=0.001,RLM0IB(3)=0.001,RLM0IB(4)=0.0005,RGB0IB=0.002,
/

&XEDT
  PRTC=10000,PPFC=1,DMPC=999999,
  DTPPF(1)=0.1,
  PCGRP(6)=5*1,
  PCGRP(11)=3*1,
  PCGRP(14)=3*1,
  PCGRP(17)=3*1,
  PPGRP(11)=1,1,1,1,1,1,1,1,1,1,1,
  PPGRP(21)=1,1,1,1,1,1,1,1,1,1,1,
  PPGRP(31)=1,1,1,1,1,1,1,1,1,1,1,
  PRCEL(1,1)=2,1,1,1,3,
  NPAGE=20,
  SN='ALPLK1','ALPLK2','ALPLK3',
    'ALPLK4','ALPLK5','ALPLK6','ALPGK',
    'ALPNFK1','ALPNFK2','ALPNFK3','DHK',
    'PK','PGMK1','PGMK2','PGMK3','PGMK4',
    'RBLK1','RBLK2','RBLK3','RBLK4','RBLK5','RBLK6',
    'RBLK7','RBLK8','RBLK9','RBLK10','RBIK1','RBIK2',
    'RBGK1','RBGK2','RBGK3','RBGK4','RBGK5',
    'SIELK1','SIELK2','SIELK3','SIELK4','SIELK5','SIELK6',
    'TLK1','TLK2','TLK3','TLK4','TLK5','TLK6','TGK','SIEGK',
    'VK1','VK2','VK3','UK1','UK2','UK3',
/

```

Table H-4. Input data for STN problem.

START : SPACE-TIME NEUTRONICS PROBLEM FOR S-III VER.3.A

```

&XCNTL
  HMTOPT(31) =1,1,
  HMTOPT(61) =2,2,
/

  === S I M M E R -3 F L U I D D Y N A M I C S D A T A ===

&XMSH
  IB=12,JB=16,NREG=7,
  DZINP(1)=3*1.16667D-1, 10*9.30000D-2, 3*1.00000D-1,
  DRINP(1)=6.06940D-2, 9.98880D-2, 1.03978D-1, 7.33712D-2, 1.12190D-1,
      8.93418D-2, 9.42044D-2, 1.12157D-1, 1.10375D-1, 1.09204D-1,
      1.08390D-1, 9.84077D-2,
/

&XTME
  TWFIN=0.02,DTSTRT=1.0D-5,DTMIN=1.0D-6,DTMAX=1.0D-3,
  CYCFIN=20000,
  NDT0=1,TCPU=3600000000.0,
  DTHINI=1.0D-4,DTHMIN=1.0D-6,DTHMAX=1.0,
  IDTH=10,
/

