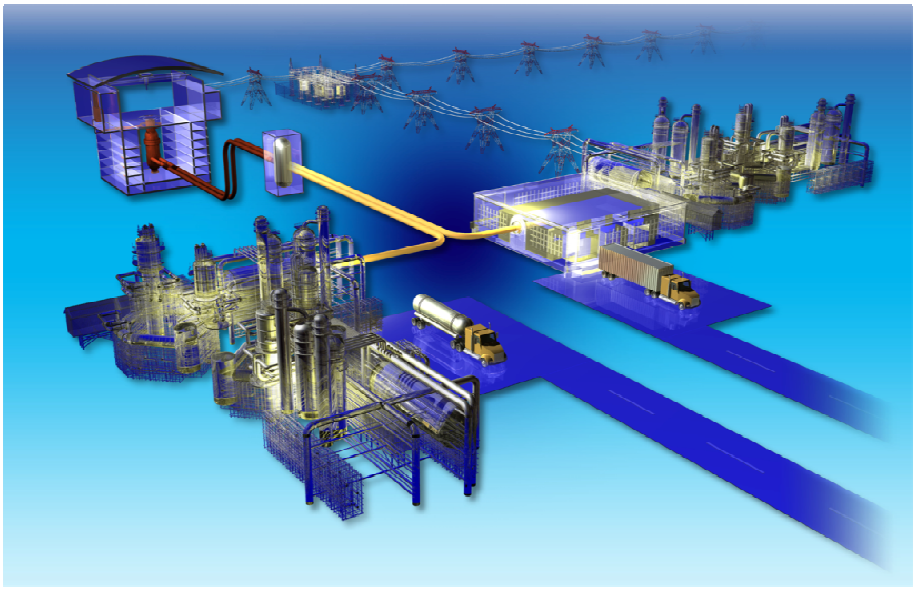
INL/EXT-10-18317

PARFUME User's Guide

September 2010



The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance

Idaho National Laboratory

INL/EXT-10-18317

PARFUME User's Guide

PARFUME Development Team

September 2010

Idaho National Laboratory
Next Generation Nuclear Plant Project
Idaho Falls, Idaho 83415

Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Next Generation Nuclear Plant Project

PARFUME User's Guide

INL/EXT-10-18317

September 2010

Approved by:

John D. Maki	9/14/10
J. T. Maki Principal Investigator	Date
Hers D Gougar	9/14/10
H. D. Gougar VHTR TDO Deputy Technical Director	Date
David Petti	9/14/10
D. A. Petti VHTR TDO Technical Director	Date
Gary D Roberts	9/14/2010
G. D. Roberts Quality Assurance	Date

ABSTRACT

PARFUME, a fuel performance analysis and modeling code, is being developed at Idaho National Laboratory (INL) for evaluating gas-reactor coated particle fuel for prismatic, pebble bed, and plate type fuel geometries. The code is an integrated mechanistic analysis tool that evaluates the thermal, mechanical, and physico-chemical behavior of (tri-isotropic [TRISO]) coated fuel particles and the probability for fuel failure given the particle-to-particle statistical variations in physical dimensions and material properties that arise during the fuel fabrication process. Using a robust finite difference numerical scheme, PARFUME is capable of performing steady-state and transient heat transfer and fission-product diffusion analyses for the fuel. Written in FORTRAN 77, PARFUME compiles in FORTRAN 90 and is easy to read, maintain, and modify. Currently, PARFUME is supported only on Linux platforms.

This document represents the initial version of the PARFUME User's Guide. The PARFUME Theory and Model Basis Report describes the theoretical aspects of the code. User information is provided, including: (1) code development, (2) capabilities and limitations, (3) installation and execution, (4) user input and output, (5) error messages, and (6) a sample problem.

CONTENTS

FIGURES

TABLES

ACRONYMS

AIAA	American Institute of Aeronautics and Astronautics
ANSI	American National Standards Institute
ATR	Advanced Test Reactor
BAF	Bacon Anisotropy Factor
BISO	bistructrual-isotropic
CAE	computer-aided engineering
CFP	coated fuel particle
CO	carbon monoxide
dtf	designed to fail
EPRI	Electric Power Research Institute
FALCON	Fuel Performance Analysis Capability
FIMA	fission per initial metallic atom
FP	fission product
FZJ	Forschungszentrum Juelich
INL	Idaho National Laboratory
IPyC	inner pyrolytic carbon
JAERI	Japan Atomic Energy Research Institute
OECD	Organization for Economic Cooperation and Development
NP-MHTGR	New Production Modular High-temperature Gas-cooled Reactor
OPyC	outer pyrolytic carbon
PARFUME	PARticle FUel ModEl
PIE	post-irradiation examination
PNNL	Pacific Northwest National Laboratory
PyC	pyrolytic carbon
R/B	release-to-birth
SiC	silicon carbide
TDO	Technology Development Office
TRISO	tristructural-isotropic
UCO	uranium carbide
UO_2	uranium oxide
VHTR	Very High Temperature Reactor

NOMENCLATURE

ε	Strain ($\mu m/\mu m$)
t	Time (s) or neutron fluence (10^{25} n/m^2, E>0.18 MeV)
E	Modulus of elasticity of a coating layer (MPa)
c	Irradiation-induced creep coefficient of a pyrocarbon layer (MPa n/m^2)$^{-1}$
σ	Stress (MPa)
μ	Poisson's ratio of a coating layer; also, mean value for a parameter having a Gaussian statistical distribution
ν	Poisson's ratio in creep for a pyrocarbon layer; also, a design parameter that varies statistically from particle to particle
ρ	Density (kg/m^3)
c_p	Specific heat capacity (J/kg-K)
k	Thermal conductivity (W/m-K)
$\dot{q}$	Volumetric heat generation rate (W/m^3)
T	Temperature (K)
C	Concentration of atoms (atoms/m^3)
Q'	Heat transport coefficient or Ludwig-Soret coefficient (dimensionless)
R	Universal gas constant (J/mol-K)
J	Diffusive atom flux (atoms/m^2-s)
D	Atom diffusivity (m^2/s)
S	Swelling strain rate (n/m^2)$^{-1}$ or source (production rate) of atoms (atoms/m^3-s)
$\overline{S}$	Average swelling strain rate over a time increment (n/m^2)$^{-1}$
U	Radial displacement (m)
r	Radial coordinate (m)
x	Distance (m)
P	Radial stress (or pressure) acting on the inner surface of a coating layer (MPa)
q	Radial stress (or pressure) acting on the outer surface of a coating layer (MPa)
α	Thermal expansion coefficient of a coating layer (K^{-1}); also, thermal diffusivity (m^2/s)
$\overline{\alpha}$	Average thermal expansion coefficient over a time increment (K^{-1})
$\dot{T}$	Rate of change in temperature [K- (10^{25}n/m^2)$^{-1}$]
$f(\Delta\nu)$	Function that describes the variation of maximum stress in the SiC layer of a cracked particle with parameter ν
$g(\Delta\nu)$	Function that describes the variation of maximum stress in the SiC layer of an uncracked particle with parameter ν
$h(\Delta\nu)$	Ratio $f(\Delta\nu)/g(\Delta\nu)$

I	Normalized integration of the stress distribution over the volume of a coating layer (m^3)
m	Weibull modulus for a coating layer
P_f	Probability of failure for a coating layer
V	Volume of a coating layer (m^3)
σ	Stress in a coating layer (MPa)
σ_c	Maximum principal stress in the volume of a coating layer (MPa)
σ_u	Stress in a coating layer for a normal spherical particle (MPa)
$\sigma_{c\bar{v}}$	Stress in the SiC layer for a multidimensional particle having all parameters set at mean values for a particle batch (MPa)
$\sigma_{u\bar{v}}$	Stress in the SiC layer for an intact spherical particle having all parameters set at mean values for a particle batch (MPa)
σ_o	Weibull characteristic strength for a coating layer (MPa-$m^{3/m}$)
σ_{ms}	Effective Weibull mean strength for a coating layer (MPa)
σ_i	i = 1,2,3, Principal stress components in three orthogonal directions (MPa)
$\Delta\nu$	Variation in parameter ν from its mean value
λ	Strength for a coating layer in a random particle as sampled from a Gaussian distribution (MPa)
λ_s	Mean strength for a coating layer having a Gaussian strength distribution (MPa)
θ	Latitude angle (radians)
ϕ	Azimuth angle (radians)

Subscripts

r	radial
t	tangential
I	IPyC layer
S	SiC layer
O	OPyC layer
a	inner surface of a coating layer
b	outer surface of a coating layer
B	buffer
k	kernel

PARFUME User's Guide

1. INTRODUCTION

PARFUME, the "PARticle FUel ModEl," is being developed as an advanced gas-cooled reactor fuel performance modeling and analysis code. This guide provides information for PARFUME Version 2.19 users, including: (1) background information, (2) capabilities and limitations, (3) installation and execution, (4) user input and output, (5) error messages, and (6) a sample problem. This document represents the initial version of the PARFUME User's Guide. The PARFUME Theory and Model Basis Report[1] describes the theoretical aspects of the code.

1.1 Background

1.1.1 Historical Development

Initial development of the coated fuel particle and its inventor, Roy Huddle, can be traced back to the Organization for Economic Cooperation and Development's (OECD's) Dragon high-temperature experimental reactor, which operated successfully from 1964 to 1975.[2] Since then, several countries have constructed gas reactors using coated fuel particles. The coated particles, composed of either pyrolytic carbon (PyC) alone (bistructural isotropic, or BISO) with two coated layers, or silicon carbide (SiC) and PyC (tri-structual isotropic, or TRISO) consisting of three coated layers, were manufactured using high-temperature chemical vapor deposition in a fluidized bed. Dragon was the first reactor to use TRISO particles, while Peach Bottom (Unit 1), a commercial power gas reactor built by the United States, was fueled with cylindrical fuel elements containing BISO particles. Eventually, the U.S. and the international community focused research efforts on TRISO fuel particles, primarily due to their performance history and reliability.

Idaho National Laboratory (INL) began development of gas reactor fuel performance codes in the early 1990s with the release of the FUEL computer code. In early 2000, the Generation IV International Forum identified several reactor technology concepts for future generation nuclear energy systems; included in the technology concepts were advanced gas reactors such as the Very High Temperature Reactor (VHTR). Consequently, a need for state-of-the-art gas reactor fuel performance codes was re-established, and development of PARFUME, the successor to the FUEL code, began.

1.1.1.1 Fuel Performance Codes

Over the years, several fuel performance analysis tools (i.e., codes), including "pellet fuel rod codes" and "fuel particle codes," have been developed. A few of the "single fuel rod" codes (i.e., non-particle) include: FRAPCON, a 1D code originally developed as a combined effort of INL and Pacific Northwest National Laboratory (PNNL), who currently oversees the development of this code; Fuel Performance Analysis Capability (FALCON), a propriety 2D code developed by the Electric Power Research Institute (EPRI); and TOUTATIS and ALCYONE, both 3D French codes being developed under the PLEIADES software environment.[3]

Prominent fuel-particle analysis codes that are in use today or are under development include: STRESS3 (UK), PANAMA (Forschungszentrum Juelich [FZJ], Germany), ATLAS (Commissariat à l'Energie Atomique [CEA], France), TIMCOAT (Massachusetts Institute of Technology [MIT], U.S.), COPA (Korea), PARFUME (INL, U.S.), and a fuel performance code developed by the Japan Atomic Energy Research Institute (JAERI).[4,5] Although most of the fuel particle codes have unique capabilities and limitations, PARFUME is recognized for its computational efficiency, closed-form stress/displacement analytical solution method, and dual-solution scheme (i.e., Monte Carlo and numerical integration) for computing failure probability.

1.1.2 Fuel Particle Description

The coating layers of a TRISO fuel particle, which surround the fuel kernel and buffer, consist of an inner pyrolytic carbon (IPyC) layer, a SiC layer, and an outer pyrocarbon (OPyC) layer. The fuel kernel is typically comprised of uranium dioxide (UO_2), although uranium oxycarbide (UCO) is under development in the United States.[6] Fuel particle diameters are on the order of 0.9 mm. A typical TRISO-coated particle is shown in Figures 1-1 and 1-2.

Coated particle fuel exhibits statistical variations in physical dimensions and material properties from particle to particle due to the nature of its fabrication process.[7] Its behavior is also inherently multidimensional, further complicating fuel particle analysis. The objective in developing PARFUME is to physically describe both the mechanical and physico-chemical behavior of the fuel particle under irradiation, while capturing the statistical nature of the fuel.

Several mechanisms have been identified that can potentially lead to particle failure, including cracking of the IPyC during irradiation, debonding of the IPyC from the SiC layer during irradiation, buildup of internal fission gas pressure, kernel/SiC interaction resulting from the amoeba effect, and thinning of the SiC layer due to fission-product/SiC interactions. The details of these phenomena and related models are explained in References 1 and 8.

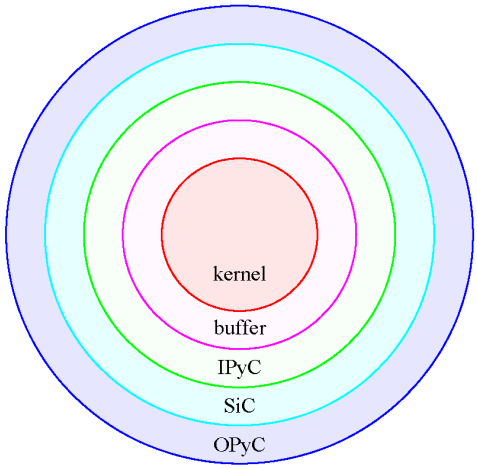


Figure 1-1. Typical TRISO-coated fuel particle geometry.

1.1.3 Basic Fuel Particle Behavior

As fuel particles undergo irradiation and temperature changes, fission gas pressure builds up in the kernel and buffer regions, while the IPyC, SiC, and OPyC act as structural layers to retain this pressure and act as a barrier to the migration of fission products (FPs). The irradiation effect on the fuel particles is shown in Figure 1-2, which shows two different particles before and after irradiation. Several phenomena result in changes to the fuel particle. The IPyC and OPyC layers both shrink and creep due to irradiation of the particle, while the SiC response is essentially limited to elastic behavior. The pressure generally increases as irradiation of the particle progresses, thereby contributing to a tensile hoop stress in the SiC layer. Failure of the particle is expected to occur if the stress in the SiC layer reaches the fracture strength of the SiC. Failure of the SiC results in an instantaneous release of elastic energy that should be sufficient to cause simultaneous failure of the PyC layers.

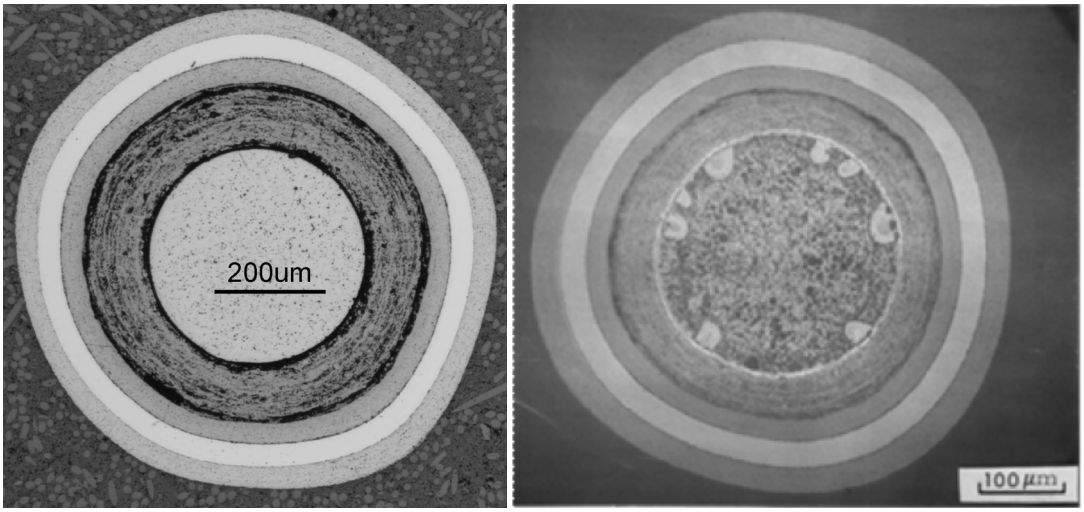


Figure 1-2. Particles before and after irradiation.

The shrinkage/swelling response of PyC is highly anisotropic and depends on the irradiation temperature and degree of anisotropy of the PyC. Studies have shown that as the irradiation temperature increases, the shrinkage increases and the stress in the IPyC increases. Offsetting the shrinkage effect is irradiation-induced creep of the PyC. Examples of shrinkage/swelling strains and creep coefficients, used to model secondary creep, for UCO particles are depicted in Figures 1-3 and 1-4.

1.1.4 Material Properties

Material properties used in PARFUME to represent the shrinkage, creep, thermal expansion, and elastic behavior of the coating layers were obtained from a report prepared by the CEGA Corporation in July 1993.[9] Due to uncertainties or incompleteness in the material data, several assumptions and approximations were required to develop the material properties.

1.1.5 Known Failure Mechanisms

Through years of fuel development and qualification programs, a number of potential fuel failure and fission-product-release mechanisms have been identified.[6] These failure mechanisms have been determined to be temperature and burn-up dependent. The mechanisms are categorized into three major failure modes: pressure vessel failure, SiC degradation, and multi-dimensional failure. Brief descriptions of the phenomena associated with each mode are presented below.

1.1.5.1 Pressure Vessel Failure Mode

A traditional failure mechanism addressed in PARFUME as well as other fuel performance codes is the pressure vessel failure of a one-dimensional spherical particle. The particle is one-dimensional because of perfect symmetry in the tangential and azimuthal directions. Early during irradiation, the shrinkage of the PyC layers puts the SiC layer in compression. As irradiation progresses, the irradiation-induced creep of the PyC layers tends to relieve some of this compressive stress. Additionally, the buildup of fission gas pressure tends to put the coating layers in tension. If the gas pressure increases enough, the tangential stress in the SiC layer could eventually become tensile. A traditional pressure vessel failure is expected to occur if the tangential stress reaches a value that exceeds the strength of the SiC for that particle.

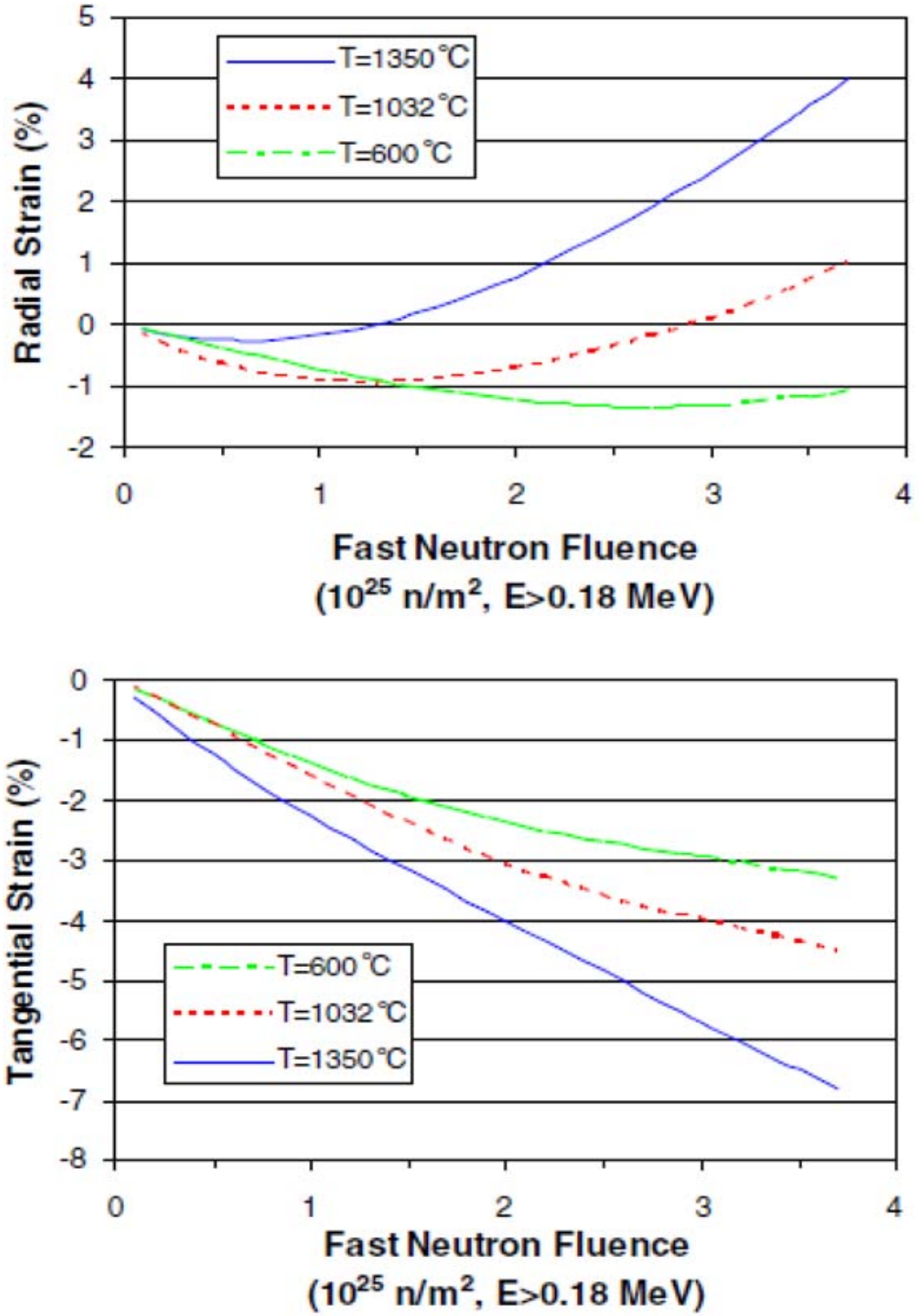


Figure 1-3. Radial and tangential irradiation-induced strains in PyC.

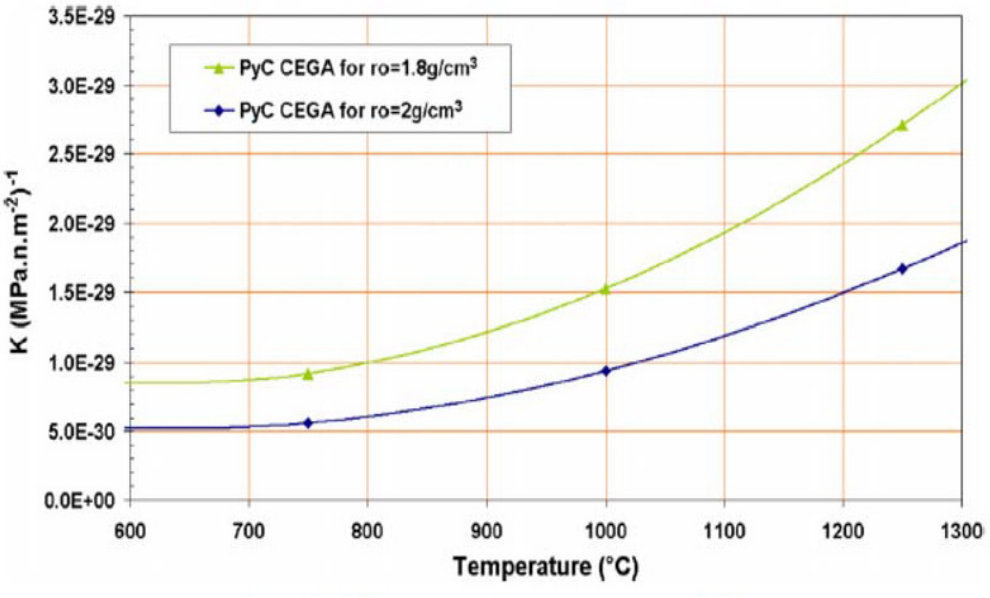


Figure 1-4. Irradiation-induced creep constant for PyC.

Fission Gas Pressure

Fission gases released during irradiation from the kernel of a coated particle depend on temperature, burnup, and time. Table 1-1 presents the normalized fission gas pressure that builds up in a 500-µm (kernel diameter) German UO_2 particle irradiated for three years at the indicated temperature and burnup. The results indicated a factor-of-eight increase in pressure as the burnup increased from 8 to 20% FIMA and the temperature increases from 1100 to 1300°C.

CO Gas Pressure

Oxygen is released during the fission process. In UO_2 coated particle fuels, there is net excess or "free" oxygen because the fission products (FPs) that are produced do not consume all of the oxygen released. The excess oxygen reacts with the buffer to form CO gas. The amount of CO produced is a function of temperature and burnup. Depending on operating conditions and fuel design, the CO contribution to total internal pressure can be as high as four times the contribution from FP gases.