&XBND
  NBC=0,
  LBCSET(1)=0,1,1,1,1,1,1,1,1,1,1,1,0,
      224*0,
      0,2,2,2,2,2,2,2,2,2,2,2,0,
/

&XBND
  NBC=1,LBCS=2,LBCP=2,LBCG=1,
  PTME(1)=0.0,1.0,
  PTAB(1)=0.12E6,0.12E6,
/

&XBND
  NBC=2, LBCS=2, LBCP=2,LBCG=1,
  PTME(1)=0.0,1.0,
  PTAB(1)=0.1E6,0.1E6,
/

&XEDT
  PRTC=100,PPFC=50,DMPC=999999,BSFC=10,
  DTPRT(1)=1.0D-1,TCPR(1)=1.0,
  DTDMP(1)=2.0D1,TCDMP(1)=1.0,
  PRCEL(1,1)=250*0,
  PRCEL(1,1)=1,1,5,
  PRCEL(1,2)=0,
  PCGRP(1)=50*0,
  PCGRP(1)=1,0,1,0,0,1,0,1,0,0,1,
  DTPPF(1)=5.0D-4,TCPPF(1)=1.0,
  PPGRP(1)=50*0,
  PPGRP(1)=1,0,0,0,0,0,0,0,0,0,0,
  PPGRP(11)=0,0,0,0,0,0,1,0,0,1,1,
  PPGRP(21)=1,0,0,1,0,0,0,0,1,1,
  PPGRP(31)=1,0,0,0,0,0,0,0,0,0,0,
  LPRGN(1)=200*0,
  NPAGE=8,
  SN(1)='ALPLK1','ALPLK2','ALPLK3','ALPLK4','ALPLK5','ALPLK6','ALPGK ',
  SN(8)='PK ','ALPSK1','ALPSK2','ALPSK3','ALPSK4','ALPSK5','ALPSK6 ',
  SN(15)='ALPSK7','ALPSK8','ALPSK9','TSK1 ','TSK2 ','TSK3 ','TSK4 ',
  SN(22)='TSK7 ','TSK8 ','TLK1 ','TLK2 ','TLK3 ','TLK4 ','TLK5 ',
  SN(29)='TLK6 ','TGK ','ALPINK','TIPINK','RBSK1 ','RBSK2 ','RBSK3 ',
  SN(36)='RBSK4 ','RBSK5 ','RBSK6 ','RBSK7 ','RBSK8 ','RBSK9 ','RBSK10 ',
  SN(43)='RBLK1 ','RBLK2 ','RBLK3 ','RBLK4 ','RBLK5 ','RBLK6 ','RBLK7 ',
  SN(50)='RBLK8 ','RBLK9 ','RBLK10','PGMK1 ','PGMK2 ','PGMK3 ','PGMK4 ',
  SN(57)='VK1 ','VK2 ','VK3 ','UK1 ','UK2 ','TSAT1 ','TSAT2 ',
  SN(64)='TSAT3 ','RBGK1 ','RBGK2 ','RBGK3 ','RBGK4 ','RBGK5 ','ALPGE ',
  SN(71)='RBIK1 ','RBIK2 ','ASMZ ','ALPNFK1','ALPNFK2','ALPNFK3','RBSK11 ',
/

```

```

&XMSC
OPTPIT=6,COURTN=0.2,
EPSP=1.0,
NITRF=150,EITRF=1.E-05,
/
&XIFA
RLMIN=5*1.D-3,RLMAX=5*1.0D-1,
RGBMIN=1.D-3,RGBMAX=1.0D-1,
ISRCBB(1)=1,ISRCDD(2)=1,
/
&XSTR
TL11G5=1.0D+20,TL12G5=1.0D+20,FL11G5=1.0D-20,FL12G5=1.0D-20,
/

<<< UPPER AXIAL BLANKET >>>
&XRGN
LRGN=1,
RGNAMB='UPPER AXIAL BLANKET',
ILB=2,IUB=9,JLB=14,JUB=16,
ALMINB(3)=4.1556D-1,
TLMINB(3)=1.15D+3,
ASMINB(1)=2.7928D-1,
ASMINB(4)=9.391D-2,4.695D-2,0.0D+0,4.696D-2,
TSINB(1)=1.3D+3,
TSINB(4)=5*1.3D+3,
TSINTB=1.3D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
TGINB=3.15D+3,
PG4INB=1.080D+5,
VINB=0.0D+0,0.0D+0,0.0D+0,
UINB=0.0D+0,0.0D+0,0.0D+0,
/

<<< CARTRIDGE >>>
&XRGN
LRGN=2,
RGNAMB='CARTRIDGE',
ILB=1,IUB=1,JLB=1,JUB=2,
ALMINB(3)=1.0D-2,
TLMINB(3)=1.15D+3,
ASMINB(5)=4.695D-2,0.0D+0,4.696D-2,
TSINB(5)=1.15D+3,1.15D+3,1.15D+3,1.15D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
PG4INB=1.080D+5,TGINB=3.15D+3,
UINB=0.0D+0,0.0D+0,0.0D+0,
VINB=1.0D+2,1.0D+2,1.0D+2,
/

<<< FUEL BULLET >>>
&XRGN
LRGN=3,
RGNAMB='FUEL BULLET',
ILB=1,IUB=1,JLB=3,JUB=3,
ALMINB(1)=5.6145D-1,0.0D+0,1.0D-2,
TLMINB(1)=4.45D+3,0.0D+0,1.15D+3,
ASMINB(5)=4.695D-2,0.0D+0,4.696D-2,
TSINB(5)=1.15D+3,1.15D+3,1.15D+3,1.15D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
PG4INB=1.080D+5,TGINB=3.15D+3,
XENRIB(1)=6*0.83,
UINB=0.0D+0,0.0D+0,0.0D+0,
VINB=1.0D+2,1.0D+2,1.0D+2,
/

<<< BURREL >>>
&XRGN
LRGN=4,
RGNAMB='BURREL',
ILB=1,IUB=1,JLB=4,JUB=16,
ALMINB(3)=1.0D-2,

```

```

TLMINB(3)=1.15D+3,
ASMINB(5)=4.695D-2,0.0D+0,4.696D-2,
TSINB(5)=1.15D+3,1.15D+3,1.15D+3,1.15D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
PG4INB=1.080D+5,TGINB=3.15D+3,
UINB=0.0D+0,0.0D+0,0.0D+0,
VINB=1.0D+2,1.0D+2,1.0D+2,
/

```