Table 1-1. Comparison of fission gas pressures in a German particle.

	Temperature °C				
Burnup (% FIMA)	1100	1150	1200	1250	1300
8	1.00	1.28	1.62	2.04	2.52
10	1.33	1.69	2.14	2.68	3.28
15	2.26	2.86	3.60	4.47	5.42
20	3.32	4.21	5.28	6.53	7.89

(Normalized to 1.0 at 8% FIMA and 1100°C)

1.1.5.2 SiC Degradation Mode

In addition to manufacturing defects, several phenomena are known to degrade the SiC layer. Thermal decomposition and localized attack of the SiC are known to occur under certain conditions. Specifically, palladium, cesium, and carbon monoxide (CO) are known to attack the SiC, while thermal decomposition of the SiC layer is known to occur at elevated temperatures. Currently, PARFUME does not model the thermal decomposition or localized attack of SiC.

Initially Defective SiC Layer

During manufacture, a small percentage of fuel particles will have a defective SiC layer. A model is planned to be included in PARFUME to predict the diffusion of FPs through the initially defective SiC layers.

Palladium Attack

Palladium (Pd) is known to attack SiC at localized reaction sites. This interaction has been the subject of extensive study. Depending on the fuel type, Pd attack of the SiC could be higher in fuels designed to operate under high-temperature conditions.

Cesium Attack

Increased cesium (Cs) release is known to occur at high burnups. The reason for the elevated release is not certainty, but some researchers have attributed the release to degradation of the SiC layer by cesium as well as other FPs.

Carbon Monoxide Attack

The excess oxygen produced during the fission process that forms CO can attack SiC.

1.1.5.3 Multi-dimensional Failure Mode

In addition to the phenomena described above, PARFUME also considers multi-dimensional behavior that has been observed in post-irradiation examination (PIE) of U.S. fuel particles that may contribute to particle failures, such as (1) cracking of the IPyC layer, (2) partial debonding of the IPyC from the SiC layer, (3) an aspherical geometry, and (4) the amoeba effect. Each failure phenomena is described below.

Cracking of the IPyC

One form of multi-dimensional behavior modeled in PARFUME is a radial shrinkage crack in the IPyC. During irradiation, shrinkage of the initially intact IPyC layer induces a significant tensile stress in that layer. If the stress exceeds the tensile strength of the IPyC layer, a radial crack develops in the IPyC. The radial crack creates local tensile stresses in the SiC layer that could lead to particle failure. The stress at this point increases as the PyC layers shrink during irradiation but eventually peaks as creep in the PyC layers overcomes the shrinkage effect.

Partial Debonding of the IPyC from the SiC

A second form of multi-dimensional behavior modeled in PARFUME is partial debonding between the IPyC and the SiC. During irradiation, shrinkage of the IPyC layer induces a radial tensile stress at the interface between the IPyC and SiC layers. If the stress exceeds the bond strength between layers, then debonding of the IPyC from the SiC occurs. The debonding process is not likely to be an instantaneous

detachment over the entire surface of the interface. Rather, it begins at an initiation point from which the layers progressively unzip during irradiation.

Particle Asphericity

A third form of multi-dimensional behavior modeled in PARFUME is asphericity. During irradiation, the faceted portion of the particle acts as a flat plate that retains the internal gas pressure. If the pressure builds up high enough, this results in a local region of tensile stress in the central portion of the plate, which can contribute to particle failures. Unlike failures caused by cracking of the IPyC or partial debonding of the IPyC, which are governed by shrinkage of the pyrocarbons, failures caused by asphericity are controlled by the internal pressure. Therefore, while failures due to IPyC cracking and debonding tend to occur early during irradiation when shrinkage stresses are at their highest, failures due to asphericity are likely to occur later when the internal pressure is highest. The Code incorporates the effects of asphericity for particles that have a flat facet but that are otherwise spherical. Because the effects of an ellipsoidal shape are small in comparison, this type of asphericity is not included in the Code.

Amoeba Effect

A final multi-dimensional failure mechanism currently considered in the code is failure of the SiC due to the amoeba effect. Kernel migration is the tendency for the fuel kernel to migrate up the temperature gradient. It has been observed in all UO_2 TRISO-coated fuel particles, and it does not involve stress levels in the coating layer. Failure due to the amoeba effect is evaluated by determining the distance that the fuel kernel migrates as a function of the temperature gradient at the particle location. Particle failure is assumed to occur when the kernel comes into contact with the SiC layer. Studies have shown that as the fuel temperature increases from 100 to 1300°C, the propensity for kernel migration increases by a factor of 1.7. Figure 1-5 shows an example of a fuel particle where the kernel has migrated towards the IPyC.

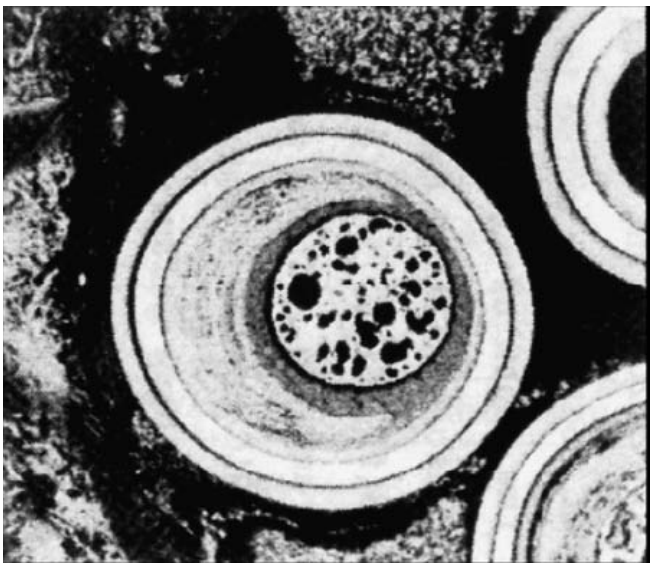


Figure 1-5. Example of kernel migration.

1.1.5.4 Potential Design Solutions

In an effort to prevent fuel particle failure by the mechanisms described above, several design changes have been considered—for example, reducing the kernel size, using UCO instead of UO_2 for the kernel, using a special type of UO_2 in which a ZrC layer is applied directly to the kernel, or replacing SiC with ZrC. The basis for these design solutions is presented in Reference 6. Additionally, replacement of SiC with ZrC has been implemented in PARFUME and is available as an option in the input data deck.

2. CAPABILITIES and LIMITATIONS

This section presents a summary of the capabilities and limitations of PARFUME. A review of the geometric and physical models used is presented to familiarize the user with the terminology associated with the fuel particle code and fuel particle terminology in general.

PARFUME is an integrated mechanistic analysis tool that evaluates the thermal, mechanical, and physico-chemical behavior of TRISO-coated fuel particles and the probability for fuel failure given the particle-to-particle statistical variations in physical dimensions and material properties that arise during the fuel fabrication process. Using a robust finite difference numerical scheme, PARFUME is capable of analyzing steady-state and transient fuel behavior. Written in FORTRAN 77, PARFUME compiles in FORTRAN 90, and it is easy to read, maintain, and modify. Currently, PARFUME is supported only on Linux platforms.

PARFUME is capable of analyzing particle behavior during reactor operations and subsequent heating/cooling operations, but the front-end post manufacturing heating/cooling operations prior to reactor operations cannot be analyzed by the code. A typical problem that PARFUME can analyze is presented in Section 6.

2.1 Code Description

2.1.1 Model Development

Model development and integration within PARFUME is a relatively complex process; therefore, the interested reader is directed to the *PARFUME Theory and Model Basis Report*[1] for the theoretical details related to physical models and methods. Nevertheless, users should have a fundamental understanding of not only the theory associated with the development of PARFUME, but a good understanding of the general solution process as well. Figure 2-4 provides an overview of the solution procedure; additional details are presented below.

2.1.2 General Solution Procedure

The general solution procedure used by PARFUME consists of the 5-step processes depicted in the flow chart of Figure 2-4. A general description of each step in the process is given below, while a detailed description of each process is provided in Reference 1.

2.1.2.1 Geometry Specification (Step 1)

This step of the process includes pre-processing steps including: geometry, mesh, and material property selection.

Geometry

The basic fuel particle geometry, described in Section 1.1.2, consists of a kernel of UO_2 or UCO surrounded by a buffer and three structural layers (IPyC, SiC, OPyC). The particles are embedded in a spherical, cylindrical, or plate-type graphite matrix; collectively, the fuel particles and matrix are referred to as a fuel element. Note that particles embedded in a spherical graphite matrix are called “pebbles”; each pebble contains several thousand coated fuel particles depending upon the fuel design. For example, each pebble for the PBMR-400 design contains approximately 15,000 fuel particles.

Within PARFUME, three fuel-element geometries (i.e., plane, spherical, and cylindrical) may be simulated in one dimension, as presented in Figure 2-1. Each geometry is modeled by averaging spherical fuel particles, void regions (i.e., coolant channels), and the graphite matrix. This modeling technique is necessary in order to capture the physical behavior of the fuel elements while eliminating the complexities (e.g., computational requirements) of modeling the detailed composition of the fuel element—for example, 15,000 coated fuel particles.

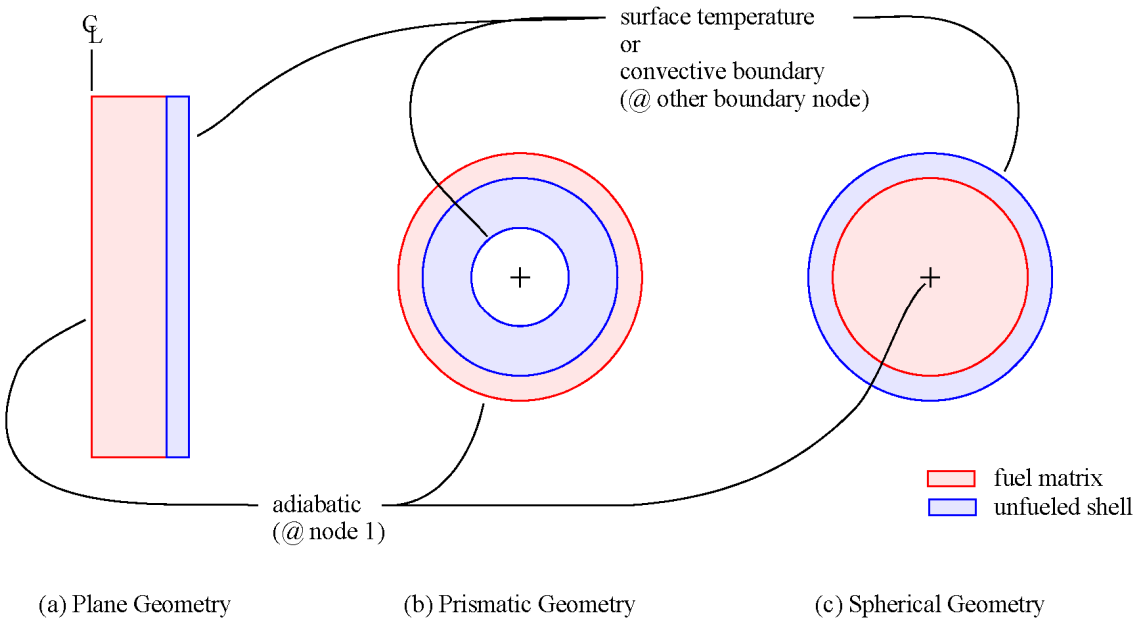


Figure 2-1. PARFUME fuel-element geometries.

A plane geometry option is provided to allow simulation of plate-type fuel. It is assumed that the plate will consist of a center-fueled region bounded on both sides by a non-fueled region. The centerline of the plate therefore represents a line of symmetry for both heat and mass transfer. Although plate-type fuel has become unpopular over the years, some reactors, such as the Advanced Test Reactor, continue to use plate-type fuel, so the plane geometry option is included in PARFUME for completeness.

A spherical geometry option is provided to allow simulation of a single pebble from a pebble bed reactor. The center of the sphere represents a line of symmetry relative to heat and mass transfer. An unfueled region, the graphite layer, representing the on the outer edge of the sphere, communicates with the fueled region on one edge and the coolant on the remaining edge.

A cylindrical geometry option is provided to allow simulation of a unit cell from a prismatic reactor core. As an approximation, an appropriate fraction of six fuel compacts represents an equivalent fueled region in the form of a ring. The outer edge of that ring is symmetric relative to both heat and mass transfer. An unfueled region representing the matrix graphite communicates with the fueled region on one edge and the coolant channel on the remaining edge. Figure 2-2 depicts the basic geometry used to develop the cylindrical fuel element geometry.

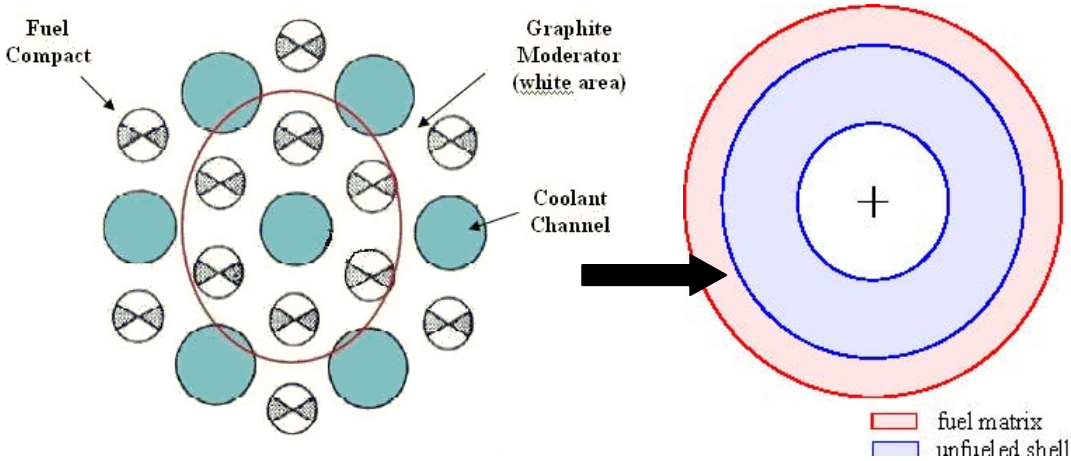


Figure 2-2. Prismatic fuel element geometry.

Mesh

PARFUME requires generation of two 1-D meshes: the "fuel particle" mesh and the "fuel element" mesh. Examples of fuel particle mesh and fuel element mesh are presented in Figure 2-3. With respect to the fuel particle mesh, the user does not specify the number of nodes, but by default, the code places nodes at 5 μm increments and on the outer surface of each layer. By default, nodes (i.e., ko, bo, io, so, oo) are placed at the interface of the geometry. However, the thickness of buffer and structural layers is small relative to the kernel, which implies that minimal differences in parameters (i.e., temperature) within a layer exist.

For the fuel element mesh, the user specifies the number of nodes. Referring to Figure 2-1, a line of symmetry relative to both heat and mass transfer exists in each geometry. Node 1 is always placed on that line of symmetry. Each geometry is then divided into intervals consistent with the number of nodes specified by the user. The last node always aligns with a boundary that may have either a surface temperature specification or a convective surface specification.

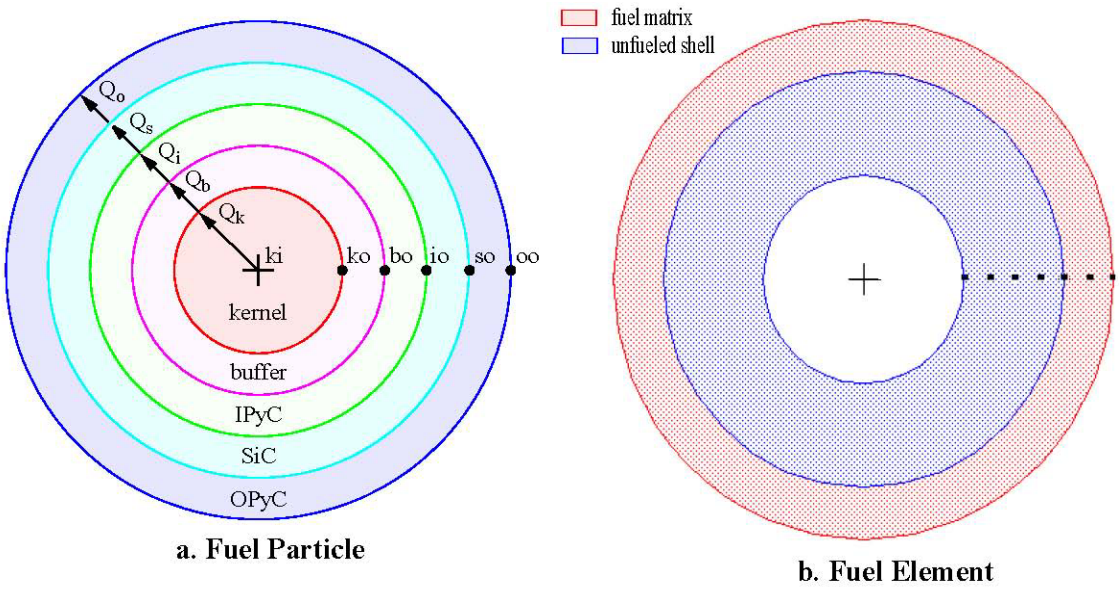


Figure 2-3. Fuel particle and fuel element mesh.

Material Properties

Material properties, both structural and thermal, in the form of models used in PARFUME to represent the shrinkage, creep, thermal expansion, and elastic behavior of the coating layers, were obtained from a report prepared by the CEGA Corporation in July 1993[9]. The range of validity of these properties forms the basis for the overall analysis limitations of PARFUME. For example:

- In general, application of the material models is limited to the range of 4×10^{25} n/m2, E > 0.18 MeV for fast neutron fluence and 600 to 1300°C for irradiation temperature.
- The densities of the dense structural PyC and the porous PyC are limited to 1.8 to 2.0 Mg/m^3 and approximately 0.9 to 1.1 Mg/m^3, respectively; the density of SiC is at least 3.18 Mg/m^3.
- Due to the scarcity of material data, it is assumed in the material models that the effects of several parameters (i.e., temperature, fluence, density) are mutually independent and their combined effect can be obtained by multiplying them together.
- Irradiation-induced creep in the PyC layers is treated as secondary creep, i.e., the creep strain rate is proportional to the level of stress in the PyC. The creep coefficient increases significantly with increases in the irradiation temperature.
- Thermal expansion of the PyCs is anisotropic and is a function of the anisotropy as represented by the Bacon Anisotropy Factor (BAF) and temperature.
- Swelling in the PyC layers is anisotropic and a function of four variables: fluence level, PyC density, degree of anisotropy (as measured by BAF), and irradiation temperature. The magnitude of the shrinkage increases as BAF increases or as the irradiation temperature increases.
- The SiC layer has an elastic modulus (stiffness) that is an order of magnitude higher than that for the PyCs.
- The dependence of Poisson ratio, ν , (for the PyC layers) on density, crystallite size, temperature and fluence is largely unknown; therefore, it is assumed that Poisson's ratio is independent of these parameters.

- Most available mechanical property test data for PyC correspond to densities of 1.5 Mg/m^3 or higher. For the buffer layer (porous PyC), which has a density of approximately 1.0 Mg/m^3, a large extrapolation of the data is required, which may significantly affect its accuracy.

Additional details, related to mechanical properties, are presented in Reference 1.

2.1.2.2 Compute Fuel Element Temperature Profile (Step 2)

Once the fuel element geometry and temperature boundary conditions are identified, the general heat conduction equation, represented by *Equation (2-1)*, is used to compute the macro temperature distribution throughout the fuel element. The volumetric heat generation rate consists of the total heat generation rate of all the particles due to fission. Energy generation due to radioactive decay of other nuclides is not modeled.

$$\rho c_p \frac{\partial T}{\partial t} = k \bullet \nabla^2 T + \dot{q} \tag{2-1}$$

2.1.2.3 Compute Fuel Particle Temperature Profile (Step 2)

Once the macro temperatures for the fuel element are determined, the general heat conduction equation is used to compute the micro temperature profile (using a quasi-steady-state assumption). Specifically, the term on the left-hand side of *Equation (2-1)* (time rate of change of temperature) is assumed to be zero, resulting in Poisson's equation. Therefore, two boundary conditions are required, i.e., the surface temperature of the particle surface and the spatial temperature gradient at the geometric line of symmetry. The particle surface temperature is obtained from the "macro" temperature distribution computed from *Equation (2-1)*, while the spatial temperature gradient at the line of symmetry is set equal to zero. The micro temperature profile accounts for all deformations in the kernel, buffer, and coating layers of the particle as well as the potential for development of a gap between the buffer and the IPyC.

2.1.2.4 Compute Particle Stress Distribution (Step 3)

Once a particle temperature profile is determined, the particle stress distribution is calculated to evaluate whether or not the particle fails. Currently, stress and displacement distribution calculations are limited to the buffer, IPyC, SiC, and OPyC, though the effect of kernel swelling is included. Strain contributions from several sources are included. Note that PARFUME does not perform stress analyses of the fuel element matrix material.

The system of equations used to compute the stress distribution in a spherical particle includes constitutive relationships (describing elastic, irradiation-induced, and thermal strain), strain-displacement equations, and the equilibrium stress equation. The two component strain equations (i.e., constitutive relationships) take into account elastic, irradiation-induced creep, irradiation-induced swelling, and thermal strain. The radial strain-rate equation, consisting of four strain terms, is shown in *Equation (2-2)*. Note that the pressure contribution to strain due to fission gases and CO is accounted for in the displacement and stress relationships presented in Reference 1.

$$\frac{\partial \varepsilon_r}{\partial t} = \frac{1}{E}\left(\frac{\partial \sigma_r}{\partial t} - 2\mu \frac{\partial \sigma_t}{\partial t}\right) + c(\sigma_r - 2v\sigma_t) + S_r + \alpha_r \dot{T} \tag{2-2}$$

Table 2-1 summarizes the strain contributions associated with each fuel particle structure. Because creep and swelling in the SiC layer are small relative to that of PyC and because of uncertainty in these properties for SiC, the SiC strains do not currently include contributions from creep or swelling. The fuel particle kernel is not considered to deform structurally, though a model is included in PARFUME to predict kernel volumetric changes over time.

Table 2-1. Fuel particle strain contributions.

Fuel Particle Component	Elastic Strain	Creep Strain	Swelling Strain	Thermal Strain
Kernel	No	No	Yes	No
Buffer	Yes	Yes	Yes	Yes
IPyC	Yes	Yes	Yes	Yes
SiC	Yes	No	No	Yes
OPyC	Yes	Yes	Yes	Yes

The stress state in a fuel particle depends on the internal gas pressure that exists during either normal reactor operation or an accident condition. Gas pressures are calculated according to the Redlich-Kwong equation of state and account for the generation of CO and the release of noble FP gases.

2.1.2.5. Compute Failure Probability (Step 4)

Once stresses have been determined, they are used in conjunction with Weibull statistics to determine particle failure probabilities in the fuel performance model. Assuming that the fuel particle failures follow a Weibull statistical distribution, the failure probability (for example, of the SiC layer) is computed by inserting the calculated stress into *Equation (2-3)*, where the characteristic strength (σ_o) and Weibull modulus (m) are determined from experimental data.

$$P_f = 1 - e^{-\int_v \left(\frac{\sigma}{\sigma_o}\right)^m \, dV} \tag{2-3}$$

The user is provided with Monte Carlo, full-integration, and fast-integration solution scheme options to determine failure probability.

2.1.2.5 Compute Fission Product Diffusion (Step 5)

The simulation of FP transport via diffusion from the fuel through the particle coating layers to the surrounding fuel element graphite matrix, and finally to the coolant boundary, is accomplished using the following fundamental transport equation of *Equation (2-4)*, where the flux is driven by FP concentration gradients and temperature gradients as shown in *Equation (2-5)*.

$$\frac{\partial C}{\partial t} = -\nabla \bullet J + S \tag{2-4}$$

$$J = -D\left(\nabla C + \frac{Q'C}{RT^2}\nabla T\right) \tag{2-5}$$

Similar to the temperature profile analyses, “micro” and “macro” diffusion analyses are performed. The micro analysis is based on a model having five different materials (kernel, buffer, IPyC, SiC, and OPyC). The macro solution is based on a model having two materials: the graphite-containing fuel particles and the surrounding graphite without fuel particles.

Results from all of the diffusion analyses are integrated over time to produce a total FP release fraction from the fuel element. This is done for each of the FPs under consideration.