```
<<< ANNULAR CORE >>>
```

```
&XRGN
```

```

LRGN=5,
RGNAMB='ANNULAR CORE',
ILB=2,IUB=9,JLB=4,JUB=13,
ALMINB(3)=3.85492D-1,
TLMINB(3)=1.15D+3,
ASMINB(1)=3.06869D-1,
ASMINB(4)=9.39D-2,4.695D-2,0.0D+0,4.696D-2,
TSINB(1)=1.3D+3,
TSINB(4)=1.15D+3,1.15D+3,1.15D+3,1.15D+3,1.15D+3,
TSINTB=1.3D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
XENRIB(1)=6*0.2275D0,
TGINB=3.15D+3,
PG4INB=1.080D+5,
VINB=0.0D+0,0.0D+0,0.0D+0,
UINB=0.0D+0,0.0D+0,0.0D+0,
/

```

```
<<< LOWER AXIAL BLANKET >>>
```

```
&XRGN
```

```

RGNAMB='LOWER AXIAL BLANKET',
LRGN=6,
ILB=2,IUB=9,JLB=1,JUB=3,
ALMINB(3)=4.15559D-1,
TLMINB(3)=1.15D+3,
ASMINB(1)=2.775422D-1,
ASMINB(4)=9.39D-2,4.695D-2,0.0D+0,4.696D-2,
TSINB(1)=1.15D+3,
TSINB(4)=1.15D+3,1.15D+3,1.15D+3,1.15D+3,1.15D+3,
TSINTB=1.15D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
PG4INB=1.080D+5,TGINB=3.15D+3,
VINB=0.0D+0,0.0D+0,0.0D+0,
UINB=0.0D+0,0.0D+0,0.0D+0,
/

```

```
<<< RADIAL BLANKET >>>
```

```
&XRGN
```

```

LRGN=7,
RGNAMB='RADIAL BLANKET',
ILB=10,IUB=12,JLB=1,JUB=16,
ALMINB(3)=7.625D-1,
TLMINB(3)=1.15D+3,
ASMINB(1)=4.5977D-3,
ASMINB(4)=9.19D-2,4.595D-2,0.0D+0,4.596D-2,
TSINB(1)=1.0D+3,
TSINB(4)=8.0D+2,8.0D+2,8.0D+2,8.0D+2,8.0D+2,
TSINTB=1.0D+3,
PSAINB=2.67D2,ALCWIB=1.0D0,ARCWIB=1.0D0,RPINIB=3.0D-3,
PG4INB=1.080D+5,TGINB=3.15D+3,
VINB=0.0D+0,0.0D+0,0.0D+0,
UINB=0.0D+0,0.0D+0,0.0D+0,
/

```

```
&XEOS
```

```

ALPHA0=0.0001,EPSTG=1.D-04,
TGMIN=300.0,
BETA(1,1)=1.50000E-01,
BETA(1,2)=1.50000E-01,
BETA(1,3)=1.50000E-01,

```

```

BETA(1,4)=1.50000E-01,
/

===SIMMER-3 NEUTRONICS DATA===

<<< NEUTRONICS OPTION FLAG >>>
&NCNTL
NIOPT(100)=1,
/

<<< NEUTRONICS MESH DATA AND CONTROL >>>
&NPAR
IT=30,JT=40,NREGB=1,12,1,16,
NCRAD=2,2*3,2,4*3,4*2, NCAXI=3,2*4,10*2,3*3,
IGM=18, NDKGRP=0,
IXSREG(1,1)=1,IXSREG(2,1)=30,IXSREG(3,1)=1,IXSREG(4,1)=40,
NFRAD(1,1)=7,3, NFRAD(1,2)=2,3,5,
NFAXI(1,2)=2,2,3,2, NFAXI(1,3)=1,3,2,1, NFAXI(1,4)=3,7,
IDIVR=1,
/