2.2 Verification and Validation

One of the most important steps in code development and application is the verification and validation (V&V) process. According to the American Institute of Aeronautics and Astronautics (AIAA), verification is "the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model," while validation is "the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model."[11]

In general, verification is the responsibility of the organization developing the code, while simulation validation primarily resides with the user. Ultimately, code verification and subsequent validation help establish the predictive capability of the code and confidence in simulation results. To date, only V&V "guidelines" have been agreed upon by professional societies, leaving the development of a detailed step-by-step V&V procedure to managers, code developers, and computational analysts.[11,12,13]

Currently, a formal V&V plan has not been established for PARFUME, although local (i.e., in-house) processes coupled with guidelines presented in several V&V documents have been utilized to establish confidence in PARFUME results. As a formal V&V plan matures, details of the V&V of PARFUME will be presented in future releases of this user guide.

2.3 Future Development

PARFUME development is a perennial process requiring, for example, a diligent effort to maintain the code up-to-date with the latest models, software, and hardware architecture. Plans will include several new models. For example, finite element stress analyses of thinned and corroded SiC layers have been performed. These analyses will be coupled with (yet to be developed) application criteria to form another failure algorithm. Also, an initially defective SiC layer model will be incorporated into PARFUME.

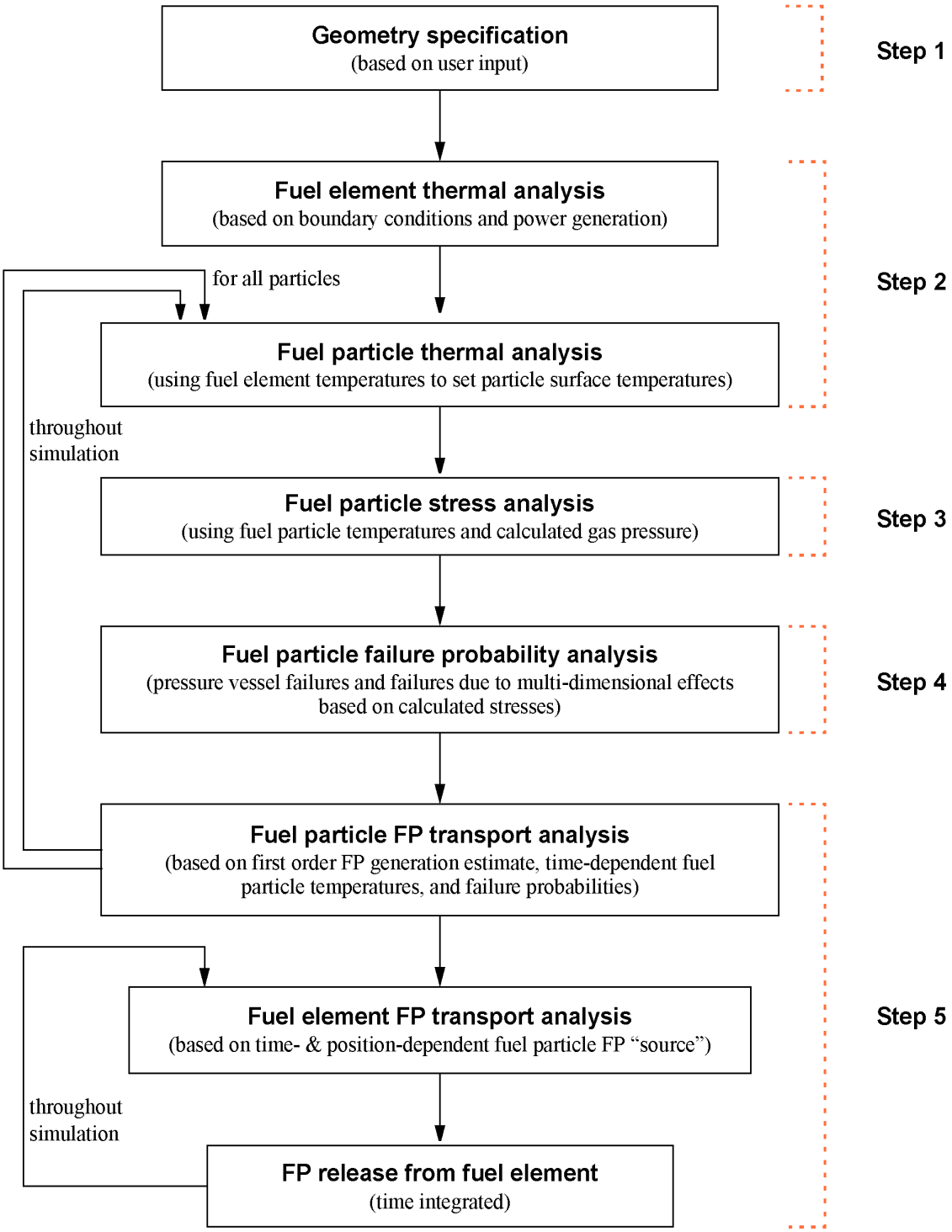


Figure 2-4. General solution procedure.

3. PARFUME CODE INPUT

This section presents a description of code input parameters; an example input deck is provided in Section 6. In addition, a summary of the input deck parameters, including default values and units, is located in Appendix A.

In this report, the input deck terminology refers to the six-digit number "XXXXXX" as the "card number." The first three digits of the card number are called the "card series," while the final three digits are called the "card sequence." For example, the card number 201001 consists of 6 digits. The digits 201 represent the card series, and the digits 001 represent the card sequence.

3.1 Run Parameters

3.1.1 CARD 100001 (Simulation Description)

3.1.1.1 "title"

This card allows users to name their simulation. This parameter is a character string, which may be up to 60 characters long.

3.1.2 CARD 101001 (Solution Schemes)

3.1.2.1 "pfss" (PARFUME Solution Scheme)

This parameter allows the user to select one of three available solution schemes: pfss = solution scheme: 0 = Monte Carlo, 1 = full integration, 2 = fast integration.

In the Monte Carlo routine of PARFUME, stresses are analyzed for a statistically sampled batch of particles. In the integration approach, the failure probability P_f for a particle batch will be formulated in terms of an integral. The fast integration method, an integration approximation, was developed to substantially reduce the time required to perform the integration with only a minimal loss of accuracy. Additional details of this solution scheme can be found in Section 5.4 of Reference 1.

3.1.2.2 "ncases"

This parameter represents the number of coated fuel particles (CFP) in a "Monte Carlo" solution scheme (i.e., sample size); if another solution scheme such as fast integration is selected, the parameter is not used. In general, the larger the value of ncases, the more likely it is that a more accurate estimate of failure probability will be obtained, but this larger sample size could result in longer computational time. A good rule-of-thumb is that ncases should be on the order of ten divided by the expected failure probability. For example, if a failure probability on the order of 1×10^{-4} is being analyzed, the value of ncases should be on the order of 1×10^{5}.

3.1.2.3 "nburp"

This parameter controls the frequency of periodic runtime updates, so the user can tell the code is running. Figure 3-1 shows the screen output using different values. Note that the "Elapsed Time (s)" screen output is based on the time the program was first executed. For example, the elapsed time data in Figure 3-1 shows that the it took the user about 2–3 seconds longer to enter the data file for the "nburp=200" simulation.

(nburp = 100)		(nburp = 200)	
Increment Completed	Elapsed Time (s)	Increment Completed	Elapsed Time (s)
100	7.	200	11.
200	8.	400	13.
300	10.	600	16.
400	11.	800	19.
500	12.	1000	22.
600	14.		
700	15.		
800	17.		
900	18.		
1000	20.		

Figure 3-1. PARFUME screen output with different “nburp” values.

3.1.2.4 “sample”

This parameter determines whether (input) parameter variations—for example, particle geometry variations such as kernel diameter standard deviation—are considered. An input value of “0” turns this option off; therefore, standard deviation is assumed to equal zero. An input value of “1” turns this option on; therefore, the standard deviation value is set based on user input values specified in card series 103 and 104.

3.1.2.5 “dtf”

This parameter is used during a FP transport analysis. It controls activation of designed-to-fail (dtf”) particle models (i.e., single-layer CFP or a BISO CFP), which are specifically designed to fail. This setting is not fully implemented in PARFUME. An input value of “0” turns this option off. An input value of “1” turns this option on. The default value is “0.”

3.1.2.6 “iseed”

This parameter allows the user to specify a “random number seed” for Monte Carlo calculations in order to initialize the random number generator; it is not used otherwise. The default value is “305.”

3.1.3 CARD 101002 (Models)

This card allows selection of models used for studying particle failure modes such as debonding, and asphericity.

3.1.3.1 “idebondp”

This parameter controls activation of the debonding models: 0 = off, 1 = on.

Additional debonding parameters are set in card series 403.

3.1.3.2 "ifacet"

This parameter controls activation of faceting models: 0 = off, 1 = on.

Additional faceting parameters are set in card series 402.

3.1.3.3 "rbvalue"

This parameter controls release-to-birth (R/B) calculations for short-term FP diffusion analysis, which is used for source-term analyses. The term "birth" represents birth from fission, and the term "release" represents the release of FPs to the environment surrounding the fuel element: ≤0 = no R/B, 1 = Kr-85m, >1 = 12 nuclides.

The 12 nuclides include: Kr-85m (m represents metastable state), Kr-87, Kr-88, Kr-89, Kr-90, Xe-131m, Xe-133, Xe-135, Xe-135m, Xe-137, Xe-138, and Xe-139. Additional details of this model can be found in Section 6 of Reference 1.

3.1.3.4 "comodel"

This parameter controls the activation of CO production models: 1 = original model (no CO production), 2 = GA (Kovaks) model, 3 = HSC model, 4 = German (Proksch) model. Additional details of this model can be found in Section 4.2.2 of Reference 1. This term allows for CO contribution to particle pressure.

3.1.3.5 "fgmodel"

This parameter controls activation of fission gas (Kr and Xe) release fraction models: 1 = original model (100% release), 2 = Booth equivalent sphere model. Additional details of fission gas release can be found in Section 4 of Reference 1. This term allows for Kr and Xe contributions to particle pressure.

3.1.3.6 "idebug"

This parameter is used for code development purposes. Contrary to its name, this parameter is not used for debugging the code. This parameter controls activation of additional output data, which is used in conjunction with ABAQUS in developing "h functions." Additional temporal data includes: particle nominal pressure and particle nominal OPyC, SiC, and IPyC temperature. If this parameter is set equal to 0, no additional output data will be included in the results file; setting this parameter equal to 1 results in additional temporal data output. Figure 3-2 is an example of the temporal outputs. Use of this parameter is not recommended. Additional information on "h functions" can be found in Section 5.2 of Reference 1.

PARTICLE nominal IPyC temp (in K) vs. ABAQUS time
0.0000E+00,1273.000, 0.1258E+05,1273.185, 0.2516E+05,1273.185, 0.3774E+05,1273.185, 0.5031E+05,1273.185, 0.6289E+05,1273.185, 0.7547E+05,1273.185, 0.8805E+05,1273.185, 0.1006E+06,1273.185, 0.1132E+06,1273.185, 0.1258E+06,1273.185, 0.1384E+06,1273.185, 0.1509E+06,1273.185, 0.1635E+06,1273.185, 0.1761E+06,1273.185, 0.1887E+06,1273.185, 0.2013E+06,1273.185, 0.2138E+06,1273.185, 0.2264E+06,1273.185, 0.2390E+06,1273.185, 0.2516E+06,1273.185, 0.2642E+06,1273.185, 0.2767E+06,1273.185, 0.2893E+06,1273.185, 0.3019E+06,1273.185, 0.3145E+06,1273.185, 0.3270E+06,1273.185, 0.3396E+06,1273.185, 0.3522E+06,1273.185, 0.3648E+06,1273.185, 0.3774E+06,1273.185, 0.3899E+06,1273.185, 0.4025E+06,1273.185, 0.4151E+06,1273.185, 0.4277E+06,1273.185, 0.4403E+06,1273.185,

Figure 3-2. Example output with "idebug" = 1.

3.2 Fuel Characteristics

3.2.1 CARD 102001 (Fuel Properties)

This card contains fuel characteristic user input.

3.2.1.1 "u235enr(%)"

This parameter represents the fuel kernel U-235 enrichment (wt%).

3.2.1.2 "ourat"

This parameter represents the oxygen-to-uranium atom ratio required for UO_2 or UCO fuel analysis.

3.2.1.3 "curat"

This parameter represents the carbon-to-uranium atom ratio required for UCO fuel analysis.

3.2.2 CARD 103001 (Kernel Properties)

The card contains the fuel particle material properties.

3.2.2.1 "kernd"

This parameter represents kernel density (Mg/m^3), which is typically supplied by the manufacturer.

3.2.2.2 "kernt"

This parameter represents the theoretical kernel density (Mg/m^3), which is typically obtained from a handbook. This parameter is used in the void volume computation. The default value is 11.03 Mg/m^3.

3.2.3 CARD 103002 (Buffer Properties)

This card contains the buffer particle material properties.

3.2.3.1 "buffd"

This parameter represents the buffer density (Mg/m^3), which is typically supplied by the manufacturer.

3.2.3.2 "bufft"

The theoretical buffer density represents the maximum densification that can occur in buffer density (Mg/m^3), which is typically obtained from a handbook. The default value is 2.25 Mg/m^3.

3.2.4 CARD 103003 (IPyC Properties)

3.2.4.1 "ipycdn"

This parameter represents the mean IPyC density (Mg/m^3).

3.2.4.2 "ipycdvar"

This parameter represents the IPyC density standard deviation (Mg/m^3).

3.2.5 CARD 103005 (OPyC Properties)

3.2.5.1 "opycdn"

This parameter represents the mean OPyC density (Mg/m^3).

3.2.5.2 "opycdvar"

This parameter represents the OPyC density standard deviation (Mg/m^3).

3.2.6 CARD 103013 (IPyC BAF)

Theoretical information on the BAF is located in Section 7 of Reference 1.

3.2.6.1 "ibafn"

This parameter represents the mean IPyC BAF, a measure of the degree of anisotropy. The larger the value, the more anisotropic the material.

3.2.6.2 "ibafvar"

This parameter represents the IPyC BAF standard deviation.

3.2.7 CARD 103015 (OPyC BAF)

Theoretical information on the BAF is located in Section 7 of Reference 1.

3.2.7.1 "obafn"

This parameter represents the mean OPyC BAF.

3.2.7.2 "obafvar"

This parameter represents the OPyC BAF standard deviation from the mean.

3.2.8 CARD 103023 (IPyC Weibull Modulus)

Theoretical information on the Weibull modulus is located in Section 7 of Reference 1.

3.2.8.1 "ipycm"

This parameter represents the IPyC Weibull modulus. The default value is 9.5.

3.2.9 CARD 103024 (SiC Weibull Modulus)

3.2.9.1 "sigm"

This parameter represents the SiC Weibull modulus. The default value is 6.0.

3.2.10 CARD 103025 (OPyC Weibull Modulus)

3.2.10.1 "opycm"

This parameter represents the OPyC Weibull modulus. The default value is 9.5.

3.2.11 CARD 103033 (Poisson's Ratio)

3.2.11.1 "cnu"

This parameter represents the Poisson's ratio in creep for PyCs. The default value is 0.5.

3.2.11.2 "cnub"

This parameter represents the Poisson's ration in creep for the buffer. The default value is 0.5.

3.2.12 CARD 103043 (Creep Amplification Factor)

3.2.12.1 "creepampn"

This parameter represents the mean creep amplification factor, which is applied to amplify (or reduce) the steady-state creep coefficient. The default value is 2.0. Additional details on this parameter are located in Section 7.1.6.1 of Reference 1.

3.2.12.2 "creepvar"

This parameter represents the standard deviation for the creep amplification factor. The default value is 0.0.

3.2.13 CARD 103054 (Zrc Modeling)

3.2.13.1 "zrc"

This parameter controls activation of the ZrC model: 0 = off, 1 = on. When the ZrC model is chosen, the material properties for SiC are replaced with the material properties for ZrC, but the geometric parameters specified by the user on the input data deck for SiC remain the same. The default value is 0.

3.2.13.2 "zrcp"

This parameter represents the fraction of ZrC theoretical density, where four options (i.e., 1, 2, 3, 4) are available to the user. Option 1 represents a value of 0.96, Option 2 represents a value of 0.85, Option 3 represents a value of 0.80, and Option 4 represents a value of 0.77. The default value is 1.

3.2.14 CARD 103061 (Defective SiC Layers)

3.2.14.1 fdef

This parameter represents a place holder variable for the fraction of initial defective SiC layers (currently not used by the code but is planned for a future model). The default value is 0.0.

3.3 Particle Geometry

3.3.1 CARD 104001 (Kernel Geometry)

3.3.1.1 "kerndia"

This parameter represents the mean kernel diameter (μm).

3.3.1.2 "kernvar"

This parameter represents the kernel diameter standard deviation (μm).

3.3.2 CARD 104002 (Buffer Geometry)

3.3.2.1 "buffthk"

This parameter represents the mean buffer thickness (μm).

3.3.2.2 "buffvar"

This parameter represents the buffer thickness standard deviation (μm) from the mean.

3.3.3 CARD 104003 (IPyC Geometry)

3.3.3.1 "ipycthk"

This parameter represents the mean IPyC thickness (μm).

3.3.3.2 "ipycvar"

This parameter represents the IPyC thickness standard deviation (μm).

3.3.4 CARD 104004 (SiC Geometry)

3.3.4.1 "sicthk"

This parameter represents the mean SiC thickness (μm).

3.3.4.2 "sicvar"

This parameter represents the SiC thickness standard deviation (μm).

3.3.5 CARD 104005 (OPyC geometry)

3.3.5.1 "opycthk"

This parameter represents the mean OPyC thickness (μm).

3.3.5.2 "opycvar"

This parameter represents the OPyC thickness standard deviation (μm).

3.4 Fuel Matrix Description

3.4.1 CARD 105001 (Fuel Element Types)

Within PARFUME, three different fuel element geometries (i.e., plane, cylindrical, and spherical) may be simulated in one dimension. Each geometry is modeled by averaging spherical fuel particles, void regions (i.e., coolant channels), and the graphite matrix. This modeling technique is necessary in order to

capture the physical behavior of the fuel elements while eliminating the complexities (i.e., computational requirements) of modeling the detailed composition of the fuel element.

Three separate options are available to specify input parameters for either the pebble bed (PEBBLEBED), prismatic (PRISMATIC), or plane geometry (PLANEGEOM) fuel element.

3.4.2 CARD 105011 (PEBBLEBED – Particle Density and Mesh)

3.4.2.1 "partnum"

This parameter represents the number of coated fuel particles (CFPs) per pebble.

3.4.2.2 "ngnfm"

This parameter represents the number of "global" nodes in the "fuel matrix" region. Referring to Figure 2-3b, "ngnfm = 3". Note that two co-located global nodes are present at the interface of the fuel matrix and shell.

3.4.2.3 "ngn"

This parameter represents the total number of "global" nodes in "fuel matrix" plus the "unfueled shell" region. Referring to Figure 2-3b, "ngn = 8". Note that two co-located global nodes are present at the interface of the fuel matrix and shell.

3.4.3 CARD 105021 (PEBBLEBED - Geometry)

3.4.3.1 "pebdia"

This parameter represents the pebble diameter (m) of a single pebble.

3.4.3.2 "pebcldtk"

This parameter represents the thickness of the non-fueled region on the outer surface of the pebble (m).

3.4.4 CARD 105031 (PEBBLEBED – Density)

3.4.4.1 "fmden"

This parameter represents the density of the fuel matrix material (Mg/m^3). The default value is 1.7.

3.4.5 3.4.5. CARD 105041 (PEBBLEBED – Uranium Contamination)

3.4.5.1 "ucontam"

This parameter represents the fraction of uranium contamination in the fuel matrix.

3.4.6 CARD 105011 (PRISMATIC – Particle Density and Mesh)

3.4.6.1 "partnum"

This parameter represents the number of CFPs per compact per meter of fuel element.

3.4.6.2 "ngnfm"

This parameter represents the number of "global" nodes in the "fuel matrix" region. Referring to Figure 2-3b, "ngnfm = 3". Note that two global nodes are present at the interface of the fuel matrix and shell.

3.4.6.3 "ngn"

This parameter represents the total number of "global" nodes in "fuel matrix" plus the "unfueled shell" region. Referring to Figure 2-3b, "ngn = 8". Note that two global nodes are present at the interface of the fuel matrix and shell.

3.4.7 CARD 105021 (PRISMATIC – Geometry)

Refer to Figure 2-2 for a description of this geometry.

3.4.7.1 "fueldia"

This parameter represents the diameter of the fuel compact (m).

3.4.7.2 "cooldia"

This parameter represents the coolant channel diameter (m).

3.4.7.3 "fuelpitch"

This parameter represents the fuel compact pitch, the center-to-center distance between fuel compacts arranged in an array.

3.4.7.4 "height"

This parameter represents the height of the fuel compact (m).

3.4.8 CARD 105031 (PRISMATIC – Density)

3.4.8.1 "fmden"

This parameter represents the density of the fuel matrix material (Mg/m^3). The default value is 1.7.

3.4.9 CARD 105041 (PRISMATIC – Uranium Contamination)

3.4.9.1 "ucontam"

This parameter represents the fraction of uranium contamination in the fuel matrix.

3.4.10 CARD 105011 (PLANEGEOM - Particle Density and Mesh)

3.4.10.1 "partnum"

This parameter represents the number of CFPs per slab per square meter of surface area.

3.4.10.2 "ngnfm"

This parameter represents the number of "global" nodes in the "fuel matrix" region. Referring to Figure 2-3b, "ngnfm = 3". Note that two global nodes are present at the interface of the fuel matrix and shell.)

3.4.10.3 "ngn"

This parameter represents the total number of "global" nodes in "fuel matrix" plus the "unfueled shell" region. Referring to Figure 2-3b, "ngn = 8". Note that two global nodes are present at the interface of the fuel matrix and shell.

3.4.11 CARD 105021 (PLANEGEOM – Geometry)

Refer to Figure 2-1 for a description of this geometry.

3.4.11.1 "fmthk"

This parameter represents the thickness of the fuel meat (m).

3.4.11.2 "cldthk"

This parameter represents the thickness of the fuel cladding (m).

3.4.11.3 "sarea"

This parameter represents the surface area of the fuel plate (m^2).

3.4.12 CARD 105031 (PLANEGEOM – Density)

3.4.12.1 "fmden"

This parameter represents the density of the fuel matrix material (Mg/m^3). The default value is 1.7.

3.4.13 CARD 105041 (PLANEGEOM - Uranium Contamination)

3.4.13.1 "ucontam"

This parameter represents the fraction of uranium contamination in the fuel matrix.

3.5 Reactor Temperature Options

3.5.1 CARD 106001 (Reactor Temperature Options)

This parameter allows the user to select a reactor temperature solution option, "rtmpopt".

Current solution schemes include: FIFD-CALC = fully implicit finite difference calculation, TEMP-DATA = allows users to input independently calculated temperatures, and VOLAVGTMP = allows users to select an adiabatic analyses.

3.5.1.1 "FIFD-CALC"

This option invokes the finite difference scheme to solve the heat conduction equation. The solution scheme is described in Section 3.1 of Reference 1.

3.5.1.2 "TEMP-DATA"

This option allows the user to input independently calculated temperatures—for example, those obtained from experimental data or computer-aided engineering (CAE) software (e.g., ABAQUS, Star-CCM+).

With respect to ABAQUS data, PARFUME reads the data, identifies the maximum and minimum temperature values for each volume element, divides the identified data into 21 bins, averages the temperatures in each bin, and utilizes the average temperatures in probability calculations. This CAE data must be in a specified format consistent with ABAQUS. Note that if this option is selected and an ABAQUS input file is not located within the same directory as the PARFUME executable file, the user will be prompted as follows:

"*Input (x.abq) file was not found*

Please enter 'x'.abq filename or QUIT"

Additionally, the CAE file name must be the same as the PARFUME input data file, and the file must have an "x.abq" file type.

3.5.1.3 VOLAVGTMP"

This option allows the user to select a volume-averaged temperature profile for heat transfer analysis in the fuel element.

3.5.2 CARD 106021 (Global Node Temperatures)

3.5.2.1 "tgi(k)"

This parameter allows users to specify temperatures (Kelvin) at the fuel matrix global nodes when the "FIFD-CALC" option is selected. When this option is selected, the values input represent the fuel element spatial temperatures.

3.5.2.2 "ntgi"

This parameter allows users to specify the associated fuel matrix node for the specified temperature when the "FIFD-CALC" option is selected. When this option is selected, the values input represent the fuel element nodes. Note that "node 1" is always located at the line of symmetry for the respective geometry (see Figure 2-1).

3.6 Diffusion Model

3.6.1 CARD 201001 (Diffusion Model)

3.6.1.1 fpspecie

This parameter turns on diffusion, where the diffusive behavior of six "long-lived" FP species—iodine (I), silver (Ag), cesium (Cs), strontium (Sr), krypton (Kr), and xenon (Xe)—can be modeled.

3.7 Environmental Parameters

3.7.1 CARD 301001 (Fluence v. Time Input)

3.7.2 "ttime"

This parameter represents the time variable and allows users to specify the time history (days) of neutron exposure.

3.7.3 "flu"

This parameter represents the fluence level and allows users to specify the time history of neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.4 CARD 302001 (Burnup v. Fluence Input)

3.7.4.1 "flu"

This parameter represents the fluence level and allows users to specify the burnup history based on neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.4.2 "bup"

This parameter represents the burnup level (%FIMA) and allows users to specify the burnup history based on neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.5 CARD 303001 (External Pressure v. Fluence Input)

3.7.5.1 "flu"

This parameter represents the fluence level and allows users to specify the burnup history based on neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.5.2 "pamb"

This parameter represents the ambient pressure (MPa) and allows users to specify the ambient pressure history based on neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.6 CARD 304001 (Boundary Temperature v- Fluence Input)

This card and its associated parameters are available only when "rtmpopt=FIFD-CALC" is selected.

3.7.6.1 "flu"

This parameter represents the fluence level and allows users to specify the boundary temperature history based on neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.6.2 "btemp"

This parameter represents the boundary temperature (K) and allows users to specify the boundary temperature history based on neutron exposure (10^{25} n/m^2, E>0.18 MeV).

3.7.7 CARD 306001 (Time Heatup Starts and Irradiation Ends)

3.7.7.1 "thus"

This parameter represents the point in time in which heatup starts (days) and irradiation ends.

3.8 Correlation Parameters and Coefficients

3.8.1 CARD 401001 (Correlation Coefficients – IPyC Cracking)

3.8.1.1 sigcr0"

This parameter represents SiC mean strength value with IPyC cracking (MPa).

3.8.1.2 "umc"

This parameter represents SiC stress for cracked CFP where all parameters are at mean values (MPa).

3.8.2 CARDS 401002 through 401012 (Correlation Coefficients “c1c”, “c2c”)

3.8.2.1 “c1c” and “c2c”

These parameters represent the polynomial coefficients necessary to correlate a 1-D PARFUME solution with a multi-dimensional solution from detailed ABAQUS calculations for IPyC cracking.

3.8.3 CARD 402001 (Correlation Coefficients – Asphericity)

3.8.3.1 “siga0”

This parameter represents the mean SiC strength in a faceted CFP (MPa).

3.8.3.2 “um”

This parameter represents the SiC stress, at the minimum value, for a faceted CFP where all parameters are at mean values (MPa).

3.8.3.3 “delum”

This parameter represents the SiC stress, at the maximum value or at the end of the solution, for a faceted CFP where all parameters are at mean values (MPa).

3.8.3.4 “aration”

This parameter represents the mean aspect ratio, which is the ratio of the maximum to minimum diameter.

3.8.3.5 “aratvar”

This parameter represents the standard deviation of the aspect ratio.

3.8.3.6 CARDS 402002 through 402013 (Coefficients “c1a”, “c2a”, “d1a”, “d2a”)

These parameters represent the polynomial coefficients to correlate a 1-D PARFUME solution with a multi-dimension solution from detailed ABAQUS calculations for asphericity.

3.8.4 CARD 403001 (Correlation Coefficients – Partial IPyC Debonding)

3.8.4.1 “sigd0”

This parameter represents the mean SiC strength for a debonded CFP (MPa).

3.8.4.2 “umd”

This parameter represents the SiC stress, at the minimum value, for a debonded CFP where all parameters are at mean values (MPa).

3.8.4.3 "bond0"

This parameter represents the IPyC bond strength, at the maximum value or at the end of the solution, for a debonded CFP where all parameters are at mean values (MPa).

3.8.4.4 "bond0var"

This parameter represents the bond strength standard deviation.

3.8.4.5 CARDS 403002 through 403013 (Coefficients "c1d" and "c2d")

These parameters represent the polynomial coefficients necessary to correlate a 1-D PARFUME solution with a multi-dimensional solution from detailed ABAQUS calculations for IPyC debonding.

4. INSTALLATION AND EXECUTION

4.1 Introduction

PARFUME is written in American National Standards Institute (ANSI) “standard” FORTRAN 77, but the code has been compiled using an Intel Visual Fortran 90 compiler. Currently, support is provided only for Linux platforms; Microsoft operating systems are not supported. Although it is expected that PARFUME v2.19 will operate properly on most Linux operating systems, the current version of the program has only been tested on SUSE 10.3.

This section presents a summary of the procedure to install and execute PARFUME on Linux platforms.

4.1.1 Transmittal Media

PARFUME is transmitted via CD-ROM disk.

4.1.2 Hardware/Software Requirements

Linux operating system

486DX or higher processor

25 MB of available hard disk space

4.1.3 Linux Quick Installation Guide

4.1.3.1 Installation/Execution Steps

Table 4-1. PARFUME installation steps.

Step No.	Description
1	Insert CD into CD-ROM drive.
2	Transfer the file ‘*.x’ to the hard drive.
3	At the prompt, type the PARFUME program version name.
4	Follow the instructions on the screen.

5. PARFUME CODE RESULTS

This section presents a summary of code outputs, error messages, and post processing. Note that a code restart option is not currently available. The complete output file data for PARFUME, including examples and parameters, is presented in Section 6.

5.1 Output Data File

The output data deck file name must be consistent with standard MS Windows file-naming protocol; in addition, the output file name is the same name as the input file name, but with a file type of "*.res".

The output data file echoes the parameters that the user input via the data file. In addition, located within the output file after the heading "Input after processing," is the input (i.e., "irradiation history derived from input") data as processed by PARFUME. Specifically, the environmental parameters, described in Table A-1 are processed and output in a table format. The output headings are described below.

5.1.1 Irradiation History Derived from Input

5.1.1.1 Step

This output heading is the number of steps, which always begins with the number 1.

5.1.1.2 ttime (days)

This output heading is the transient time.

5.1.1.3 flut (e25 n/m2)

This output heading is the fast fluence specified in 10^{25} n/m^2, E>0.18 MeV.

5.1.1.4 bupt (%FIMA)

This output heading is the burnup specified in percent fissions per initial metal atom (%FIMA).

5.1.1.5 xprest (mpa)

This output heading is external pressure specified in MPa.

5.1.1.6 btempt (k)

This output heading is the boundary temperature specified in degrees Kelvin.

5.2 Post Processing

The output data is not in a format to be read directly into a post processing program such as Tecplot or Visit, although the data, with some minor manipulation, can be put into a data format required by MS Excel for data manipulation and graphical display. For example, opening the output data file using MS Excel with "delimited" file type selected and "space" delimiter selected will produce a manageable file for data analysis and plotting.

5.3 Error Messages

PARFUME will issue a warning for most, but not all, erroneous user inputs; nevertheless, users are expected to be familiar with PARFUME and the expectation of realistic inputs. Although it is not practical to list all the error messages that a user might encounter while running PARFUME, a few of the most common error messages are presented and discussed below.

5.3.1 Missing Card

In the event that the user fails to include the necessary cards for the simulation, PARFUME will provide the following error message:

failed while reading input because
----
did not find cards 102001
failed because inputs below are invalid

U235ENR (U235 enrichment %)
OURAT (oxygen to uranium atom ratio)
CURAT (carbon to uranium atom ratio)

5.3.2 Invalid Inputs Example

In this example, a value of -14% was entered in the input data deck. The subsequent error message is:

failed because inputs below are invalid

U235ENR (U235 enrichment %)

5.3.3 Missing Input Data File

In the event that the input data file is not located in the same directory as the executable or an incorrect input data file name is used, the following error message will be displayed:

Enter input ('x'.dat) filename:
sample#1.dat
Input (sample#1.dat) file was not found
Please enter 'x'.dat filename or QUIT
sample#1.dat
Input (sample#1.dat) file was not found
Please enter 'x'.dat filename or QUIT
QUIT

5.3.4 Missing ABAQUS data file

With respect to ABAQUS data, PARFUME reads the data, identifies the maximum and minimum temperature values for each volume element, divides the identified data into 21 bins, averages the temperatures in each bin, and utilizes the average temperatures in probability calculations. This CAE data must be in a specified format consistent with the ABAQUS standard output format. Note that if this option is selected and an ABAQUS input file is not located within the same directory as the PARFUME executable file, the user will be prompted as follow:

"*Input (x.abq) file was not found*

Please enter 'x'.abq filename or QUIT"

Additionally, the CAE file name must be the same the PARFUME input data file; and the file must have an "x.abq" file type.

5.3.5 Fuel Element Node Mismatch

This error occurred due to a mismatch between the input variables "ngn" and "ngti."

failed during history processing because
---
init temp sequential expansion .ne. NGN fluence in boundary htc history > EOLFLU

6. SAMPLE PROBLEMS

The sample problem presented below was executed using PARFUME Version 1.1. Nearly identical results will be obtained with PARFUME Version 2.19.

6.1 Sample Problem #1

In this problem, a fuel element with pebble bed geometry and TRISO CFPs is irradiated for 351 days, at a temperature of 1113.2 K and pressure of 0.1 MPa, to an accumulated fluence of 5×10^{25} n/m^2 (E>0.18 MeV). One day later, after cooling to approximately 573 K, it is placed in an oven and heated to 1873 K at an ambient pressure of 0.1 MPa. The fast integration solution scheme is used, and the following models are activated: Kr-85m R/B, HSC CO production, and Booth equivalent sphere fission gas release. Additional details, including environmental conditions, particle geometry, and run parameters are specified in the input data deck below. The fuel element environmental history is presented in Figures 6-1, 6-2, and 6-3.

6.1.1 Input Data Deck (prob#1_.dat)

```
*####################################################################*
************** GENERAL OPTIONS (SOLVERS/MODELS) **************
* CARD 100001 (simulation name)
*       title
100001   'Sample Problem #1' *
* CARD 101001 (run parameters)
*            pfss     ncases   nburp   sample   dtf   iseed
101001           2   10000000   100        1 *
* CARD 101002 (models)
*         idebondp    ifacet   rbvalue   comodel  fgmodel  idebug
101002           0         0         1         3        2       0

********************** MATERIAL PROPERTIES **********************
* CARD  101002  (fuel  characteristics)
*          u235enr (%)  ourat  curat
102001           9.82      2.     0.
* CARD 103001 (kernel properties)
*          kernd(g/cm^3) kernt(g/cm^3)
103001             10.81
* CARD 103002 (buffer properties)
*          buffd(g/cm^3) bufft(g/cm^3)
103002               1.
```

```
* CARD 103003 (IPyC properties)
*         ipycdn(g/cm^3)  ipycdvar(g/cm^3)
103003              1.9               0.
* CARD 103005  (OPyC properties)
*         opycdn(g/cm^3)   opycdvar(g/cm^3)
103005             1.88                0.
*
* CARD 103013  (IPyC Bacon anisotropic factor)
*         ibafn   ibafvar
103013    1.053        0.
* CARD 103015  (OPyC  Bacon  anisotropic  factor)
*         obafn   obafvar
103015    1.019        0. *
*
* CARD 103023  (IPyC  Weibull  modulus)
*          ipycm
103023     9.50
* CARD 103024  (SiC  Weibull  modulus)
*          sigm
103024     8.02
* CARD 103025  (OPyC  Weibull  modulus)
*          opycm
103025     9.50
*
* CARD  103033  (Poisson's  ratio)
*           cnu      cnub
103033      0.5       0.5
* CARD  103043  (creep  amplification  factor)
*           creepampn      creepvar
103043         2.0           0.0 *
* CARD  103054  (Enable  ZrC)
*          zrc         zrcp
103054      0           1 *
*
```

```
* CARD  103061  (defective  SiC  layers)
*          fdef
103061     0.0
******************** FUEL PARTICLE GEOMETRY ********************

* CARD  104001  (kernel  geometry)
*           kerndia(e-6 m)   kernvar(e-6 m)
104001                497.               0.
*104001                497.             14.1

* CARD 104002 (buffer geometry)
*          buffthk(e-6 m)   buffvar(e-6 m)
104002                94.               0.
*104002                94.             10.3

* CARD 104003 (IPyC geometry)
*           ipycthk(e-6 m)   ipycvar(e-6 m)
104003                 41.               0.
*104003                 41.               4.

* CARD 104004 (SiC geometry)
*           sicthk(e-6 m)     sicvar(e-6 m)
104004                36.               0.
*104004                36.               1.7

* CARD 104005 (OPyC geometry)

*           opycthk(e-6 m)     opycvar(e-6 m)
104005                 40.                0.
*104005                 40.                2.2

* (variance ignored, it has little impact on results, saves cpu time)


******************** FUEL ELEMENT DESCRIPTION ********************
```

```
* CARD 105001  (Pebblebed)
105001    PEBBLEBED
* CARD 105011 (Pebblebed)
*         partnum(particles/pebble)    ngnfm   ngn
105011                         1631.        7    10
* CARD 105021  (Pebblebed)
*         pebdia(m)   pebcldtk(m)
105021       .02600        .00300
* CARD  105031  (Pebblebed)
*          fmden(g/cm^3)
105031              1.75

* CARD 105041  (Pebblebed)
*         ucontam 105041    1.82E-6

******************** FUEL ELEMENT ENVIRONMENT ********************

* CARD 106001  (fuel temperature option)
*           rtmpopt
106001    FIFD-CALC
* CARD 106021 (global node temperatures)
*         tgi(k)  ntgi
106021    1113.2    10
* CARD 201001  (fission product transport description)
*         fpspecie
201001          Ag
*
* CARD  SERIES 301XXX  (fluence v- time input)
*          timeirr(days)   flu(e25 n/m^2)
301001              351.              5.0
301002              352.        5.0000003
301003          352.0208        5.0000003062
301004          352.0833        5.0000003250
301005          352.3125        5.0000003937
```

```
301006          352.3333        5.0000004000
301007          352.8958        5.0000005687
301008          353.2083        5.0000006625
301009          365.8750        5.0000041625
*
* CARD SERIES  302XXX  (burnup v- fluence  input)
*         flu(e25 n/m^2)    bup(%FIMA)
302001              5.0          11.1
302002         5.0000041625       11.1
*
* CARD  SERIES  303XXX  (external pressure v- fluence input)
*        external  pressure v- fluence input
*          flu(e25 n/m^2)  pamb(MPa)
303001                0.         .1
*
* CARD SERIES 304XXX  (boundary temperature v- fluence input)
*         flu(e25 n/m^2)  btemp(k)
304001              5.0       1113.2
304002         5.0000001        999.667
304003         5.0000002        786.333
304004          5.0000003        573.
304005         5.0000003062     573.
304006         5.0000003125     823.
304007         5.0000003187    1073.
304008         5.0000003250    1323.
304009         5.0000003937    1323.
304010         5.0000004       1523.
304011         5.0000005687    1523.
304012         5.0000006156    1698.
304013         5.0000006625    1873.
304014         5.0000041625   1873.

* CARD SERIES 306XXX  (time heatup starts and irradiation ends)
*        thus(days)
306001         352.
```

```
*
******************** CORRELATION COEFFICIENTS ********************
* CARD SERIES  401XXX  (correlation coefficients for ipyc cracking)
*         sigcr0(MPa)    umc(MPa)
401001         1543.87     228.394
*              c1c             c2c
  401002        0.0000          0.0000      * for fuel particle radial posit
  401003        0.0000          0.0000      * for kernel diameter
  401004        0.0000          0.0000      * for buffer thickness
  401005      2.002910e-2   -1.104311e-4    * for ipyc thickness
  401006      4.751676e-3    2.421231e-4    * for sic thickness
  401007     -1.572899e-2    2.521020e-4    * for opyc thickness
  401008         0.0000        0.0000       * for ipyc density
  401009         0.0000        0.0000       * for opyc density
  401010         0.0000        0.0000       * for ipyc baf
  401011         0.0000        0.0000       * for opyc baf
  401012         0.0000        0.0000       * for creep coeff amplication
*
* CARD SERIES 402XXX  (correlation coefficients for ipyc asphericity)
*         siga0(MPa)   um(MPa)  delum(MPa)  aration   aratvar
402001          1000.     1000.       1000.       1. 0.
*        c1a         c2a           d1a        d2a
  402002  0.0000     0.0000        0.0000      0.0000     * fuel part rad pos
  402003  0.0000     0.0000        0.0000      0.0000 * for kernel diamet
  402004  0.0000     0.0000        0.0000      0.0000 * for buffer thickn
  402005  0.0000     0.0000        0.0000      0.0000 * for ipyc thicknes
  402006  0.0000     0.0000        0.0000      0.0000 * for sic thickness
  402007  0.0000     0.0000        0.0000      0.0000 * for opyc thicknes
  402008  0.0000     0.0000        0.0000      0.0000 * for ipyc density
  402009  0.0000     0.0000        0.0000      0.0000 * for opyc density
  402010  0.0000     0.0000        0.0000      0.0000 * for ipyc baf
  402011  0.0000     0.0000        0.0000      0.0000 * for opyc baf
  402012  0.0000     0.0000        0.0000      0.0000 * for creep coef
  402013  0.0000     0.0000        0.0000      0.0000 * for asphericity
```

```
* CARD SERIES 403XXX  (correlation coefficients for ipyc debonding)
*          sigd0(MPa)    umd(MPa)   bond0(MPa)   bond0var(MPa)
403001         1000.       100.        100.             0.
*              c1d           c2d
  403002       0.0000          0.0000   * for fuel particle radial posit
  403003       0.0000          0.0000   * for kernel diameter
  403004       0.0000          0.0000   * for buffer thickness
  403005       0.0000          0.0000   * for ipyc thickness
  403006       0.0000          0.0000   * for sic thickness
  403007       0.0000          0.0000   * for opyc thickness
  403008       0.0000          0.0000   * for ipyc density
  403009       0.0000          0.0000   * for opyc density
  403010       0.0000          0.0000   * for ipyc baf
  403011       0.0000          0.0000   * for opyc baf
  403012       0.0000          0.0000   * for creep coeff amplication
  403013       0.0000          0.0000   * for asphericity effects
  *
.
 ######################################################################
```

6.1.2 Input Data Deck Notes

1. Parameters not specified on the input data deck—for example, values for variables—will default to those specified on Table A-1, located in the Appendix. For example on card number 101001, a value for the variable “dtf” is not specified, so the variable “dtf” will default to a value of “0” (design-to-fail analysis is turned off).
2. Note the end of file period ‘.’ required at the end of the file.
3. Card number 10602X could have been specified as shown below:

```
*          fuel element temperature options
*              rtmpopt
106001       FIFD-CALC
*                    tgi(k)       ntgi
106021       1113.2            1
106022       1113.2            2
106023       1113.2            3
106024       1113.2            4
```

```
106025      1113.2          5
106026      1113.2          6
106027      1113.2          7
106028      1113.2          8
106029      1113.2          9
106030      1113.2          10
```

4. Note that the some users may choose to sanitize the data deck of comments and some input parameters that will default to the desired value. An example of such a data deck is presented in Section 6.1.2.1.

6.1.2.1 Example "Sanitized" Data Deck (prob#1_.dat)

```
* $RCSfile:  $
*   $Source:  $
*   $Revision:  $
*   $Date:  $
*   $Author: $
*
*     hidden options
*       casenum
*
*     title
100001  'TEST AG'
*
*
*     run parameters
*           pfss      ncases      nburp      sample
101001         2    10000000       1000           1
*    idebondp      ifacet    rbvalue     comodel     fgmodel    idebug
101002     0           0          1           3           2          0
*
*
*     fuel characteristics
*       u235enr(%)  ourat  curat
```

```
 102001     9.82      2.     0.
*
*
*      particle material  properties
*         kernd(g/cm^3)
103001            10.81
*         buffd(g/cm^3)
103002               1.
*        ipycdn(g/cm^3)   ipycdvar(g/cm^3)
103003             1.9                 0.
*        opycdn(g/cm^3)   opycdvar(g/cm^3)
103005            1.88                 0.
*
*        ibafn  ibafvar
103013   1.053        0.
*        obafn  obafvar
103015   1.019        0.
*
*         sigm
103024    8.02
*
*
*      particle geometry
*         kerndia(e-6 m)   kernvar(e-6 m)
104001             497.               0.
*104001              497.             14.1
*         buffthk(e-6 m)   buffvar(e-6 m)
104002              94.               0.
*104002               94.             10.3
*         ipycthk(e-6 m)   ipycvar(e-6 m)
104003              41.               0.
*104003               41.               4.
*          sicthk(e-6 m)    sicvar(e-6 m)
104004              36.               0.
```

```
*104004               36.               1.7
*         opycthk(e-6 m)    opycvar(e-6 m)
104005               40.                0.
*104005               40.               2.2
* to save cpu, variance was ignored because it has little impact
*
*
*      fuel element description
*          reactor
105001   PEBBLEBED
*        partnum(particles/pebble)     ngnfm     ngn
105011                        1631.         7      10
*        pebdia(m)  pebcldtk(m)
105021      .02600       .00300
*105021      .03190       .00595 *
*        fmden(g/cm^3)
105031            1.75
*
*        ucontam
105041   1.82E-6
*
*
*      fuel element temperature options
*           rtmpopt
106001    FIFD-CALC
*         tgi(k)    ntgi
106021    1113.2      10
*
*
*         fission product transport description
*           fpspecie
201001            Ag
*
*
```

```
*         fluence v- time input
*           timeirr(days)  flu(e25 n/m^2)
301001               351.             5.0
301002               352.       5.0000003
301003           352.0208       5.0000003062
301004           352.0833       5.0000003250
301005           352.3125       5.0000003937
301006           352.3333       5.0000004000
301007           352.8958       5.0000005687
301008           353.2083       5.0000006625
301009           365.8750       5.0000041625
*
*
*     burnup v- fluence input
*       flu(e25 n/m^2)  bup(%FIMA)
302001             5.0        11.1
302002    5.0000041625        11.1
*
*
*     external pressure v- fluence input
*       flu(e25 n/m^2)  pamb(MPa)
303001              0.         .1
*
*
*     boundary temperature v- fluence input
*       flu(e25 n/m^2)  btemp(k)
304001             5.0       1113.2
304002       5.0000001        999.667
304003       5.0000002        786.333
304004       5.0000003        573.
304005       5.0000003062     573.
304006       5.0000003125     823.
304007       5.0000003187    1073.
304008       5.0000003250    1323.
```

```
304009       5.0000003937    1323.
304010       5.0000004       1523.
304011       5.0000005687    1523.
304012       5.0000006156    1698.
304013       5.0000006625    1873.
304014       5.0000041625    1873.
*
*      time heatup starts (& irradiation ends)
*        thus(days)
306001        352.
*
*
*      correlation function coefficients for ipyc cracking
*        sigcr0(MPa)  umc(MPa)
401001       1543.87   228.394
*
*                  c1c           c2c
401005      2.002910e-2   -1.104311e-4     * for ipyc thickness
401006      4.751676e-3    2.421231e-4     * for sic thickness
401007     -1.572899e-2    2.521020e-4     * for opyc thickness
*
*
        correlation function coefficients for asphericity
          siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001         1000.    1000.       1000.       1.       0.
*
*
*       correlation function coefficients for partial ipyc debonding
*         sigd0(MPa)  umd(MPa)  bond0(MPa)  bond0var(MPa)
403001         1000.      100.        100.             0.
*
.
```

6.1.3 User Screen Output (prob#1_.dat)

```
hammkd@inl383782:~/Documents/PARFUME/user_guide/sample_prob#1> ./pf.x
  12/02/09                    07:53:58
PARFUME  :  INL Particle Fuel Performance Model - v1.10
   ------    Providing statistical calculations of failure
              probabilities for TRISO-coated fuel particles
Enter input  ('x'.dat)  filename:
prob#1_.dat
**********************************
 Processing input from set number          1
 12/02/09                    07:53:58
 Start of multiple integration for    4 variables over    11 divisions
   (which requires a total of       390 increments)
 Increment   Elapsed
 Completed   Time (s)
 ---------   -------
       100         9.
       200        12.
       300        15.
       400        18.
       500        21.
       600        24.
       700        27.
       800        30.
       900        33.
      1000        36.
      1100        39.
      1200        42.

End of multiple integration for        1284 increments

  Probability of SiC failure                      1.235427E-07
    Contribution due to amoeba effect    0.000000E+00
    Contribution due to IPyC cracking    1.142557E-07
```

```
   Contribution due to IPyC debonding   0.000000E+00
   Contribution due to pressure         9.287065E-09
 Probability of IPyC cracking         4.799876E-01
 Probability of IPyC debonding        0.000000E+00
 Buffer/IPyC contact due to gap closure was predicted in           0
 increments
 Buffer shrinkage was limited by theoretical density during        0
 increments
 IPyC reached the stress/swelling data limit at 1350 C in        459
 increments
 OPyC reached the stress/swelling data limit at 1350 C in        459
 increments
 Calculation time:      44.5730000000003     seconds
 Average number of increments per second =     8.74969151728619
 Normal  end  of  processing  for  set  number                     1
 ****************************************
 Null input set detected: Normal end of PARFUME
hammkd@inl383782:~/Documents/PARFUME/user_guide/sample_prob#1> ll
```

6.1.4 Screen Output Notes

1. On the screen output, the word “increments” actually represents integration points; furthermore, the number of integration points represents the number of particles analyzed.
2. Note that the screen output “which requires a total of 390 increments” actually represents 390 integration points (i.e., particles for deterministic analyses, full integration and fast integration). This value is used by code developers to provide an estimate of the number of integration points. The actual number of integration points is 408, specified on the screen output: “IPyC reached the stress/swelling data limit at 1350°C in 408 increments.”
3. With the variable sample = 1 (i.e., standard deviation included in analysis), the diffusion model included in the analysis (i.e., fspecie parameter specified), and no user input for any of the input variables having a standard deviation, four variables are specified on the screen output following “Start of multiple integration …” (i.e., three strength variables: IPyC, SiC, and OPyC and particle radial position in the matrix).
4. With the variable sample = 0 (i.e., standard deviation not included in analysis) and the diffusion model included in the analysis (i.e., fspecie parameter specified), and no user input for any of the input variables having a standard deviation, three variables are specified on the screen output following “Start of multiple integration …” (i.e., three strength variables: IPyC, SiC, and OPyC). There is no distribution for the particles; therefore, all particles are at the same radial position in the matrix).