<<< EDIT CONTROLS >>>
&NEDT
IEDXST=1, IEDSFT=1, INVPRT=1, INVREG=6,
IRGBND(1,1)=1,IRGBND(2,1)=2,IRGBND(3,1)=8,IRGBND(4,1)=11,
IRGBND(1,2)=1,IRGBND(2,2)=2,IRGBND(3,2)=12,IRGBND(4,2)=40,
IRGBND(1,3)=3,IRGBND(2,3)=24,IRGBND(3,3)=1,IRGBND(4,3)=11,
IRGBND(1,4)=3,IRGBND(2,4)=24,IRGBND(3,4)=12,IRGBND(4,4)=31,
IRGBND(1,5)=3,IRGBND(2,5)=24,IRGBND(3,5)=32,IRGBND(4,5)=40,
IRGBND(1,6)=25,IRGBND(2,6)=30,IRGBND(3,6)=1,IRGBND(4,6)=40,
/

<<< INITIAL CONDITIONS >>>
&NINI
POWER=9.00000D+08,

DECAY(1)=1.290D-02, 3.110D-02, 1.340D-01, 3.310D-01,
1.260D+00, 3.210D+00

BETAD(1)= 8.85063E-05, 8.75324E-04, 7.55629E-04, 1.50649E-03,
6.93011E-04, 1.85063E-04,
DSPECT(1,1) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,2) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,3) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,4) = 0.00000E+00, 6.68590E-03, 4.95520E-03, 1.26630E-02,
8.36640E-03, 1.47280E-02,
DSPECT(1,5) = 5.31570E-03, 1.34939E-01, 6.80800E-02, 1.11298E-01,
6.85230E-02, 7.48210E-02,
DSPECT(1,6) = 1.58609E-01, 4.57160E-01, 3.89470E-01, 3.71631E-01,
3.42475E-01, 4.22890E-01,
DSPECT(1,7) = 4.16740E-01, 2.86778E-01, 3.34028E-01, 3.00795E-01,
3.01489E-01, 2.98223E-01,
DSPECT(1,8) = 3.83051E-01, 1.12014E-01, 1.84462E-01, 1.74638E-01,
2.76471E-01, 1.83388E-01,
DSPECT(1,9) = 3.62860E-02, 2.41990E-03, 1.90043E-02, 2.89642E-02,
2.68721E-03, 5.95510E-03,
DSPECT(1,10) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,11) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,12) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,13) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,14) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,15) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,

```

```

DSPECT(1,16) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,17) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
DSPECT(1,18) = 0.00000E+00, 0.00000E+00, 0.00000E+00, 0.00000E+00,
0.00000E+00, 0.00000E+00,
/

```

<<< QUASI-STATIC DATA >>>

```

&NQUS
IWTF=0,
DTSH=1.0D-4,DTSMAX=1.0D-2,
EPS4=2.00000D-02,EPS5=5.00000D-01,
EPS7=2.00000D+00,EPS8=1.00000D+06,EPS9=5.00000D-01,
EPS10=1.00000D-02,EPS17=8.51600D-02,EPS18=1.00000D+02,
EPSG=1.00000D-03,EPSPHY=1.00000D-05,
/

```

<<< CONVERGENCE PRECISION >>>

```

&NCNV
ITLMOU=70,ITLMIN=10,
EPSO=1.00000D-03,EPSP=1.00000D-04,EPSFAC=1.50000D+01,
EPSMIN=1.00000D-06,ERRFXU=1.00000D-06,
/

```

<<< SHIELDING FACTER RELATED DATA >>>