5. Note that “11 divisions” represent the maximum number of parts that the normal distribution for variables (such as particle diameter, thickness, density, radial position, BAF, creep amplification) is separated into for the analysis.
6. Note that strength (i.e., IPyC, SiC, OPyC) defaults to being an integration variable when the diffusion model is selected. In this case, the number of integration points is not 11 (unlike the default value of 11 for the other integration points); the number of integration points, which is approximately 4–7, is determined by a subroutine.

6.1.5 Output Data (prob#1_01.res)

The results from this simulation are presented in graphical form followed by portions of the numerical results, which begin in Section 6.1.5.2.

6.1.5.1 Graphical Analysis of Results

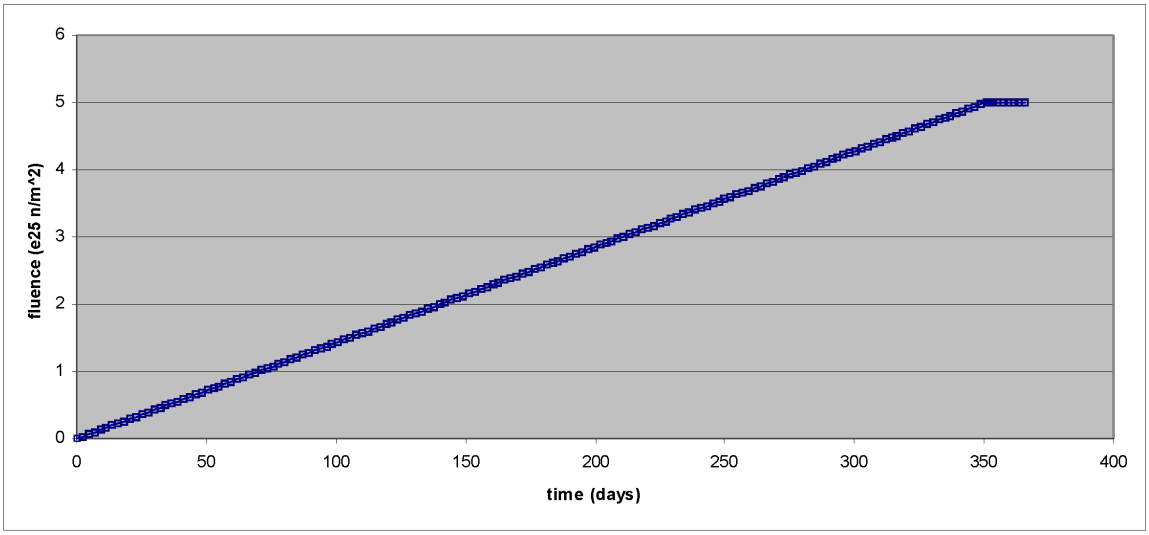


Figure 6-1. Accumulated irradiation history.

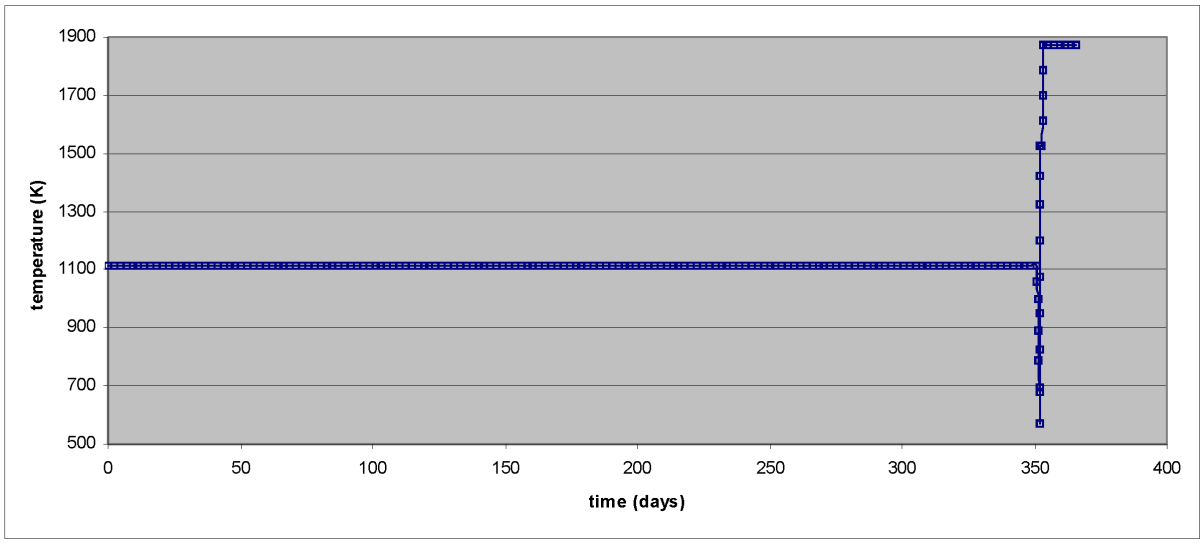


Figure 6-2. Fuel element surface temperature history.

Note that upon removal from the reactor, the fuel element cools prior to heatup in the oven. Additionally, PARFUME does not model the heat generated due to the decay of radioactive nuclides; therefore, the only energy generation occurs as the result of the heat due to the oven.

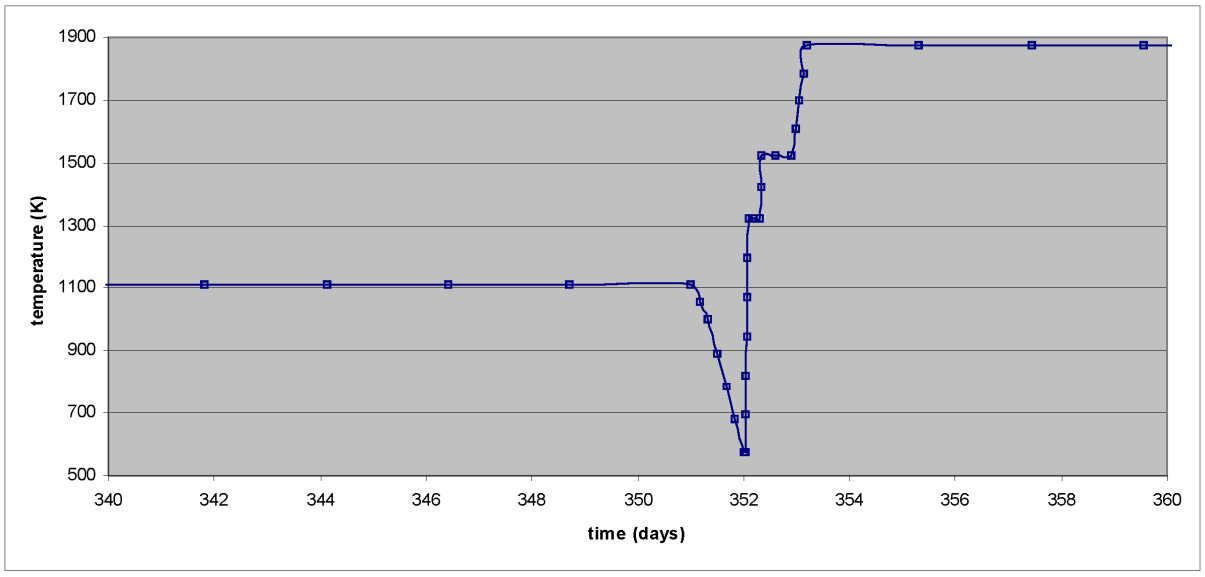


Figure 6-3. Fuel element surface temperature history (heatup).

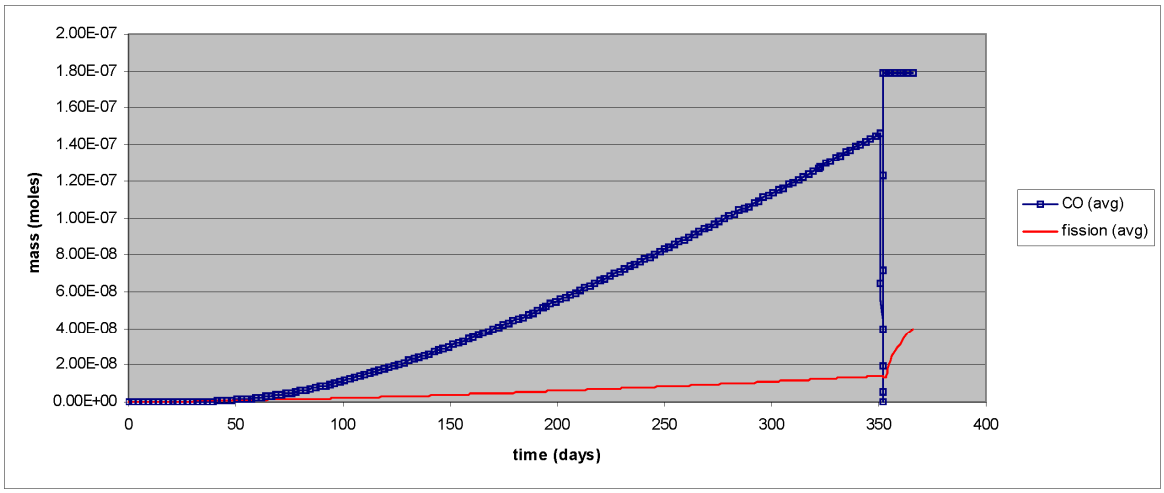


Figure 6-4. Moles of gas produced.

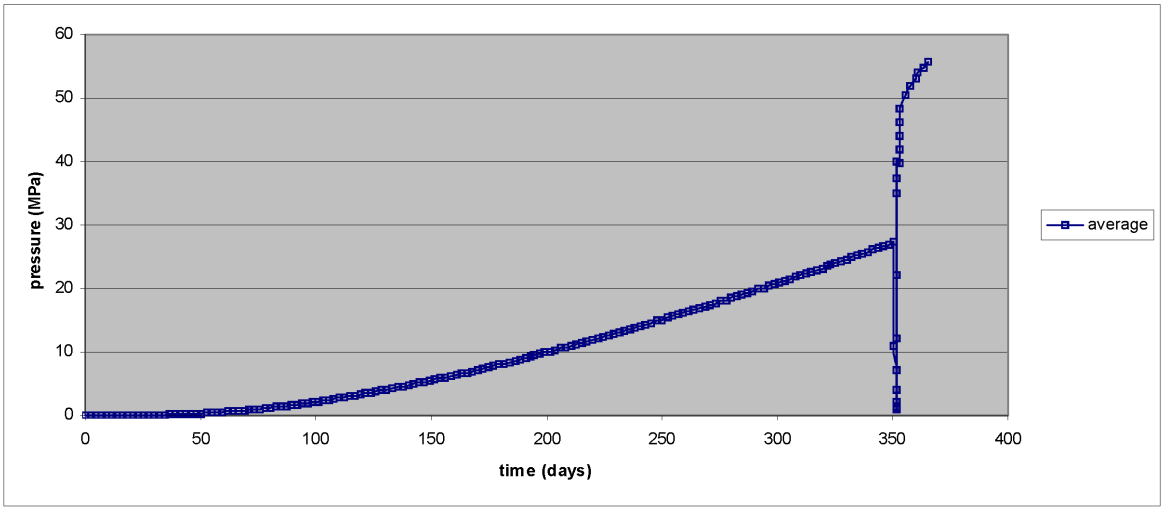


Figure 6-5. Particle internal pressure.

Particle internal pressure buildup due to CO and FP gas production as shown in Figure 6-4. Note that the increase in pressure at 350 days is due to the particle temperature increase due to heatup in the oven.

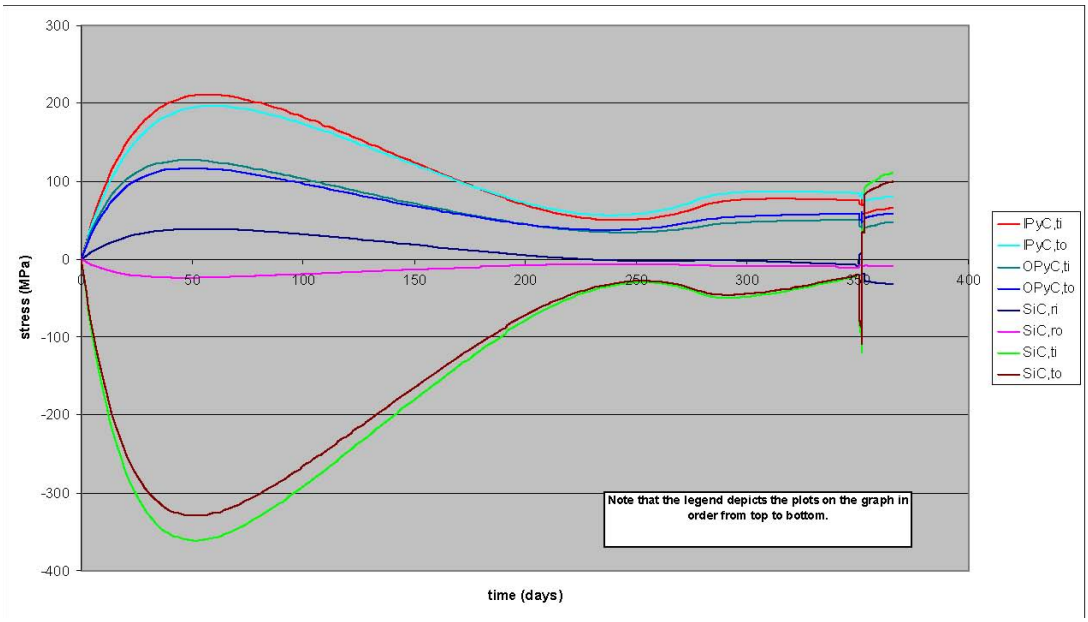


Figure 6-6. Particle nominal stress history.

The IPyC and OPyC layers exhibit shrink and creep due to irradiation; the SiC remains rigid, experiencing only elastic deformation. In addition, as shown in Figure 6-5, the pressure in the particle gradually increases due to gas buildup. During the first 55 days of irradiation, the magnitude of the stresses increase due to shrinkage of the IPyC and OPyC layers, while the SiC layer experiences compressive stresses as the result of the OPyC layer shrinking into the SiC and the IPyC shrinkage away from the SiC layer. Furthermore, the gradual increase in pressure does not significantly contribute (i.e., offset) the tensile hoop stress in the pyrocarbon layers. As irradiation continues past 55 days, the magnitude of the stresses decreases as the result of material creep. Eventually, the pressure load becomes significant; specifically, the pressure stress counters the SiC compressive stresses, resulting in a decrease in the magnitude of the SiC stress. The stress magnitude increases past 350 days due to the increase in fuel element temperature as a result of head addition in the oven. Failure of the particle is expected to occur if the stress in the SiC layer reaches the SiC fracture strength.

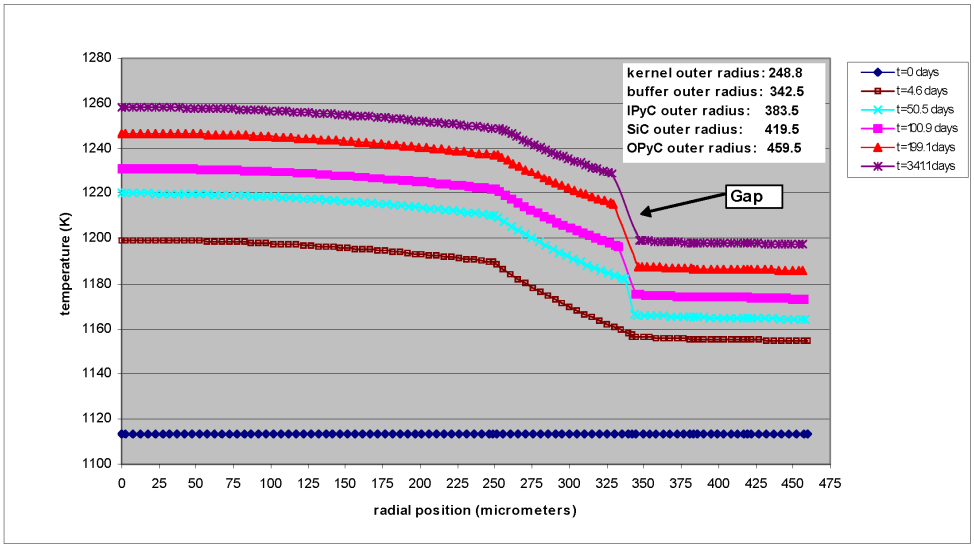


Figure 6-7. Particle radial temperature profile.

As expected, a parabolic temperature gradient occurs in the fuel kernel due to heat generation from fission within the kernel; a linear temperature profile is observed in the buffer due to no energy generation within the buffer. A gap at the interface of the buffer and IPyC layer begins to form at 4.6 days. Since the thermal properties of the PyC layers and SiC layer are similar, a large temperature gradient does not develop.

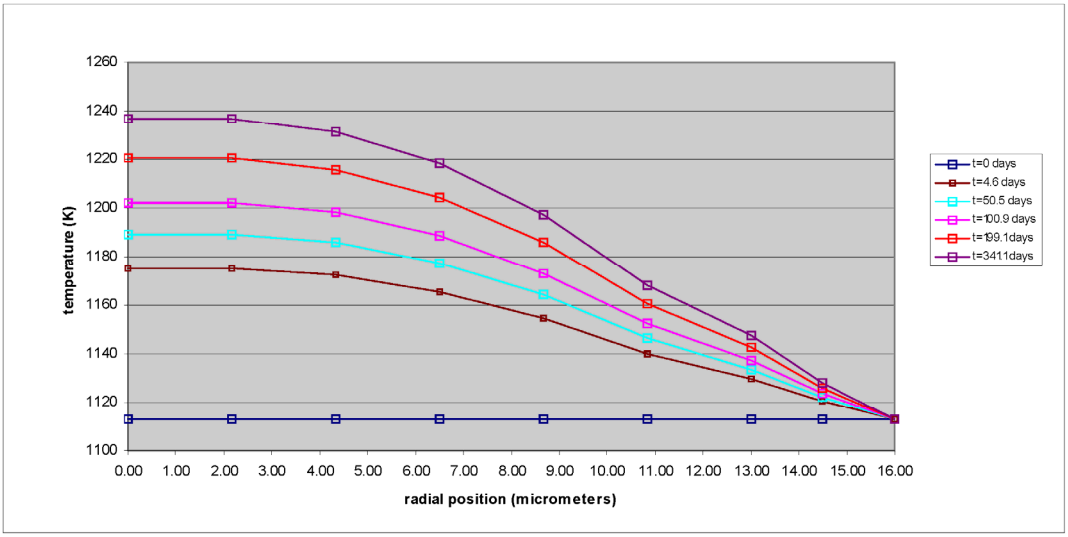


Figure 6-8. Fuel element temperature profile.

As expected, a parabolic temperature gradient occurs in the fueled region of the fuel element due to heat generation from fission. A linear temperature profile develops in the unfueled region. Also note that the user input value for the number of global nodes is 10; since the outer node of the fueled region overlaps the inner node of the unfueled region, data associated with only nine nodes is plotted.

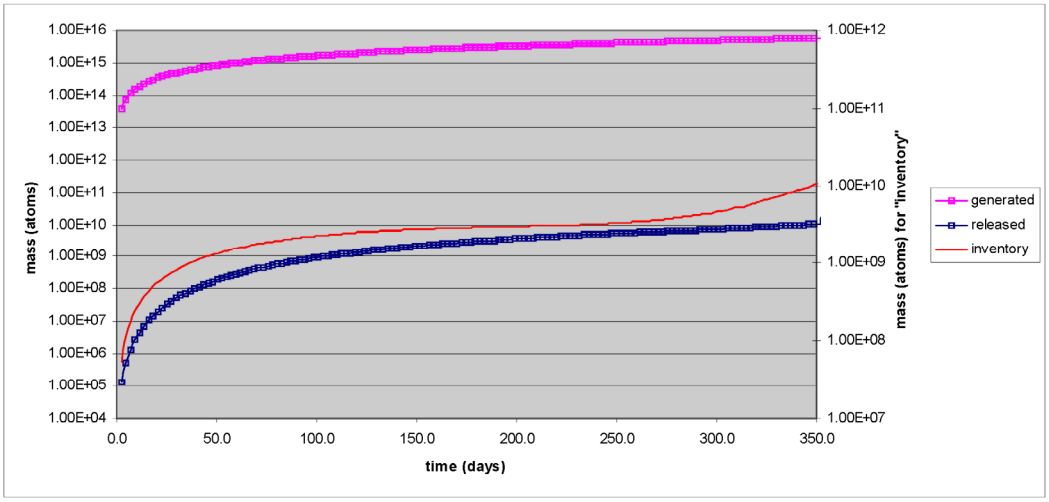


Figure 6-9. "AG" global FP diffusion release history.

The amount of silver (Ag) released as a fraction of Ag generated increases from 3×10^{-9} at 2.3 days to 2×10^{-6} after 350 days. Note that the value for "inventory" of Ag is incorrect.

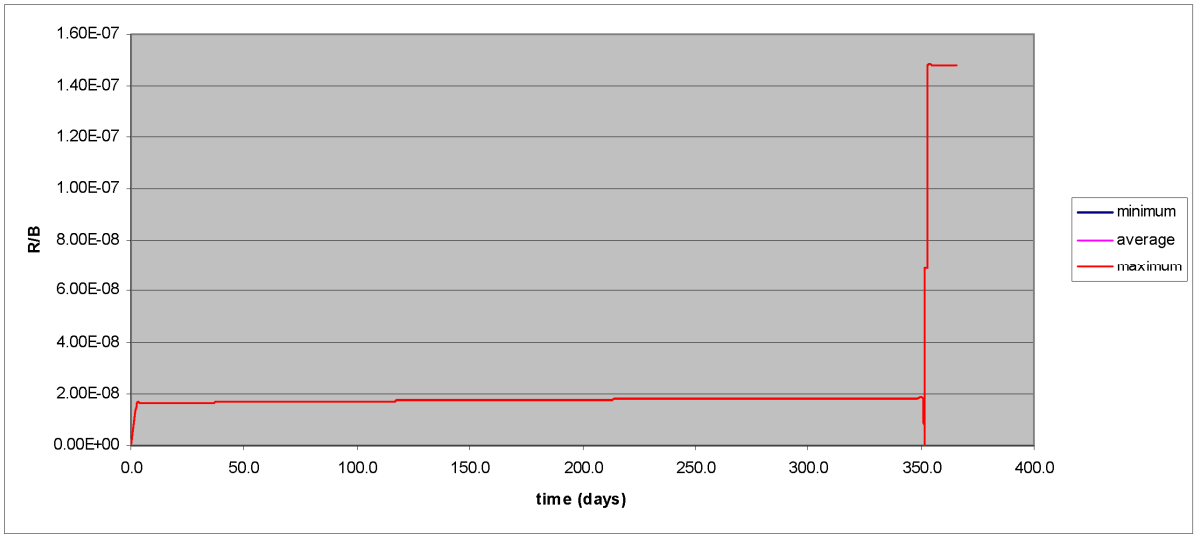


Figure 6-10. Kr-85m release-to-birth ratio.