```

&NSHL
ITLMBG=10, EPSBKG=1.00D-03,
/

```

<<< ISOTOPIC DATA >>>

```

&NISO
ISOTOP='FERT','FISS','STEEL','COOL','CONT','FISS',
NCMIX(1,1)=1,NCMIX(2,1)=2,NCMIX(3,1)=3,NCMIX(4,1)=4,NCMIX(5,1)=5,
THDENS(1)=9.805D+3,THDENS(2)=9.805D+3,THDENS(3)=7.256D+03,
THDENS(4)=7.776D+02,THDENS(5)=2.520D+03,
LNMN(1)=1,LNMN(2)=1,LNMN(3)=1,LNMN(4)=1,LNMN(5)=1,
LMC(1,1)=1,LMC(1,2)=2,LMC(1,3)=3,LMC(1,4)=4,LMC(1,5)=5,
AVDENS(1,1)=6.50946E+00,
AVDENS(1,2)=6.47066E+00,
AVDENS(1,3)=7.79209E+00,
AVDENS(1,4)=2.03691E+00,
AVDENS(1,5)=1.41569E+01,
/

```

APPENDIX I

POSTPROCESSOR BFSCAN

The bfscan program is a postprocessor aiming at grasping a quick look at the SIMMER-III result immediately. Since the first priority of bfscan is a quick response, bfscan uses only the character-based user interface. In order to improve the speed of response, bfscan stores all the contents of a post-processing file (SIMBF) in memory. Therefore, the maximum number of the time steps depends on the size of work array in bfscan, the number of the meshes and variables in the post-processing file. Although bfscan does not use graphic drivers, it not only displays values of the variables, but also plots the time transients, radial and axial distribution and contours of variables using character-based, pseudo-graphics. This program also has an interface to postscript format, and thus the plotted results can be displayed or printed with smooth lines. The simple description on the usage of bfscan is documented in the following.

1. NAME

bfscan

2. SYNOPSIS

bfscan [-t] [file1 file2 . . .]

3. FLAGS

-t bfscan will display a prompt “tstart, tstep, tend =” and then a user enters the first time, time interval, and the final time to read the post-processing file. This option is useful to process only a part of a very large post-processing file.

4. PARAMETERS

[file1 file2 . . .] Specifies the names of post-processing files to be read. Default is “SIMBF”. The brackets [] means that the parameters in this brackets can be omitted.

5. USAGE

Bfscan displays the prompting message “ENTER COMMAND >” after displaying information from the post-processing file. The user can control bfscan by typing the commands following this message. Several commands can be input on the same line at once using the delimiter “;”.

(1) mode

Bfscan has two display modes: “numerical display mode” and “plotting mode”. These two display modes are invoked by typing “**disp**” and “**plot**” command, respectively. In the “numerical display mode”, bfscan displays the value of the variables in a specified format on the screen. In the “plotting mode”, bfscan displays the graphs of the variables using character based pseudo graphics.