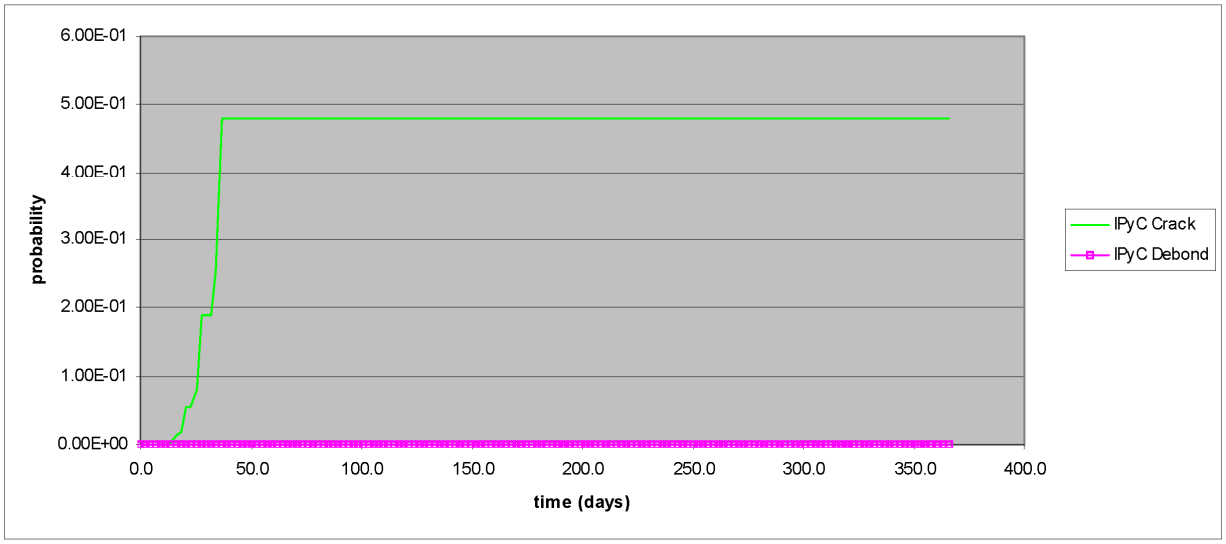


Figure 6-11. IPyC failure probability.

Note that the probability for IPyC failure due to cracking is less than 0.5, and the probability for IPyC failure due to debonding is 0 since the debonding model was not selected by the user.

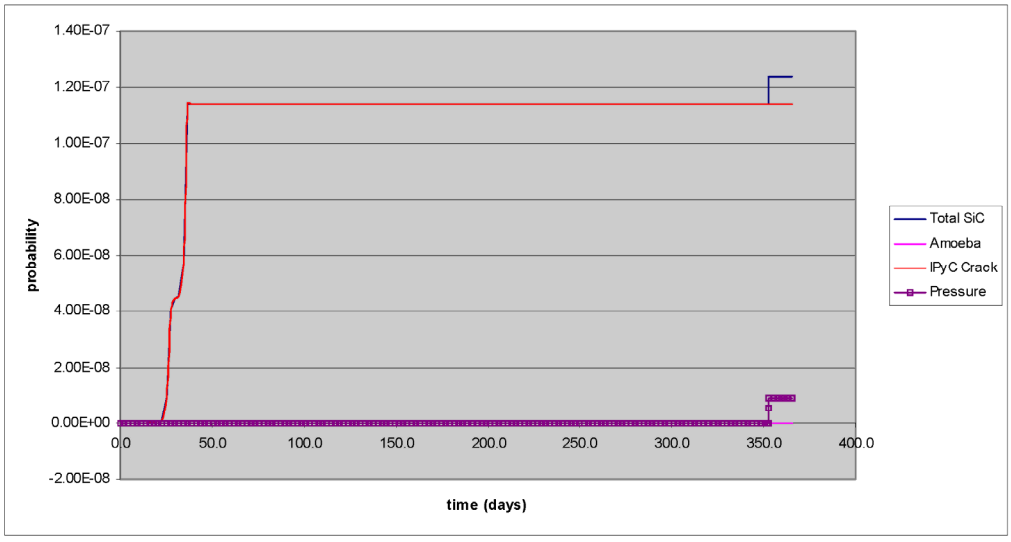


Figure 6-12. SiC failure probability.

Note that the probability for SiC failure due to cracking of the IPyC is less than 1.2e-7, yet the probability for IPyC failure due to cracking is less than 0.5 (see Figure 6-11). In addition, the increase in failure probability during the first 50 days correlates with the increased stress magnitudes described in Figure 6-6.

6.1.5.2 Numerical Results

The results are compiled in an output file named "prob#1_01.res" which includes an input echo, irradiation history derived from input, and the output data such as failure probability, particle and fuel element temperature, and particle internal pressure. The input echo includes the parameter values input by the user and the default parameters, which may not have been included by the user in the input deck. In addition, irradiation history is derived from user input is provided to assist the user in evaluating whether or not the environmental conditions included in the input deck are the expected conditions by the user.

```
12/02/09 07:53:58


PARFUME  : INL Particle Fuel Performance Model - v1.10
------    Providing statistical calculations of failure
              probabilities for TRISO-coated fuel particles

 **********************************


Processing input from set number             1


12/02/09                   07:53:58


Input echo
==========
*
*PARFUME V??? Input Data Deck
*
*#########################################################################


*************** GENERAL OPTIONS (SOLVERS/MODELS) ***************
*  CARD 100001 (simulation name)
*        title
100001     'Sample Problem #1'
*
* CARD 101001 (run parameters)
*             pfss      ncases      nburp      sample      dtf      iseed
101001           2    10000000       100           1
*
```

```
* CARD 101002 (models)
*         idebondp     ifacet     rbvalue     comodel     fgmodel     idebug
101002           0          0           1           3           2           0
*
********************* MATERIAL PROPERTIES *********************
* CARD 101002 (fuel characteristics)
*         u235enr(%)     ourat     curat
102001          9.82        2.        0.
*
* CARD 103001 (kernel properties)
*         kernd(g/cm^3) kernt(g/cm^3)
103001            10.81
* CARD 103002 (buffer properties)
*         buffd(g/cm^3) bufft(g/cm^3)
103002               1.
* CARD 103003 (IPyC properties)
*         ipycdn(g/cm^3) ipycdvar(g/cm^3)
103003               1.9               0.
* CARD 103005 (OPyC properties)
*         opycdn(g/cm^3) opycdvar(g/cm^3)
103005              1.88               0.
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*         ibafn ibafvar
103013    1.053      0.
* CARD 103015 (OPyC Bacon anisotropic factor)
*         obafn obafvar
103015    1.019      0.
*
* CARD 103023 (IPyC Weibull modulus)
 *        ipycm
103023    9.50
* CARD 103024 (SiC Weibull modulus)
*         sigm
```

```
103024    8.02
* CARD 103025 (OPyC Weibull modulus)
*         opycm
103025    9.50 *
* CARD 103033 (Poisson's ratio)
*         cnu     cnub
103033    0.5     0.5
* CARD 103043 (creep amplification factor)
*         creepampn     creepvar
103043       2.0          0.0
*
* CARD 103054 (Enable ZrC)
*          zrc     zrcp
103054      0       1
*
* CARD 103061 (defective SiC layers)
*         fdef
103061    0.0
*
******************** FUEL PARTICLE GEOMETRY *********************
* CARD 104001 (kernel geometry)
*         kerndia(e-6 m)    kernvar(e-6 m)
104001              497.                0.
*104001              497.             14.1
* CARD 104002 (buffer geometry)
*         buffthk(e-6 m)   buffvar(e-6 m)
104002               94.               0.
*104002               94.            10.3 *
*
* CARD 104003 (IPyC geometry)
*         ipycthk(e-6 m)   ipycvar(e-6 m)
104003               41.               0.
*104003               41.               4.
* CARD 104004 (SiC geometry)
```

```
*         sicthk(e-6 m)   sicvar(e-6 m)
104004              36.             0.
*104004              36.            1.7
* CARD 104005 (OPyC geometry)
*         opycthk(e-6 m)   opycvar(e-6 m)
104005               40.              0.
*104005               40.             2.2
* (to save cpu, variance was ignored because it has little impact on resu
*
******************** FUEL ELEMENT DESCRIPTION ********************
 * CARD 105001 (Pebblebed)
105001 PEBBLEBED
* CARD 105011 (Pebblebed)
*         partnum(particles/pebble)     ngnfm     ngn
105011                         1631.         7      10
* CARD 105021 (Pebblebed)
*         pebdia(m)     pebcldtk(m)
105021       .02600          .00300
* CARD 105031 (Pebblebed)
*         fmden(g/cm^3)
105031             1.75
* CARD 105041 (Pebblebed)
*         ucontam
105041    1.82E-6
*
******************** FUEL ELEMENT ENVIRONMENT ********************
* CARD 106001 (fuel temperature option)
*           rtmpopt
 106001    FIFD-CALC
* CARD 106021 (global node temperatures)
*         tgi(k)     ntgi
106021    1113.2       10
* CARD 201001 (fission product transport description)
*         fpspecie
```

```
201001          Ag *
* CARD SERIES 301XXX  (fluence v- time input)
*         timeirr(days)   flu(e25 n/m^2)
301001             351.              5.0
301002             352.        5.0000003
301003         352.0208        5.0000003062
301004         352.0833        5.0000003250
301005         352.3125        5.0000003937
301006         352.3333        5.0000004000
301007         352.8958        5.0000005687
301008         353.2083        5.0000006625
301009         365.8750        5.0000041625
*
*
* CARD SERIES 302XXX   (burnup v- fluence input)
*         flu(e25 n/m^2)    bup(%FIMA)
302001               5.0          11.1
302002         5.0000041625       11.1
*
*
* CARD SERIES 303XXX  (external pressure v- fluence input)
*       external pressure v- fluence input
*         flu(e25 n/m^2)  pamb(MPa)
303001               0.         .1
*
* CARD SERIES 304XXX  (boundary temperature v- fluence input)
*         flu(e25 n/m^2)  btemp(k)
304001             5.0     1113.2
304002        5.0000001      999.667
304003        5.0000002      786.333
304004        5.0000003      573.
304005        5.0000003062   573.
304006        5.0000003125   823.
304007        5.0000003187  1073.
```

```
304008        5.0000003250  1323.
304009        5.0000003937  1323.
304010        5.0000004     1523.
304011        5.0000005687  1523.
304012        5.0000006156  1698.
304013        5.0000006625  1873.
304014        5.0000041625  1873.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*         thus(days)
306001          352.

******************** CORRELATION COEFFICIENTS ********************
* CARD SERIES 401XXX  (correlation coefficients for ipyc cracking)
*         sigcr0(MPa)   umc(MPa)
401001        1543.87    228.394
*              c1c             c2c
401002         0.0000         0.0000       * for fuel particle radial posit
401003         0.0000         0.0000       * for kernel diameter
401004         0.0000         0.0000       * for buffer thickness
401005       2.002910e-2    -1.104311e-4   * for ipyc thickness
401006       4.751676e-3     2.421231e-4   * for sic thickness
401007      -1.572899e-2     2.521020e-4   * for opyc thickness
401008         0.0000         0.0000       * for ipyc density
401009         0.0000         0.0000       * for opyc density
401010         0.0000         0.0000       * for ipyc baf
401011         0.0000         0.0000       * for opyc baf
401012         0.0000         0.0000       * for creep coeff amplication

 *
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*          siga0(MPa)    um(MPa)    delum(MPa)    aration    aratvar
402001          1000.      1000.         1000.         1.         0.
*        c1a        c2a        d1a        d2a
```

```
402002    0.0000     0.0000    0.0000      0.0000        * fuel part rad pos
402003    0.0000     0.0000    0.0000      0.0000        * for kernel diamet
402004    0.0000     0.0000    0.0000      0.0000        * for buffer thickn
402005    0.0000     0.0000    0.0000      0.0000        * for ipyc thicknes
402006    0.0000     0.0000    0.0000      0.0000        * for sic thickness
402007    0.0000     0.0000    0.0000      0.0000        * for opyc thicknes
402008    0.0000     0.0000    0.0000      0.0000        * for ipyc density
402009    0.0000     0.0000    0.0000      0.0000        * for opyc density
402010    0.0000     0.0000    0.0000      0.0000        * for ipyc baf
402011    0.0000     0.0000    0.0000      0.0000        * for opyc baf
402012    0.0000     0.0000    0.0000      0.0000        * for creep coef
402013    0.0000     0.0000    0.0000      0.0000        * for asphericity
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
*         sigd0(MPa)    umd(MPa)    bond0(MPa)    bond0var(MPa)
403001         1000.        100.          100.              0.
              c1d             c2d
403002        0.0000           0.0000           * for fuel particle radial
position
403003        0.0000           0.0000           * for kernel diameter
403004        0.0000           0.0000           * for buffer thickness
403005        0.0000           0.0000           * for ipyc thickness
403006        0.0000           0.0000           * for sic thickness
403007        0.0000           0.0000           * for opyc thickness
403008        0.0000           0.0000           * for ipyc density
403009        0.0000           0.0000           * for opyc density
403010        0.0000           0.0000           * for ipyc baf
403011        0.0000           0.0000           * for opyc baf
403012        0.0000           0.0000           * for creep coeff
amplication
403013        0.0000           0.0000           * for asphericity effects
*


.
```

```
Input after processing
======================
*       title
100001    Sample Problem #1
*
*
*       run parameters
*            pfss       ncases       nburp       sample       dtf       iseed
101001          2     10000000         100            1         0         305
*        idebondp       ifacet     rbvalue      comodel   fgmodel      idebug
101002          0            0           1            3         2           0
*
*
*       fuel characteristics
*         u235enr(%)    ourat    curat
102001         9.820     2.00     0.00
*
**       particle material properties
*          kernd(g/cm^3)     kernt(g/cm^3)
103001            10.810            11.030
*          buffd(g/cm^3)     bufft(g/cm^3)
103002             1.000             2.250
*         ipycdn(g/cm^3)  ipycdvar(g/cm^3)
103003             1.900             0.000
*         opycdn(g/cm^3)  opycdvar(g/cm^3)
103005             1.880             0.000
*
*          ibafn           ibafvar
103013     1.053             0.000
*          obafn           obafvar
103015     1.019             0.000
*
*          ipycm
103023     9.500
```

```
*          sigm
103024     8.020
*          opycm
103025     9.500
*
*            cnu         cnub
103033     0.500       0.500
*
*          creepampn      creepvar
103043          2.00          0.00
*
*          zrc         zrcp
103054       0           1
*
*          fdef
103061     0.00
* *
*          particle geometry
*             kerndia(e-6 m)    kernvar(e-6 m)
104001                  497.0               0.0
*             buffthk(e-6 m)    buffvar(e-6 m)
104002                   94.0               0.0
*             ipycthk(e-6 m)    ipycvar(e-6 m)
104003                   41.0               0.0
*              sicthk(e-6 m)     sicvar(e-6 m)
104004                   36.0               0.0
*             opycthk(e-6 m)    opycvar(e-6 m)
104005                   40.0               0.0
**
*          fuel matrix description
*             reactor
105001     PEBBLEBED
*          partnum (particles/pebble)     ngnfm     ngn
105011                       1.63E+03         7      10
```

```
*          pebdia(m)      pebcldtk(m)
105021        0.026            0.0030
*
*          fmden(g/cm^3)
105031              1.75
*
*          ucontam
105041   1.820E-06
*
**         fuel matrix temperature options
*          rtmpopt
106001    FIFD-CALC *
*
*        initial fuel matrix temperatures
*          temperature(k)    node
              1113.20          1
              1113.20          2
              1113.20          3
              1113.20          4
              1113.20          5
              1113.20          6
              1113.20          7
              1113.20          8
              1113.20          9
              1113.20         10
*
```

*	irradiation history derived from input				
		flut	bupt	xprest	
*step	ttime (days)	(e25 n/m^2, E>.18 MeV)	(% FIMA)	(mps)	btempt (k)
1	0.000	0.000	0.000	0.100	1113.200
2	2.294	0.033	0.073	0.100	1113.200
3	4.588	0.065	0.145	0.100	1113.200
4	6.882	0.098	0.218	0.100	1113.200
5	9.176	0.131	0.290	0.100	1113.200
6	11.471	0.163	0.363	0.100	1113.200
7	13.765	0.196	0.435	0.100	1113.200
8	16.059	0.229	0.508	0.100	1113.200
9	18.353	0.261	0.580	0.100	1113.200
10	20.647	0.294	0.653	0.100	1113.200
11	22.941	0.327	0.725	0.100	1113.200
12	25.235	0.359	0.798	0.100	1113.200
13	27.529	0.392	0.871	0.100	1113.200
14	29.824	0.425	0.943	0.100	1113.200
15	32.118	0.458	1.016	0.100	1113.200
16	34.412	0.490	1.088	0.100	1113.200
17	36.706	0.523	1.161	0.100	1113.200
18	39.000	0.556	1.233	0.100	1113.200
19	41.294	0.588	1.306	0.100	1113.200
20	43.588	0.621	1.378	0.100	1113.200
21	45.882	0.654	1.451	0.100	1113.200
22	48.176	0.686	1.524	0.100	1113.200
23	50.471	0.719	1.596	0.100	1113.200
24	52.765	0.752	1.669	0.100	1113.200
25	55.059	0.784	1.741	0.100	1113.200
26	57.353	0.817	1.814	0.100	1113.200
27	59.647	0.850	1.886	0.100	1113.200
28	61.941	0.882	1.959	0.100	1113.200
29	64.235	0.915	2.031	0.100	1113.200
30	66.529	0.948	2.104	0.100	1113.200
31	68.824	0.980	2.176	0.100	1113.200

*	irradiation history derived from input				
		flut	bupt	xprest	
*step	ttime (days)	(e25 n/m^2, E>.18 MeV)	(% FIMA)	(mps)	btempt (k)
32	71.118	1.013	2.249	0.100	1113.200
33	73.412	1.046	2.322	0.100	1113.200
34	75.706	1.078	2.394	0.100	1113.200
35	78.000	1.111	2.467	0.100	1113.200
36	80.294	1.144	2.539	0.100	1113.200
37	82.588	1.176	2.612	0.100	1113.200
38	84.882	1.209	2.684	0.100	1113.200
39	87.176	1.242	2.757	0.100	1113.200
40	89.471	1.275	2.829	0.100	1113.200
41	91.765	1.307	2.902	0.100	1113.200
42	94.059	1.340	2.975	0.100	1113.200
43	96.353	1.373	3.047	0.100	1113.200
44	98.647	1.405	3.120	0.100	1113.200
45	100.941	1.438	3.192	0.100	1113.200
46	103.235	1.471	3.265	0.100	1113.200
47	105.529	1.503	3.337	0.100	1113.200
48	107.824	1.536	3.410	0.100	1113.200
49	110.118	1.569	3.482	0.100	1113.200
50	112.412	1.601	3.555	0.100	1113.200
51	114.706	1.634	3.627	0.100	1113.200
52	117.000	1.667	3.700	0.100	1113.200
53	119.294	1.699	3.773	0.100	1113.200
54	121.588	1.732	3.845	0.100	1113.200
55	123.882	1.765	3.918	0.100	1113.200
56	126.176	1.797	3.990	0.100	1113.200
57	128.471	1.830	4.063	0.100	1113.200
58	130.765	1.863	4.135	0.100	1113.200
59	133.059	1.895	4.208	0.100	1113.200
60	135.353	1.928	4.280	0.100	1113.200
61	137.647	1.961	4.353	0.100	1113.200
62	139.941	1.993	4.425	0.100	1113.200
63	142.235	2.026	4.498	0.100	1113.200

*	irradiation history derived from input				
		flut	bupt	xprest	
*step	ttime (days)	(e25 n/m^2, E>.18 MeV)	(% FIMA)	(mps)	btempt (k)
64	144.529	2.059	4.571	0.100	1113.200
65	146.824	2.092	4.643	0.100	1113.200
66	149.118	2.124	4.716	0.100	1113.200
67	151.412	2.157	4.788	0.100	1113.200
68	153.706	2.190	4.861	0.100	1113.200
69	156.000	2.222	4.933	0.100	1113.200
70	158.294	2.255	5.006	0.100	1113.200
71	160.588	2.288	5.078	0.100	1113.200
72	162.882	2.320	5.151	0.100	1113.200
73	165.176	2.353	5.224	0.100	1113.200
74	167.471	2.386	5.296	0.100	1113.200
75	169.765	2.418	5.369	0.100	1113.200
76	172.059	2.451	5.441	0.100	1113.200
77	174.353	2.484	5.514	0.100	1113.200
78	176.647	2.516	5.586	0.100	1113.200
79	178.941	2.549	5.659	0.100	1113.200
80	181.235	2.582	5.731	0.100	1113.200
81	183.529	2.614	5.804	0.100	1113.200
82	185.824	2.647	5.876	0.100	1113.200
83	188.118	2.680	5.949	0.100	1113.200
84	190.412	2.712	6.022	0.100	1113.200
85	192.706	2.745	6.094	0.100	1113.200
86	195.000	2.778	6.167	0.100	1113.200
87	197.294	2.810	6.239	0.100	1113.200
88	199.588	2.843	6.312	0.100	1113.200
89	201.882	2.876	6.384	0.100	1113.200
90	204.176	2.908	6.457	0.100	1113.200
91	206.471	2.941	6.529	0.100	1113.200
92	208.765	2.974	6.602	0.100	1113.200
93	211.059	3.007	6.675	0.100	1113.200
94	213.353	3.039	6.747	0.100	1113.200
95	215.647	3.072	6.820	0.100	1113.200

*	irradiation history derived from input				
		flut	bupt	xprest	
*step	ttime (days)	(e25 n/m^2, E>.18 MeV)	(% FIMA)	(mps)	btempt (k)
96	217.941	3.105	6.892	0.100	1113.200
97	220.235	3.137	6.965	0.100	1113.200
98	222.529	3.170	7.037	0.100	1113.200
99	224.824	3.203	7.110	0.100	1113.200
100	227.118	3.235	7.182	0.100	1113.200
101	229.412	3.268	7.255	0.100	1113.200
102	231.706	3.301	7.327	0.100	1113.200
103	234.000	3.333	7.400	0.100	1113.200
104	236.294	3.366	7.473	0.100	1113.200
105	238.588	3.399	7.545	0.100	1113.200
106	240.882	3.431	7.618	0.100	1113.200
107	243.176	3.464	7.690	0.100	1113.200
108	245.471	3.497	7.763	0.100	1113.200
109	247.765	3.529	7.835	0.100	1113.200
110	250.059	3.562	7.908	0.100	1113.200
111	252.353	3.595	7.980	0.100	1113.200
112	254.647	3.627	8.053	0.100	1113.200
113	256.941	3.660	8.125	0.100	1113.200
114	259.235	3.693	8.198	0.100	1113.200
115	261.529	3.725	8.271	0.100	1113.200
116	263.824	3.758	8.343	0.100	1113.200
117	266.118	3.791	8.416	0.100	1113.200
118	268.412	3.824	8.488	0.100	1113.200
119	270.706	3.856	8.561	0.100	1113.200
120	273.000	3.889	8.633	0.100	1113.200
121	275.294	3.922	8.706	0.100	1113.200
122	277.588	3.954	8.778	0.100	1113.200
123	279.882	3.987	8.851	0.100	1113.200
124	282.176	4.020	8.924	0.100	1113.200
125	284.471	4.052	8.996	0.100	1113.200
126	286.765	4.085	9.069	0.100	1113.200
127	289.059	4.118	9.141	0.100	1113.200

*	irradiation history derived from input				
		flut	bupt	xprest	
*step	ttime (days)	(e25 n/m^2, E>.18 MeV)	(% FIMA)	(mps)	btempt (k)
128	291.353	4.150	9.214	0.100	1113.200
129	293.647	4.183	9.286	0.100	1113.200
130	295.941	4.216	9.359	0.100	1113.200
131	298.235	4.248	9.431	0.100	1113.200
132	300.529	4.281	9.504	0.100	1113.200
133	302.824	4.314	9.576	0.100	1113.200
134	305.118	4.346	9.649	0.100	1113.200
135	307.412	4.379	9.722	0.100	1113.200
136	309.706	4.412	9.794	0.100	1113.200
137	312.000	4.444	9.867	0.100	1113.200
138	314.294	4.477	9.939	0.100	1113.200
139	316.588	4.510	10.012	0.100	1113.200
140	318.882	4.542	10.084	0.100	1113.200
141	321.176	4.575	10.157	0.100	1113.200
142	323.471	4.608	10.229	0.100	1113.200
143	325.765	4.641	10.302	0.100	1113.200
144	328.059	4.673	10.375	0.100	1113.200
145	330.353	4.706	10.447	0.100	1113.200
146	332.647	4.739	10.520	0.100	1113.200
147	334.941	4.771	10.592	0.100	1113.200
148	337.235	4.804	10.665	0.100	1113.200
149	339.529	4.837	10.737	0.100	1113.200
150	341.824	4.869	10.810	0.100	1113.200
151	344.118	4.902	10.882	0.100	1113.200
152	346.412	4.935	10.955	0.100	1113.200
153	348.706	4.967	11.027	0.100	1113.200
154	351.000	5.000	11.100	0.100	1113.200
155	351.167	5.000	11.100	0.100	1056.433
156	351.333	5.000	11.100	0.100	999.667
157	351.500	5.000	11.100	0.100	893.000
158	351.667	5.000	11.100	0.100	786.333
159	351.833	5.000	11.100	0.100	679.666

```
*       irradiation history derived from input
```