Bfscan also has two working modes: “time mode” and “space mode”. These two working modes are invoked by typing “**time**” and “**space**” command, respectively. The “time mode” is used to display and plot the time transient of the variables. The “space mode” is used to display the spatial distribution of the variables. The “space” mode is subdivided into three axis modes, namely “x-axis”, “z-axis” and “contour” mode. These modes are invoked by typing “**radial**”, “**axial**” and “**contour**” command, respectively. If one of these commands is used, the working mode is changed to the “space mode” automatically.

(2) cell address

The commands “**i**” and “**j**” are also used to specify the cell address where the variables are displayed and plotted. The synopsis of these commands is as follows.

i I1 [I2]

j J1 [J2]

I1, I2, J1 and J2 are the location of the left most, right-most, lower-most and top-most side of the region.

(3) variable name

v [V1, V2, V3 . . .]

specifies the name of variables (V1, V2 and V3...). If only command “**v**” is input, the list of variable names will appear in the display.

(4) time

The time is specified by the following commands.

“**t**” [TIME] where TIME is the time (s) when the variables are displayed.

“**f**” and “**b**” command advances and puts back the time step, respectively.

(5) plotting

plot [N] where N is the number of the variables plotted in a graph.

(6) scale

The scaling of the graph is specified by the following commands.

x [XMIN XMAX | auto] and **y** [YMIN YMAX | auto] , where XMIN and XMAX are the minimum and maximum value for x axis and YMIN and YMAX are the minimum and maximum value for y axis. The parameter “auto” means the auto-scaling.

(7) number of columns

The number of columns and rows of the variable table is specified by

nx NX and **ny** [NY] , where NX and NY are the number of columns and rows. The default values are NX=5 and NY=30.

(8) file output

The command “**psyche**” saves the value of the variables to a file. The number and format of the variables depends on the displaying mode and working mode. In “time mode”, the first column is the time and the remaining columns are the variables. In “space mode”, the first column is the location and the remaining columns are the variables.

(9) printing

The command “**print**” sends the same text displayed in the display to the printer. The synopsis is as follows;

print [printer_queue]: where printer_queue is the queue name of the printer in your system.

(10) postscript interface

Bfscan provides the interface to postscript format. The following commands are used to print and display the graphs with postscript printer or postscript browser.

psprt [printer_queue]: prints the same graph in the display with postscript printer.

psprt2 : Two graphs will be printed in one page. This command specifies the first graph and store the information in a working file.

psprt22 [printer_queue]: Two graphs will be printed in one page. This command specifies the second graph and invokes the actual printing.

psfile: output the plot with PostScript file.

epsfile: output the plot with Encapsulated PostScript file.

gv or **gs:** The graphs will be displayed on the screen using **gv** (GhostView command) or **gs** (GhostScript) command. These commands are only available if these utilities are installed in your system.

psenv: Bfscan displays several prompts to modify the size and location of graphs, the title of the graph, etc.

psanim [tstart tend tstep] [printer_queue] : print the graphs with postscript from tstart to tend by tstep.

ipt [M]: specifies the horizontal figure number M in each paper for psprt2(psanim) mode.

jpt [N]: specifies the perpendicular figure number N in each paper for psprt2(psanim) mode.

pscale [horizontal size [vertical size]] : specifies the size of graph.

porign [x [y]] : specifies the location of the origin of the file.

ytitle [y-axis name] : specifies the title of the y-axis.

mtitle [main title] : specifies the main title.

mf [main title size (cm)] : specifies the size of main title (default value: 0.5cm).

6. INSTALLATION

(1) buffer memory size

The parameter MNB in param.h is the size of the buffer memory in which all the information from the postprocessing file is stored. This parameter must be determined carefully depending on the size of the memory in your computer and postprocessing file.

(2) system dependent routines

The system dependent routine fdate_ (NOW) is used in bfscan, where NOW is a 36 bytes character variable. This routine returns the current date in NOW(12:13), hour in NOW(15:16) and minute in NOW(18:19). This routine is used to generate a unique file name to output the information from bfscan. The routine fdate_(NOW) is used in subroutines “frame_pst.f”, “psfile.f”, “epsfile.f”, “psy_file.f” and “txtfile.f”.

The system dependent routine is “system”. This routine is rather general and may be installed in your system but essential for bfscan to execute. This routine executes the UNIX commands given through its argument.

(3) output utilities

The Unix commands “lpr”, “enscript”, and “more” are used in bfscan. If you intend to display the graphs with postscript on your display, you need install Unix utility “gs (GhostScript)” or “gv (GhostView)” into your system.

(4) help file

Bfscan provides a simple on-line help. In order to activate this function, you must put the help file “man/bfscan.hlp” in your system and modify the path name in the subroutine “interpret.f”.

7. EXAMPLE

The following command

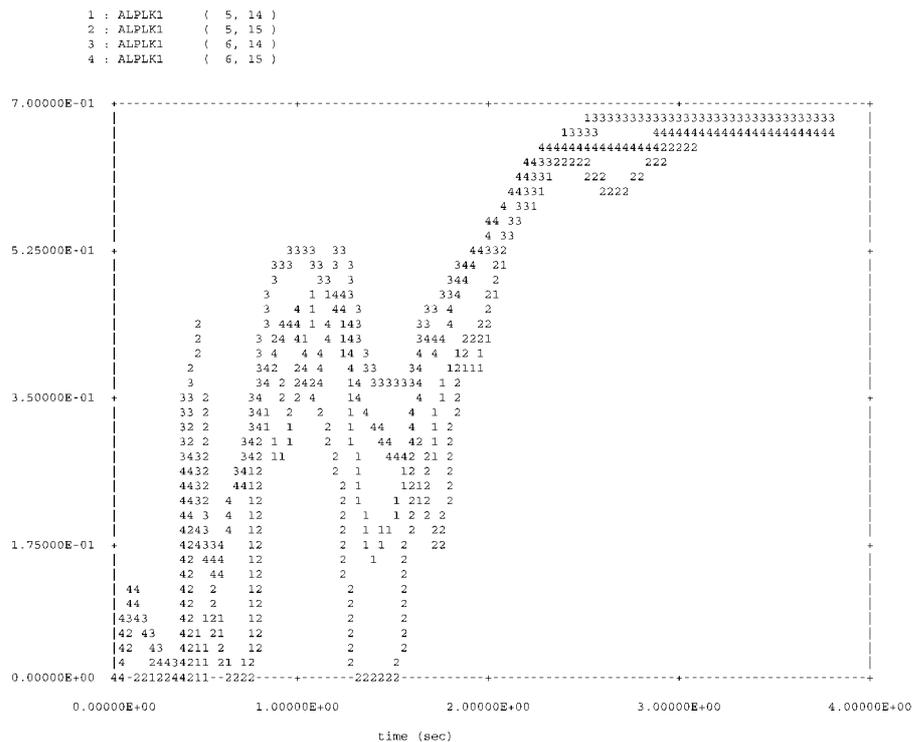
ENTER COMMAND > **time;disp; ik; i 5 6; j 14 15 ;v ALPLK1**

results in the following table.

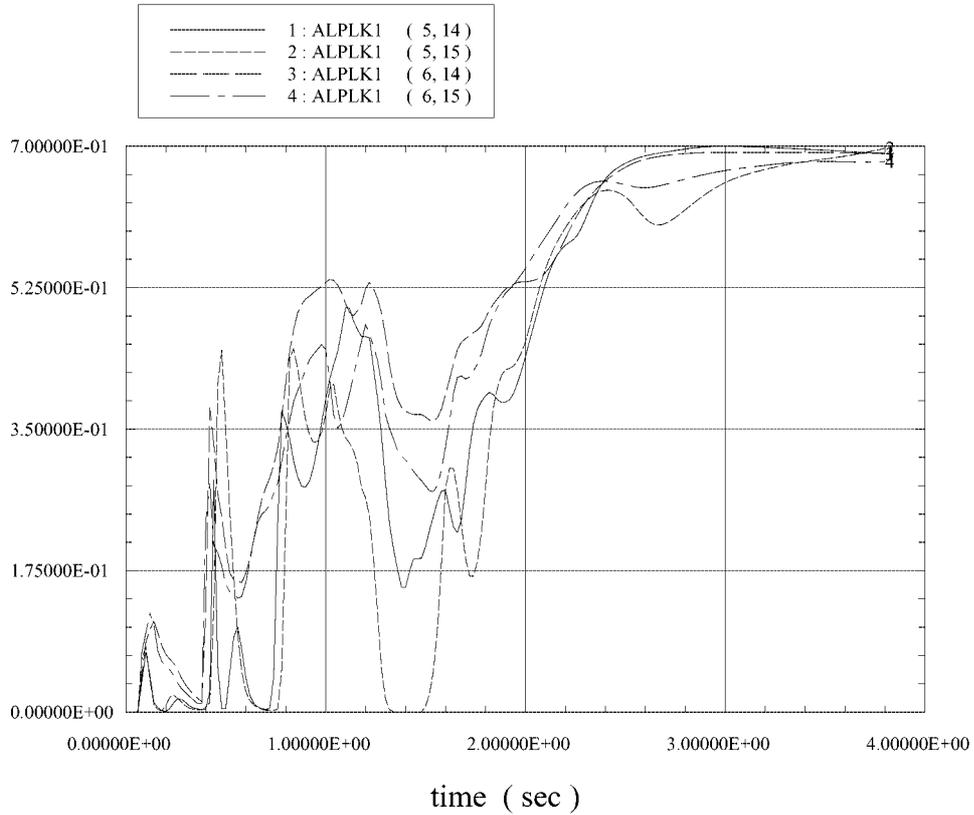
TIME	ALPLK1 (5, 14)	ALPLK1 (5, 15)	ALPLK1 (6, 14)	ALPLK1 (6, 15)
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2.01524E-02	5.67145E-08	1.53373E-07	3.66895E-07	8.80669E-07
4.01200E-02	1.41471E-08	1.19391E-07	7.45932E-07	1.58870E-06
6.01200E-02	8.30902E-07	2.99125E-04	2.30771E-06	6.92858E-04
8.01200E-02	3.83024E-02	6.58103E-02	4.74317E-02	7.43889E-02