*step	ttime (days)	flut (e25 n/m^2, E>.18 MeV)	bupt (% FIMA)	xprest (mps)	btempt (k)
160	352.000	5.000	11.100	0.100	573.000
161	352.010	5.000	11.100	0.100	573.000
162	352.021	5.000	11.100	0.100	573.000
163	352.031	5.000	11.100	0.100	698.000
164	352.042	5.000	11.100	0.100	823.000
165	352.052	5.000	11.100	0.100	948.000
166	352.062	5.000	11.100	0.100	1073.000
167	352.073	5.000	11.100	0.100	1198.000
168	352.083	5.000	11.100	0.100	1323.000
169	352.198	5.000	11.100	0.100	1323.000
170	352.313	5.000	11.100	0.100	1323.000
171	352.323	5.000	11.100	0.100	1423.000
172	352.333	5.000	11.100	0.100	1523.000
173	352.615	5.000	11.100	0.100	1523.000
174	352.896	5.000	11.100	0.100	1523.000
175	352.974	5.000	11.100	0.100	1610.500
176	353.052	5.000	11.100	0.100	1698.000
177	353.130	5.000	11.100	0.100	1785.500
178	353.208	5.000	11.100	0.100	1873.000
179	355.319	5.000	11.100	0.100	1873.000
180	357.431	5.000	11.100	0.100	1873.000
181	359.542	5.000	11.100	0.100	1873.000
182	359.653	5.000	11.100	0.100	1873.000
183	363.764	5.000	11.100	0.100	1873.000
184	365.875	5.000	11.100	0.100	1873.000

```
*       time heatup starts
*         thus(days)
306001      352.000
*
*       correlation function coefficients for ipyc cracking
*         sigcr0(mpa)    umc(mpa)
```

```
401001      1543.870    228.394
*                 c1c            c2c
401002     0.00000          0.00000        * for fuel prtcle radial position
401003     0.00000          0.00000        * for kernel diameter
401004     0.00000          0.00000        * for buffer thickness
401005    2.002910E-02   -1.104311E-04     * for ipyc thickness
401006    4.751676E-03    2.421231E-04     * for sic thickness
401007   -1.572899E-02    2.521020E-04     * for opyc thickness
401008     0.00000          0.00000        * for ipyc density
401009     0.00000          0.00000        * for opyc density
401010     0.00000          0.00000        * for ipyc baf
401011     0.00000          0.00000        * for opyc baf
401012     0.00000          0.00000        * for creep coeff amplification
*      correlation function coefficients for asphericity
        siga0(mpa)   um(mpa)   delum(mpa)   aration   aratvar
402001    1000.000  1000.000     1000.000     1.000     0.000
*               c1a          c2a        d1a         d2a
402002   0.00000   0.00000   0.00000   0.00000    * for fuel prtcle radial
position
402003   0.00000   0.00000   0.00000   0.00000    * for kernel diameter
402004   0.00000   0.00000   0.00000   0.00000    * for buffer thickness
402005   0.00000   0.00000   0.00000   0.00000    * for ipyc thickness
402006   0.00000   0.00000   0.00000   0.00000    * for sic thickness
402007   0.00000   0.00000   0.00000   0.00000    * for opyc thickness
402008   0.00000   0.00000   0.00000   0.00000    * for ipyc density
402009   0.00000   0.00000   0.00000   0.00000    * for opyc density
402010   0.00000   0.00000   0.00000   0.00000    * for ipyc baf
402011   0.00000   0.00000   0.00000   0.00000    * for opyc baf
402012   0.00000   0.00000   0.00000   0.00000    * for creep coeff
amplification
402013   0.00000   0.00000   0.00000   0.00000    * for asphericity effects
*
*      correlation function coefficients for partial ipyc debonding
*        sigcr0(mpa)   umd(mpa)   bond0(mpa)   bond0var(mpa)
403001      1000.000    100.00      100.00      0.000
*                 c1d            c2d
```

```
403002      0.00000    0.00000         * for fuel prtcle radial position
403003      0.00000    0.00000         * for kernel diameter
403004      0.00000    0.00000         * for buffer thickness
403005      0.00000    0.00000         * for ipyc thickness
403006      0.00000    0.00000         * for sic thickness
403007      0.00000    0.00000         * for opyc thickness
403008      0.00000    0.00000         * for ipyc density
403009      0.00000    0.00000         * for opyc density
403010      0.00000    0.00000         * for ipyc baf
403011      0.00000    0.00000         * for opyc baf
403012      0.00000    0.00000         * for creep coeff amplification
403013      0.00000    0.00000         * for asphericity effects
*
.
Start of multiple integration for       4 variables over       11 divisions
  (which requires a total of          390 increments)

Increment      Elapsed
Completed      Time (s)
---------      -------
   100               9.
   200              12.
   300              15.
   400              18.
   500              21.
   600              24.
   700              27.
   800              30.
   900              33.
  1000              36.
  1100              39.
  1200              42.

End of multiple integration for      390 increments
```

```
Probability of SiC failure                1.235427E-07
Contribution due to amoeba effect         0.000000E+00
Contribution due to IPyC cracking         1.142557E-07
Contribution due to IPyC debonding        0.000000E+00
Contribution due to pressure              9.287065E-09
Probability of IPyC cracking              4.799876E-01
Probability of IPyC debonding             0.000000E+00
Buffer/IPyC contact due to gap closure was predicted in increments      0
Buffer shrinkage was limited by theoretical density during increments   0
IPyC reached the stress/swelling data limit at 1350°C in increments     459
OPyC reached the stress/swelling data limit at 1350°C in increments     459
Calculation time: 44.5730000000003 Average      seconds
number of increments per second =              8.74969151728619
 Normal end of processing for set number
                                                  1
****************************************
```

Failure probabilities vs time (s) and fast fluence (10^25 n/m^2, E>.18 MeV)

			- - - - CONTRIBUTION TO TOTAL DUE TO - - -					
TIME	FLU	TOTAL	AMOEBA	IPyC CRACK	IPyC DEBND	PRESSURE	IPyC CRACK	IPyC DEBND
0.000000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1.982118E+05	3.2680E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	7.8722E-10	0.0000E+00
3.964235E+05	6.5359E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	5.7001E-07	0.0000E+00
5.946353E+05	9.8039E-02	4.9211E-14	0.0000E+00	4.9211E-14	0.0000E+00	0.0000E+00	2.6837E-05	0.0000E+00
7.928471E+05	1.3072E-01	2.6025E-12	0.0000E+00	2.6025E-12	0.0000E+00	0.0000E+00	2.5401E-04	0.0000E+00
9.910588E+05	1.6340E-01	1.8908E-11	0.0000E+00	1.8908E-11	0.0000E+00	0.0000E+00	1.1108E-03	0.0000E+00
1.189271E+06	1.9608E-01	6.8908E-11	0.0000E+00	6.8908E-11	0.0000E+00	0.0000E+00	3.4312E-03	0.0000E+00
1.387482E+06	2.2876E-01	1.5372E-10	0.0000E+00	1.5372E-10	0.0000E+00	0.0000E+00	1.2764E-02	0.0000E+00
1.585694E+06	2.6144E-01	3.8517E-10	0.0000E+00	3.8517E-10	0.0000E+00	0.0000E+00	1.9217E-02	0.0000E+00
1.783906E+06	2.9412E-01	7.1770E-10	0.0000E+00	7.1770E-10	0.0000E+00	0.0000E+00	5.5732E-02	0.0000E+00
1.982118E+06	3.2680E-01	7.1770E-10	0.0000E+00	7.1770E-10	0.0000E+00	0.0000E+00	5.5732E-02	0.0000E+00
2.180329E+06	3.5948E-01	9.4016E-09	0.0000E+00	9.4016E-09	0.0000E+00	0.0000E+00	8.0129E-02	0.0000E+00
2.378541E+06	3.9216E-01	4.0765E-08	0.0000E+00	4.0765E-08	0.0000E+00	0.0000E+00	1.8889E-01	0.0000E+00
2.576753E+06	4.2484E-01	4.4439E-08	0.0000E+00	4.4439E-08	0.0000E+00	0.0000E+00	1.8889E-01	0.0000E+00
2.774965E+06	4.5752E-01	4.5370E-08	0.0000E+00	4.5370E-08	0.0000E+00	0.0000E+00	1.8889E-01	0.0000E+00
2.973176E+06	4.9020E-01	5.7241E-08	0.0000E+00	5.7241E-08	0.0000E+00	0.0000E+00	2.5353E-01	0.0000E+00
3.171388E+06	5.2288E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
3.369600E+06	5.5556E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
3.567812E+06	5.8824E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
3.766024E+06	6.2092E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
3.964235E+06	6.5359E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
4.162447E+06	6.8627E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
4.360659E+06	7.1895E-01	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
			DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT					
3.049020E+07	5.0000E+00	1.1426E-07	0.0000E+00	1.1426E-07	0.0000E+00	0.0000E+00	4.7999E-01	0.0000E+00
3.049695E+07	5.0000E+00	1.1981E-07	0.0000E+00	1.1426E-07	0.0000E+00	5.5518E-09	4.7999E-01	0.0000E+00
3.050370E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.051045E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.051720E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.069960E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.088200E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.106440E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.124680E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.142920E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00
3.161160E+07	5.0000E+00	1.2354E-07	0.0000E+00	1.1426E-07	0.0000E+00	9.2871E-09	4.7999E-01	0.0000E+00

PARTICLE nominal stress histories (MPa) vs time (s) and fast fluence (10^25 n/m^2, E>.18 MeV)

TIME	FLU	IPC/SiC,ri	SiC/OPC,ro	IPyC, ti	IPyC, to	SiC,ti	SiC,to	OPyC,ti	OPyC,to
0.000000E+00	0.0000E+00	-1.3180E-01	-1.0023E-01	-6.8728E-02	-6.2138E-02	-5.6648E-01	-5.2296E-01	-98795E-02	-9.8909E-02
1.982118E+05	3.2680E-02	4.4161E+00	-3.5948E+00	2.3030E+01	2.0833E+01	-4.6503E+01	-4.2498E+01	1.8399E+01	1.6523E+01
3.964235E+05	6.5359E-02	8.6031E+00	-6.7322E+00	4.4975E+01	4.0589E+01	-8.8861E+01	-8.1193E+01	3.5040E+01	3.1465E+01
5.946353E+05	9.8039E-02	1.2401E+01	-9.4550E+00	6.4902E+01	5.8603E+01	-1.2649E+02	-1.1556E+02	4.9492E+01	4.4482E+01
7.928471E+05	1.3072E-01	1.5837E+01	-1.1812E+01	8.2952E+01	7.4993E+01	-1.5985E+02	-1.4602E+02	6.2015E+01	5.5803E+01
9.910588E+05	1.6340E-01	1.8937E+01	-1.3847E+01	9.9264E+01	8.9872E+01	-1.8936E+02	-1.7297E+02	7.2841E+01	6.5629E+01
1.189271E+06	1.9608E-01	2.1727E+01	-1.5598E+01	1.1397E+02	1.0335E+02	-2.1541E+02	-1.9674E+02	8.2176E+01	7.4141E+01
1.387482E+06	2.2876E-01	2.4230E+01	-1.7100E+01	1.2720E+02	1.1553E+02	-2.3833E+02	-2.1767E+02	9.0200E+01	8.1495E+01
1.585694E+06	2.6144E-01	2.6468E+01	-1.8384E+01	1.3905E+02	1.2650E+02	-2.5845E+02	-2.3602E+02	9.7073E+01	8.7830E+01
1.783906E+06	2.9412E-01	2.8462E+01	-1.9475E+01	1.4965E+02	1.3636E+02	-2.7603E+02	-2.5207E+02	1.0293E+02	9.3266E+01
1.982118E+06	3.2680E-01	3.0230E+01	-2.0396E+01	1.5908E+02	1.4519E+02	-2.9134E+02	-2.6603E+02	1.0791E+02	9.7912E+01
2.180329E+06	3.5948E-01	3.1792E+01	-2.1169E+01	1.6745E+02	1.5308E+02	-3.0460E+02	-2.7812E+02	1.1209E+02	1.0186E+02
2.378541E+06	3.9216E-01	3.3163E+01	-2.1812E+01	1.7484E+02	1.6008E+02	-3.1600E+02	-2.8852E+02	1.1560E+02	1.0520E+02
2.576753E+06	4.2484E-01	3.4359E+01	-2.2340E+01	1.8133E+02	1.6628E+02	-3.2575E+02	-2.9740E+02	1.1850E+02	1.0799E+02
2.774965E+06	4.5752E-01	3.5394E+01	-2.2767E+01	1.8700E+02	1.7174E+02	-3.3399E+02	-3.0491E+02	1.2087E+02	1.1031E+02
2.973176E+06	4.9020E-01	3.6281E+01	-2.3106E+01	1.9191E+02	1.7652E+02	-3.4088E+02	-3.1119E+02	1.2277E+02	1.1220E+02
3.171388E+06	5.2288E-01	3.7033E+01	-2.3368E+01	1.9612E+02	1.8066E+02	-3.4656E+02	-3.1636E+02	1.2426E+02	1.1372E+02
3.369600E+06	5.5556E-01	3.7660E+01	-2.3561E+01	1.9970E+02	1.8423E+02	-3.5113E+02	-3.2052E+02	1.2539E+02	1.1491E+02
3.567812E+06	5.8824E-01	3.8173E+01	-2.3693E+01	2.0270E+02	1.8726E+02	-3.5472E+02	-3.2379E+02	1.2620E+02	1.1581E+02
				DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT					
2.596574E+07	4.2810E+00	-2.2593E+00	-9.4244E+00	7.6562E+01	8.6553E+01	-4.7798E+01	-4.4216E+01	4.7179E+01	5.5165E+01
2.616395E+07	4.3137E+00	-2.4520E+00	-9.4727E+00	7.6794E+01	8.6766E+01	-4.7073E+01	-4.3562E+01	4.7446E+01	5.5436E+01
2.636216E+07	4.3464E+00	-2.6561E+00	-9.5171E+00	7.6969E+01	8.6923E+01	-4.6262E+01	-4.2832E+01	4.7694E+01	5.5685E+01
2.656038E+07	4.3791E+00	-2.8694E+00	-9.5585E+00	7.7097E+01	8.7033E+01	-4.5383E+01	-4.2038E+01	4.7925E+01	5.5918E+01
2.675859E+07	4.4118E+00	-3.0906E+00	-9.5974E+00	7.7186E+01	8.7106E+01	-4.4446E+01	-4.1192E+01	4.8144E+01	5.6136E+01
2.695680E+07	4.4444E+00	-3.3182E+00	-9.6344E+00	7.7243E+01	8.7148E+01	-4.3462E+01	-4.0304E+01	4.8352E+01	5.6344E+01
2.715501E+07	4.4771E+00	-3.5512E+00	-9.6697E+00	7.7275E+01	8.7165E+01	-4.2439E+01	-3.9380E+01	4.8551E+01	5.6542E+01
2.735322E+07	4.5098E+00	-3.7893E+00	-9.7033E+00	7.7283E+01	8.7159E+01	-4.1377E+01	-3.8420E+01	4.8741E+01	5.6731E+01
2.755144E+07	4.5425E+00	-4.0335E+00	-9.7334E+00	7.7261E+01	8.7124E+01	-4.0260E+01	-3.7411E+01	4.8912E+01	5.6901E+01
2.774965E+07	4.5752E+00	-4.2843E+00	-9.7597E+00	7.7207E+01	8.7057E+01	-3.9085E+01	-3.6347E+01	4.9062E+01	5.7050E+01
2.794786E+07	4.6078E+00	-4.5405E+00	-9.7830E+00	7.7127E+01	8.6965E+01	-3.7860E+01	-3.5239E+01	4.9196E+01	5.7182E+01
2.814607E+07	4.6405E+00	-4.8014E+00	-9.8039E+00	7.7025E+01	8.6851E+01	-3.6596E+01	-3.4095E+01	4.9317E+01	5.7301E+01
2.834428E+07	4.6732E+00	-5.0663E+00	-9.8230E+00	7.6905E+01	8.6720E+01	-3.5299E+01	-3.2920E+01	4.9428E+01	5.7411E+01
2.854249E+07	4.7059E+00	-5.3347E+00	-9.8407E+00	7.6769E+01	8.6574E+01	-3.3974E+01	-3.1721E+01	4.9531E+01	5.7512E+01
2.874071E+07	4.7386E+00	-5.6061E+00	-9.8573E+00	7.6621E+01	8.6416E+01	-3.2626E+01	-3.0501E+01	4.9628E+01	5.7608E+01
2.893892E+07	4.7712E+00	-5.8800E+00	-9.8730E+00	7.6463E+01	8.6248E+01	-3.1259E+01	-2.9263E+01	4.9720E+01	5.7699E+01
2.913713E+07	4.8039E+00	-6.1562E+00	-9.8881E+00	7.6295E+01	8.6072E+01	-2.9875E+01	-2.8010E+01	4.9809E+01	5.7787E+01
2.933534E+07	4.8366E+00	-6.4345E+00	-9.9026E+00	7.6120E+01	8.5888E+01	-2.8478E+01	-2.6744E+01	4.9894E+01	5.7871E+01
2.953355E+07	4.8693E+00	-6.7145E+00	-9.9167E+00	7.5939E+01	8.5699E+01	-2.7068E+01	-2.5466E+01	4.9978E+01	5.7954E+01
2.973176E+07	4.9020E+00	-6.9961E+00	-9.9305E+00	7.5753E+01	8.5505E+01	-2.5647E+01	-2.4179E+01	5.0059E+01	5.8034E+01

PARTICLE nominal temperature histories (in K)

Time (s)	TP(1)	TP(2)	TP(3)	TP(4)	TP(5)	TP(6)	TP(7)	TP(8)	TP(9)	TP(10)	TP(11)	TP(12)
0.000000E+00	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20
1.982118E+05	1197.48	1197.48	1197.47	1197.46	1197.43	1197.40	1197.36	1197.32	1197.26	1197.20	1197.13	1197.05
3.964235E+05	1199.37	1199.37	1199.36	1199.35	1199.32	1199.29	1199.25	1199.21	1199.15	1199.09	1199.02	1198.94
5.946353E+05	1200.96	1200.96	1200.95	1200.93	1200.91	1200.88	1200.84	1200.79	1200.74	1200.67	1200.60	1200.53
7.928471E+05	1202.74	1202.74	1202.73	1202.72	1202.70	1202.66	1202.63	1202.58	1202.52	1202.46	1202.39	1202.31
9.910588E+05	1204.67	1204.67	1204.66	1204.65	1204.62	1204.59	1204.55	1204.50	1204.45	1204.39	1204.32	1204.24
1.189271E+06	1206.68	1206.68	1206.68	1206.66	1206.64	1206.61	1206.57	1206.52	1206.46	1206.40	1206.33	1206.25
1.387482E+06	1208.73	1208.73	1208.72	1208.71	1208.69	1208.65	1208.61	1208.57	1208.51	1208.45	1208.38	1208.30
1.585694E+06	1210.73	1210.73	1210.72	1210.71	1210.68	1210.65	1210.61	1210.57	1210.51	1210.45	1210.38	1210.30
1.783906E+06	1212.58	1212.57	1212.57	1212.55	1212.53	1212.50	1212.46	1212.41	1212.35	1212.29	1212.22	1212.14
1.982118E+06	1214.15	1214.15	1214.14	1214.13	1214.10	1214.07	1214.03	1213.99	1213.93	1213.87	1213.80	1213.72
2.180329E+06	1215.39	1215.39	1215.39	1215.37	1215.35	1215.32	1215.28	1215.23	1215.17	1215.11	1215.04	1214.96
2.378541E+06	1216.30	1216.30	1216.30	1216.28	1216.26	1216.22	1216.19	1216.14	1216.08	1216.02	1215.95	1215.87
2.576753E+06	1216.94	1216.94	1216.93	1216.91	1216.89	1216.86	1216.82	1216.77	1216.72	1216.65	1216.58	1216.50
2.774965E+06	1217.38	1217.38	1217.37	1217.36	1217.33	1217.30	1217.26	1217.21	1217.16	1217.10	1217.02	1216.95
2.973176E+06	1217.71	1217.71	1217.70	1217.68	1217.66	1217.63	1217.59	1217.54	1217.49	1217.42	1217.35	1217.27
3.171388E+06	1217.98	1217.98	1217.97	1217.96	1217.94	1217.90	1217.86	1217.82	1217.76	1217.70	1217.63	1217.55
3.369600E+06	1218.25	1218.25	1218.24	1218.23	1218.20	1218.17	1218.13	1218.08	1218.03	1217.97	1217.89	1217.82
3.567812E+06	1218.53	1218.53	1218.52	1218.51	1218.48	1218.45	1218.41	1218.36	1218.31	1218.25	1218.18	1218.10
3.766024E+06	1218.84	1218.84	1218.83	1218.82	1218.79	1218.76	1218.72	1218.67	1218.62	1218.56	1218.48	1218.41

DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT

Time (s)	TP(97)	TP(98)	TP(99)	TP(100)	TP(101)	TP(102)	TP(103)	TP(104)
0.000000E+00	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20
1.982118E+05	1154.38	1154.28	1154.19	1154.09	1154.00	1153.91	1153.82	1153.78
3.964235E+05	1155.17	1155.07	1154.97	1154.88	1154.79	1154.70	1154.61	1154.57
5.946353E+05	1155.67	1155.57	1155.48	1155.38	1155.29	1155.20	1155.12	1155.07
7.928471E+05	1156.17	1156.08	1155.98	1155.89	1155.80	1155.71	1155.62	1155.58
9.910588E+05	1156.67	1156.58	1156.48	1156.39	1156.30	1156.21	1156.12	1156.08
1.189271E+06	1157.17	1157.07	1156.98	1156.89	1156.79	1156.71	1156.62	1156.58
1.387482E+06	1157.67	1157.57	1157.48	1157.38	1157.29	1157.20	1157.12	1157.07
1.585694E+06	1158.16	1158.06	1157.97	1157.88	1157.79	1157.70	1157.61	1157.57
1.783906E+06	1158.65	1158.56	1158.46	1158.37	1158.28	1158.19	1158.10	1158.06
1.982118E+06	1159.14	1159.05	1158.95	1158.86	1158.77	1158.68	1158.59	1158.55
2.180329E+06	1159.63	1159.53	1159.44	1159.35	1159.26	1159.17	1159.08	1159.04
2.378541E+06	1160.12	1160.02	1159.92	1159.83	1159.74	1159.65	1159.57	1159.52
2.576753E+06	1160.60	1160.50	1160.41	1160.31	1160.22	1160.13	1160.05	1160.01
2.774965E+06	1161.08	1160.98	1160.88	1160.79	1160.70	1160.61	1160.53	1160.49
2.973176E+06	1161.55	1161.46	1161.36	1161.27	1161.18	1161.09	1161.00	1160.96
3.171388E+06	1162.03	1161.93	1161.83	1161.74	1161.65	1161.56	1161.48	1161.44
3.369600E+06	1162.50	1162.40	1162.31	1162.21	1162.12	1162.04	1161.95	1161.91
3.567812E+06	1162.96	1162.87	1162.77	1162.68	1162.59	1162.50	1162.42	1162.37
3.766024E+06	1163.43	1163.33	1163.24	1163.14	1163.05	1162.97	1162.88	1162.84

PARTICLE nominal radii histories (in micrometers)