1.00120E-01	7.43258E-02	8.02179E-02	8.71633E-02	9.81804E-02
1.20120E-01	4.59532E-02	4.07787E-02	1.01584E-01	1.22152E-01
1.40068E-01	1.22321E-02	9.30354E-03	1.12523E-01	1.08077E-01
1.60068E-01	5.56516E-03	3.27428E-03	9.82165E-02	7.59971E-02
1.80068E-01	1.80821E-03	1.58738E-03	8.20831E-02	6.27149E-02
2.00068E-01	7.86609E-04	7.91638E-03	7.15769E-02	5.68924E-02
2.20023E-01	4.46940E-03	1.84746E-02	6.55529E-02	5.23156E-02
2.40108E-01	1.16553E-02	2.07534E-02	6.02524E-02	4.54057E-02
2.60054E-01	1.64169E-02	1.69472E-02	5.18828E-02	3.58316E-02
2.80054E-01	1.57422E-02	1.21104E-02	4.15170E-02	2.87433E-02
3.00054E-01	1.18414E-02	7.67550E-03	3.34530E-02	2.38727E-02
3.20129E-01	7.58068E-03	4.69201E-03	2.72084E-02	1.93014E-02
3.40043E-01	4.88124E-03	3.34525E-03	2.17699E-02	1.47575E-02
3.60184E-01	3.70868E-03	2.91963E-03	1.69301E-02	1.05169E-02
3.80184E-01	3.42609E-03	2.85345E-03	1.31282E-02	1.07640E-02
4.00184E-01	3.58206E-03	5.63966E-03	1.27546E-01	2.36122E-01
4.20184E-01	2.55109E-02	1.17579E-02	3.76777E-01	2.82595E-01
4.40050E-01	2.87430E-01	1.26811E-01	3.32153E-01	2.06120E-01
4.60050E-01	5.64574E-02	4.06064E-01	2.69766E-01	1.97131E-01
4.80050E-01	4.08212E-03	4.47737E-01	2.41634E-01	1.81246E-01
5.00050E-01	4.37089E-03	3.49608E-01	2.02161E-01	1.58231E-01
5.20050E-01	4.87612E-02	2.48663E-01	1.72442E-01	1.48899E-01
5.40050E-01	9.26092E-02	1.67135E-01	1.63919E-01	1.46580E-01
5.60050E-01	1.05251E-01	9.60099E-02	1.61530E-01	1.40880E-01
5.80050E-01	7.81253E-02	5.04181E-02	1.60224E-01	1.42901E-01

ENTER COMMAND > **time;plot 4; ik; i 5 6; j 14 15 ;v ALPLK1**

displays the following graph.



This graph can be displayed using postscript browser by typing
 ENTER COMMAND > **gv (or gs)**
 which results in the following graph.



The “space mode” works as follows. The commands

ENTER COMMAND > **space;disp; i 5 11; j 12 18;v ALPGK**
 output the following table.

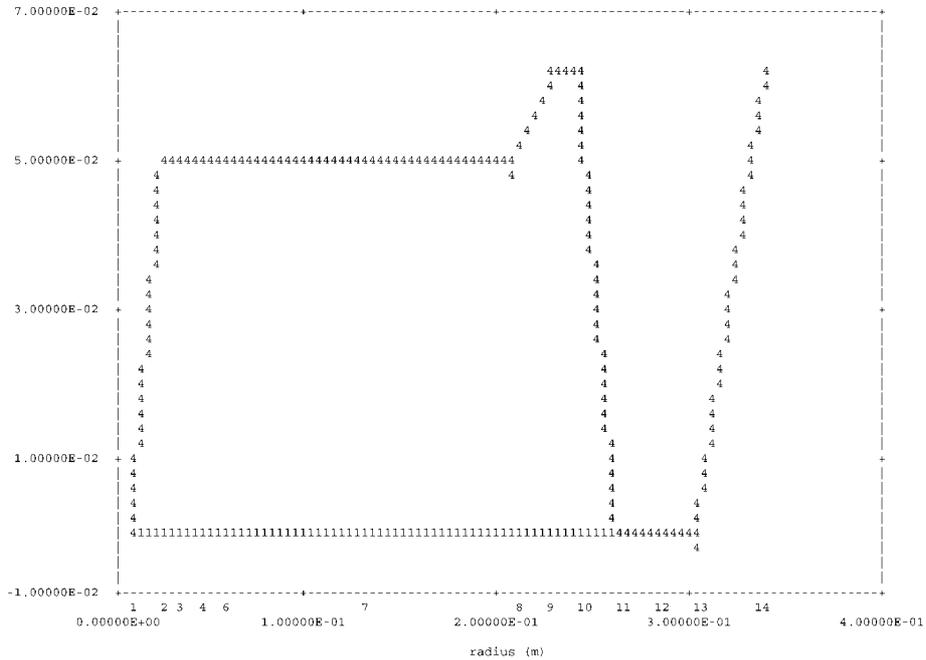
```
variable =ALPGK      time = 0.00000E+00  cycle = 0
J  I      5      6      7      8      9      10      11
18| 1.00000E+00 1.00000E+00 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
17| 1.00000E+00 1.00000E+00 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
16| 1.00000E+00 1.00000E+00 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
15| 1.00000E+00 1.00000E+00 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
14| 1.00000E+00 1.00000E+00 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
13| 1.00000E+00 1.00000E+00 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
12| 5.13929E-02 5.13929E-02 5.13929E-02 5.13929E-02 6.32929E-02 6.32929E-02 -1.00000E-20
```

ENTER COMMAND > **i 1 14;j 6 9;radial**
 plots the radial (x-axis) distribution as follows.

```

1 : ALPGK ( 1- 14, 6)
2 : ALPGK ( 1- 14, 7)
3 : ALPGK ( 1- 14, 8)
4 : ALPGK ( 1- 14, 9)
    
```

TIME = 0.00000E+00 (sec) CYCLE = 0



The contour plotting is also possible.
ENTER COMMAND > j 1 38;contour

ALPGK(1- 14, 1- 38) TIME = 0.00000E+00