Time (s)	RP(1)	RP(2)	RP(3)	RP(4)	RP(5)	RP(6)	RP(7)	RP(8)	RP(9)	RP(10)	RP(11)	RP(12)
0.000000E+00	0.00	2.48	7.46	12.43	17.39	22.36	27.33	32.30	37.27	42.24	47.21	52.18
1.982118E+05	0.00	2.49	7.46	12.43	17.40	22.37	27.34	32.31	37.28	42.25	47.22	52.19
3.964235E+05	0.00	2.49	7.46	12.43	17.40	22.37	27.34	32.31	37.28	42.25	47.22	52.20
5.946353E+05	0.00	2.49	7.46	12.43	17.40	22.37	27.35	32.32	37.29	42.26	47.23	52.21
7.928471E+05	0.00	2.49	7.46	12.43	17.41	22.38	27.35	32.32	37.30	42.27	47.24	52.22
9.910588E+05	0.00	2.49	7.46	12.43	17.41	22.38	27.36	32.33	37.30	42.28	47.25	52.23
1.189271E+06	0.00	2.49	7.46	12.44	17.41	22.39	27.36	32.34	37.31	42.29	47.26	52.24
1.387482E+06	0.00	2.49	7.46	12.44	17.42	22.39	27.37	32.34	37.32	42.29	47.27	52.25
1.585694E+06	0.00	2.49	7.47	12.44	17.42	22.40	27.37	32.35	37.33	42.30	47.28	52.26
1.783906E+06	0.00	2.49	7.47	12.44	17.42	22.40	27.38	32.35	37.33	42.31	47.29	52.27
1.982118E+06	0.00	2.49	7.47	12.45	17.43	22.40	27.38	32.36	37.34	42.32	47.30	52.28
2.180329E+06	0.00	2.49	7.47	12.45	17.43	22.41	27.39	32.37	37.35	42.33	47.31	52.29
2.378541E+06	0.00	2.49	7.47	12.45	17.43	22.41	27.39	32.37	37.35	42.33	47.32	52.30
2.576753E+06	0.00	2.49	7.47	12.45	17.44	22.42	27.40	32.38	37.36	42.34	47.32	52.31
2.774965E+06	0.00	2.49	7.47	12.46	17.44	22.42	27.40	32.39	37.37	42.35	47.33	52.32
2.973176E+06	0.00	2.49	7.48	12.46	17.44	22.43	27.41	32.39	37.38	42.36	47.34	52.33
3.171388E+06	0.00	2.49	7.48	12.46	17.45	22.43	27.41	32.40	37.38	42.37	47.35	52.34
3.369600E+06	0.00	2.49	7.48	12.46	17.45	22.43	27.42	32.40	37.39	42.38	47.36	52.35
3.567812E+06	0.00	2.49	7.48	12.47	17.45	22.44	27.42	32.41	37.40	42.38	47.37	52.36
3.766024E+06	0.00	2.49	7.48	12.47	17.46	22.44	27.43	32.42	37.40	42.39	47.38	52.37

DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT

Time (s)	RP(97)	RP(98)	RP(99)	RP(100)	RP(101)	RP(102)	RP(103)	RP(104)
0.000000E+00	427.00	432.00	437.00	442.00	447.00	452.00	457.00	459.50
1.982118E+05	427.00	432.00	437.00	442.00	447.00	452.00	457.00	459.50
3.964235E+05	427.04	432.04	437.03	442.03	447.03	452.02	457.02	459.52
5.946353E+05	427.00	431.99	436.98	441.97	446.97	451.96	456.95	459.45
7.928471E+05	426.96	431.94	436.93	441.92	446.90	451.89	456.88	459.37
9.910588E+05	426.92	431.90	436.88	441.86	446.85	451.83	456.81	459.30
1.189271E+06	426.89	431.86	436.84	441.81	446.79	451.76	456.74	459.23
1.387482E+06	426.86	431.83	436.80	441.76	446.73	451.70	456.67	459.16
1.585694E+06	426.83	431.79	436.75	441.72	446.68	451.64	456.60	459.09
1.783906E+06	426.80	431.76	436.71	441.67	446.63	451.58	456.54	459.02
1.982118E+06	426.78	431.73	436.68	441.63	446.58	451.53	456.47	458.95
2.180329E+06	426.76	431.70	436.64	441.58	446.53	451.47	456.41	458.88
2.378541E+06	426.73	431.67	436.61	441.54	446.48	451.41	456.35	458.82
2.576753E+06	426.72	431.64	436.57	441.50	446.43	451.36	456.29	458.75
2.774965E+06	426.70	431.62	436.54	441.46	446.39	451.31	456.23	458.69
2.973176E+06	426.68	431.60	436.51	441.43	446.34	451.26	456.17	458.63
3.171388E+06	426.67	431.57	436.48	441.39	446.30	451.20	456.11	458.57
3.369600E+06	426.65	431.55	436.45	441.35	446.25	451.16	456.06	458.51
3.567812E+06	426.64	431.53	436.43	441.32	446.21	451.11	456.00	458.45
3.766024E+06	426.62	431.51	436.40	441.29	446.17	451.06	455.95	458.39

Particle internal pressures (MPa) vs fast fluence (10^25 n/m^2, E>.18 MeV) and transient time (s)

FLU	TIME	Pavg	Pmax
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3.2680E-02	1.9821E+05	2.2215E-03	2.3475E-03
6.5359E-02	3.9642E+05	5.1711E-03	5.5421E-03
9.8039E-02	5.9464E+05	8.6608E-03	9.3358E-03
1.3072E-01	7.9285E+05	1.2599E-02	1.3644E-02
1.6340E-01	9.9106E+05	1.6936E-02	1.8405E-02
1.9608E-01	1.1893E+06	2.1651E-02	2.3603E-02
2.2876E-01	1.3875E+06	2.6769E-02	2.9284E-02
2.6144E-01	1.5857E+06	3.2395E-02	3.5601E-02
2.9412E-01	1.7839E+06	3.8728E-02	4.2824E-02
3.2680E-01	1.9821E+06	4.6053E-02	5.1324E-02
3.5948E-01	2.1803E+06	5.4712E-02	6.1525E-02
3.9216E-01	2.3785E+06	6.5067E-02	7.3864E-02
4.2484E-01	2.5768E+06	7.7471E-02	8.8762E-02
4.5752E-01	2.7750E+06	9.2260E-02	1.0661E-01
DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT			
4.9673E+00	3.0128E+07	2.6986E+01	3.1516E+01
5.0000E+00	3.0326E+07	2.7282E+01	3.1862E+01
5.0000E+00	3.0341E+07	1.0945E+01	1.1217E+01
5.0000E+00	3.0355E+07	7.0578E+00	7.3262E+00
5.0000E+00	3.0370E+07	2.2250E+00	2.4554E+00
5.0000E+00	3.0384E+07	1.4244E+00	1.6270E+00
5.0000E+00	3.0398E+07	1.2366E+00	1.4131E+00
5.0000E+00	3.0413E+07	9.7611E-01	1.1281E+00
5.0000E+00	3.0414E+07	9.8017E-01	1.1328E+00
5.0000E+00	3.0415E+07	9.8017E-01	1.1328E+00
5.0000E+00	3.0416E+07	1.1893E+00	1.3733E+00
5.0000E+00	3.0416E+07	1.4215E+00	1.6418E+00
5.0000E+00	3.0417E+07	3.9790E+00	4.2338E+00
5.0000E+00	3.0418E+07	1.2101E+01	1.2437E+01
5.0000E+00	3.0419E+07	2.2166E+01	2.2613E+01
5.0000E+00	3.0420E+07	3.5113E+01	3.5718E+01
5.0000E+00	3.0430E+07	3.4900E+01	3.5518E+01
5.0000E+00	3.0440E+07	3.4900E+01	3.5310E+01
5.0000E+00	3.0441E+07	3.7480E+01	3.7915E+01
5.0000E+00	3.0442E+07	3.9897E+01	4.0516E+01
5.0000E+00	3.0466E+07	3.9734E+01	4.0354E+01

Gas Moles Produced vs Fast Fluence (10^25 n/m^2, E>.18 MeV) and Transient Time (s)

FLU	TIME	COavg	COmax	FGavg	FGmax
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3.2680E-02	1.9821E+05	1.2711E-38	1.3653E-37	1.3287E-11	1.3806E-11
6.5359E-02	3.9642E+05	7.2958E-24	2.5874E-23	3.0945E-11	3.2579E-11
9.8039E-02	5.9464E+05	7.1826E-19	1.7282E-18	5.1790E-11	5.4901E-11
1.3072E-01	7.9285E+05	2.4820E-16	4.9193E-16	7.5281E-11	8.0164E-11
1.6340E-01	9.9106E+05	8.7765E-15	1.5485E-14	1.0111E-10	1.0803E-10
1.9608E-01	1.1893E+06	9.8337E-14	1.6053E-13	1.2908E-10	1.3828E-10
2.2876E-01	1.3875E+06	5.6800E-13	8.7695E-13	1.5905E-10	1.7076E-10
2.6144E-01	1.5857E+06	2.1587E-12	3.1945E-12	1.9090E-10	2.0535E-10
2.9412E-01	1.7839E+06	6.1829E-12	8.8462E-12	2.2455E-10	2.4193E-10
3.2680E-01	1.9821E+06	1.4481E-11	2.0154E-11	2.5988E-10	2.8040E-10
3.5948E-01	2.1803E+06	2.9235E-11	3.9768E-11	2.9682E-10	3.2064E-10
3.9216E-01	2.3785E+06	5.2743E-11	7.0401E-11	3.3526E-10	3.6255E-10
4.2484E-01	2.5768E+06	8.7257E-11	1.1466E-10	3.7512E-10	4.0606E-10
4.5752E-01	2.7750E+06	1.3489E-10	1.7499E-10	4.1634E-10	4.5109E-10

Data Intentionally Removed To Reduce Page Count

4.9673E+00	3.0128E+07	1.4453E-07	1.6218E-07	1.3834E-08	1.5770E-08
5.0000E+00	3.0326E+07	1.4603E-07	1.6383E-07	1.3972E-08	1.5931E-08
5.0000E+00	3.0341E+07	6.4890E-08	6.4900E-08	1.3973E-08	1.5931E-08
5.0000E+00	3.0355E+07	4.0021E-08	4.0025E-08	1.3973E-08	1.5932E-08
5.0000E+00	3.0370E+07	5.3455E-09	5.3481E-09	1.3973E-08	1.5932E-08
5.0000E+00	3.0384E+07	2.3646E-11	2.3676E-11	1.3973E-08	1.5932E-08
5.0000E+00	3.0398E+07	5.2208E-17	5.2364E-17	1.3973E-08	1.5932E-08
5.0000E+00	3.0413E+07	4.4033E-29	4.4302E-29	1.3011E-08	1.4995E-08
5.0000E+00	3.0414E+07	4.3392E-29	4.3394E-29	1.3011E-08	1.4995E-08
5.0000E+00	3.0415E+07	4.3389E-29	4.3389E-29	1.3011E-08	1.4995E-08
5.0000E+00	3.0416E+07	9.6955E-16	1.0036E-15	1.3011E-08	1.4995E-08
5.0000E+00	3.0416E+07	2.6345E-10	2.6684E-10	1.3011E-08	1.4995E-08
5.0000E+00	3.0417E+07	1.9141E-08	1.9218E-08	1.3011E-08	1.4995E-08
5.0000E+00	3.0418E+07	7.1637E-08	7.1730E-08	1.3011E-08	1.4995E-08
5.0000E+00	3.0419E+07	1.2331E-07	1.2339E-07	1.3011E-08	1.4995E-08
5.0000E+00	3.0420E+07	1.7870E-07	1.7870E-07	1.3011E-08	1.4995E-08

Particle Volume-averaged & Centerline Temperatures (k) vs Fast Fluence (10^25 n/m^2, E>.18MeV) and Transient Time (s)

FLU	TIME	TCLmin	TCLavg	TCLmax
0.0000E+00	0.0000E+00	1.1132E+03	1.1132E+03	1.1132E+03
3.2680E-02	1.9821E+05	1.1830E+03	1.1975E+03	1.2178E+03
6.5359E-02	3.9642E+05	1.1834E+03	1.1994E+03	1.2204E+03
9.8039E-02	5.9464E+05	1.1847E+03	1.2010E+03	1.2223E+03
1.3072E-01	7.9285E+05	1.1861E+03	1.2027E+03	1.2243E+03
1.6340E-01	9.9106E+05	1.1877E+03	1.2047E+03	1.2264E+03
1.9608E-01	1.1893E+06	1.1895E+03	1.2067E+03	1.2287E+03
2.2876E-01	1.3875E+06	1.1913E+03	1.2087E+03	1.2309E+03
2.6144E-01	1.5857E+06	1.1931E+03	1.2107E+03	1.2331E+03
2.9412E-01	1.7839E+06	1.1949E+03	1.2126E+03	1.2351E+03
3.2680E-01	1.9821E+06	1.1964E+03	1.2142E+03	1.2367E+03
3.5948E-01	2.1803E+06	1.1977E+03	1.2154E+03	1.2381E+03
3.9216E-01	2.3785E+06	1.1987E+03	1.2163E+03	1.2390E+03

7. Data Intentionally Removed To Reduce Page Count

5.0000E+00	3.0417E+07	9.4692E+02	9.4723E+02	9.4746E+02
5.0000E+00	3.0418E+07	1.0719E+03	1.0723E+03	1.0725E+03
5.0000E+00	3.0419E+07	1.1970E+03	1.1973E+03	1.1975E+03
5.0000E+00	3.0420E+07	1.3221E+03	1.3224E+03	1.3225E+03
5.0000E+00	3.0430E+07	1.3230E+03	1.3230E+03	1.3230E+03
5.0000E+00	3.0440E+07	1.3230E+03	1.3230E+03	1.3230E+03
5.0000E+00	3.0441E+07	1.4224E+03	1.4225E+03	1.4227E+03
5.0000E+00	3.0442E+07	1.5224E+03	1.5226E+03	1.5227E+03
5.0000E+00	3.0466E+07	1.5230E+03	1.5230E+03	1.5230E+03
5.0000E+00	3.0490E+07	1.5230E+03	1.5230E+03	1.5230E+03
5.0000E+00	3.0497E+07	1.6104E+03	1.6105E+03	1.6105E+03
5.0000E+00	3.0504E+07	1.6980E+03	1.6980E+03	1.6980E+03
5.0000E+00	3.0510E+07	1.7855E+03	1.7855E+03	1.7855E+03
5.0000E+00	3.0517E+07	1.8730E+03	1.8730E+03	1.8730E+03
5.0000E+00	3.0700E+07	1.8730E+03	1.8730E+03	1.8730E+03
5.0000E+00	3.0882E+07	1.8730E+03	1.8730E+03	1.8730E+03
5.0000E+00	3.1064E+07	1.8730E+03	1.8730E+03	1.8730E+03

GLOBAL Fuel Element Temperature Histories (in K)

Time (s)	TG(1)	TG(2)	TG(3)	TG(4)	TG(5)	TG(6)	TG(7)	TG(8)	TG(9)	TG(10)
0.000000E+00	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20	1113.20
1.982118E+05	1174.01	1174.01	1171.27	1164.43	1153.78	1139.41	1129.39	1129.39	1120.25	1113.20
3.964235E+05	1175.37	1175.37	1172.55	1165.50	1154.57	1139.86	1129.65	1129.65	1120.35	1113.20
5.946353E+05	1176.11	1176.11	1173.26	1166.13	1155.07	1140.19	1129.85	1129.85	1120.44	1113.20
7.928471E+05	1176.85	1176.85	1173.96	1166.76	1155.58	1140.52	1130.06	1130.06	1120.53	1113.20
9.910588E+05	1177.58	1177.58	1174.67	1167.38	1156.08	1140.85	1130.27	1130.27	1120.62	1113.20
1.189271E+06	1178.31	1178.31	1175.36	1168.01	1156.58	1141.17	1130.47	1130.47	1120.71	1113.20
1.387482E+06	1179.03	1179.03	1176.06	1168.63	1157.07	1141.50	1130.67	1130.67	1120.80	1113.20
1.585694E+06	1179.76	1179.76	1176.75	1169.24	1157.57	1141.83	1130.88	1130.88	1120.89	1113.20
1.783906E+06	1180.47	1180.47	1177.44	1169.85	1158.06	1142.15	1131.08	1131.08	1120.98	1113.20
1.982118E+06	1181.19	1181.19	1178.12	1170.46	1158.55	1142.47	1131.28	1131.28	1121.06	1113.20
2.180329E+06	1181.90	1181.90	1178.80	1171.07	1159.04	1142.80	1131.49	1131.49	1121.15	1113.20
2.378541E+06	1182.60	1182.60	1179.48	1171.67	1159.52	1143.12	1131.69	1131.69	1121.24	1113.20
2.576753E+06	1183.31	1183.31	1180.15	1172.27	1160.01	1143.43	1131.89	1131.89	1121.33	1113.20
2.774965E+06	1184.00	1184.00	1180.82	1172.87	1160.49	1143.75	1132.08	1132.08	1121.42	1113.20
2.973176E+06	1184.69	1184.69	1181.49	1173.46	1160.96	1144.07	1132.28	1132.28	1121.50	1113.20
3.171388E+06	1185.38	1185.38	1182.14	1174.05	1161.44	1144.38	1132.48	1132.48	1121.59	1113.20

DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT

3.041819E+07	1071.95	1071.95	1071.99	1072.09	1072.26	1072.47	1072.63	1072.63	1072.76	1073.00
3.041909E+07	1197.02	1197.02	1197.06	1197.15	1197.30	1197.51	1197.65	1197.65	1197.78	1198.00
3.042000E+07	1322.09	1322.09	1322.13	1322.22	1322.36	1322.55	1322.68	1322.68	1322.80	1323.00
3.042990E+07	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00
3.043980E+07	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00	1323.00
3.044070E+07	1422.36	1422.36	1422.38	1422.44	1422.54	1422.68	1422.77	1422.77	1422.86	1423.00
3.044160E+07	1522.43	1522.43	1522.45	1522.51	1522.60	1522.71	1522.80	1522.80	1522.87	1523.00
3.046590E+07	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00
3.049020E+07	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00	1523.00
3.049695E+07	1610.44	1610.44	1610.45	1610.45	1610.46	1610.47	1610.48	1610.48	1610.49	1610.50
3.050370E+07	1697.95	1697.95	1697.95	1697.96	1697.97	1697.98	1697.98	1697.98	1697.99	1698.00
3.051045E+07	1785.46	1785.46	1785.46	1785.47	1785.47	1785.48	1785.49	1785.49	1785.49	1785.50
3.051720E+07	1872.97	1872.97	1872.97	1872.97	1872.98	1872.99	1872.99	1872.99	1872.99	1873.00
3.069960E+07	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00
3.088200E+07	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00
3.106440E+07	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00
3.124680E+07	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00
3.142920E+07	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00
3.161160E+07	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00	1873.00

Global fission product release histories

Time (s)	- -	(atoms)	- -	Ag rf
0.000000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1.982118E+05	5.3624E+07	3.8166E+13	1.3517E+05	3.5417E-09
3.964235E+05	1.1493E+08	7.6331E+13	5.4576E+05	7.1499E-09
5.946353E+05	1.7827E+08	1.1450E+14	1.3606E+06	1.1883E-08
7.928471E+05	2.4240E+08	1.5266E+14	2.6952E+06	1.7655E-08
9.910588E+05	3.0681E+08	1.9083E+14	4.6527E+06	2.4382E-08
1.189271E+06	3.7124E+08	2.2899E+14	7.3241E+06	3.1984E-08
1.387482E+06	4.3548E+08	2.6716E+14	1.0790E+07	4.0388E-08
1.585694E+06	4.9939E+08	3.0532E+14	1.5121E+07	4.9525E-08
1.783906E+06	5.6284E+08	3.4349E+14	2.0380E+07	5.9331E-08
1.982118E+06	6.2570E+08	3.8166E+14	2.6620E+07	6.9748E-08
2.180329E+06	6.8873E+08	4.1982E+14	3.3893E+07	8.0732E-08
2.378541E+06	7.5387E+08	4.5799E+14	4.2252E+07	9.2256E-08
2.576753E+06	8.1566E+08	4.9615E+14	5.1732E+07	1.0427E-07
2.774965E+06	8.7628E+08	5.3432E+14	6.2361E+07	1.1671E-07
2.973176E+06	9.3794E+08	5.7248E+14	7.4166E+07	1.2955E-07
3.171388E+06	1.0063E+09	6.1065E+14	8.7204E+07	1.4281E-07

DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT

3.369600E+06	1.0653E+09	6.4881E+14	1.0149E+08	1.5643E-07
3.567812E+06	1.1232E+09	6.8698E+14	1.1704E+08	1.7037E-07
3.766024E+06	1.1800E+09	7.2514E+14	1.3385E+08	1.8459E-07
3.964235E+06	1.2357E+09	7.6331E+14	1.5194E+08	1.9905E-07
4.162447E+06	1.2904E+09	8.0148E+14	1.7131E+08	2.1374E-07
4.360659E+06	1.3441E+09	8.3964E+14	1.9195E+08	2.2861E-07
4.558871E+06	1.3966E+09	8.7781E+14	2.1387E+08	2.4364E-07
4.757082E+06	1.4481E+09	9.1597E+14	2.3706E+08	2.5881E-07
4.955294E+06	1.4985E+09	9.5414E+14	2.6152E+08	2.7409E-07
5.153506E+06	1.5478E+09	9.9230E+14	2.8725E+08	2.8948E-07
5.351718E+06	1.5961E+09	1.0305E+15	3.1423E+08	3.0494E-07
5.549929E+06	1.6433E+09	1.0686E+15	3.4246E+08	3.2046E-07
5.748141E+06	1.6894E+09	1.1068E+15	3.7192E+08	3.3604E-07

Kr-85m R/B

Time (s)	R/Bmin	R/Bavg	R/Bmax
0.000000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1.982118E+05	1.6428E-08	1.6428E-08	1.6428E-08
3.964235E+05	1.6458E-08	1.6458E-08	1.6458E-08
5.946353E+05	1.6479E-08	1.6479E-08	1.6479E-08
7.928471E+05	1.6500E-08	1.6500E-08	1.6500E-08
9.910588E+05	1.6520E-08	1.6520E-08	1.6520E-08
1.189271E+06	1.6541E-08	1.6541E-08	1.6541E-08
1.387482E+06	1.6562E-08	1.6562E-08	1.6562E-08
1.585694E+06	1.6582E-08	1.6582E-08	1.6582E-08
1.783906E+06	1.6603E-08	1.6603E-08	1.6603E-08
1.982118E+06	1.6623E-08	1.6623E-08	1.6623E-08
2.180329E+06	1.6643E-08	1.6643E-08	1.6643E-08
2.378541E+06	1.6663E-08	1.6663E-08	1.6663E-08
2.576753E+06	1.6683E-08	1.6683E-08	1.6683E-08

DATA INTENTIONALLY REMOVED TO REDUCE PAGE COUNT

3.044070E+07	5.1184E-08	5.1184E-08	5.1184E-08
3.044160E+07	6.8475E-08	6.8475E-08	6.8475E-08
3.046590E+07	6.8519E-08	6.8519E-08	6.8519E-08
3.049020E+07	6.8519E-08	6.8519E-08	6.8519E-08
3.049695E+07	8.5727E-08	8.5727E-08	8.5727E-08
3.050370E+07	1.0474E-07	1.0474E-07	1.0474E-07
3.051045E+07	1.2539E-07	1.2539E-07	1.2539E-07
3.051720E+07	1.4750E-07	1.4750E-07	1.4750E-07
3.069960E+07	1.4750E-07	1.4750E-07	1.4750E-07
3.088200E+07	1.4750E-07	1.4750E-07	1.4750E-07
3.106440E+07	1.4750E-07	1.4750E-07	1.4750E-07
3.124680E+07	1.4750E-07	1.4750E-07	1.4750E-07
3.142920E+07	1.4750E-07	1.4750E-07	1.4750E-07
3.161160E+07	1.4750E-07	1.4750E-07	1.4750E-07

```
Null input set detected: Normal end of PARFUME
```

6.1.6 Output data notes (prob#1_01.res)

1. The output data can be imported into MS Excel for post processing, but the user must manipulate some text in order to prepare the data for plotting.
2. The global fuel element radial positions are not part of the output; therefore, the user must reconstruct the radial positions using input parameters associated with variables “ngnfm” and “ngn.” Keep in mind that the outermost node of the fueled region overlaps the inner most node of the unfueled region. So if, for example, the user desires to plot fuel element temperature profile versus radial position, the total number of nodes representing the radial positions are ngn-1.
3. Time is output in units of seconds; therefore, the user must convert from seconds to the desired unit of time.
4. Note that PARFUME only models energy production from fission (i.e., 200 MeV/fission). That is, it does not model energy production from the decay of radionuclides.
5. The computed value for “inventory” in the Ag Global Fission Product Diffusion Release History is incorrect.

7. REFERENCES

1. Miller, G. K., D. A. Petti, J. T. Maki, and D. L. Knudson, 2009, *PARFUME Theory and Model Basis Report*, INL/EXT-08-14497, Idaho National Laboratory, September 2009.
2. Verfondern, K., H. Nabielek, and J. M. Kendall, 2007, "Coated Particle Fuel for High Temperature Gas Cooled Reactors," *Nuclear Engineering and Technology*, Vol. 39, No. 5, pp. 603–605.
3. Williamson, R. L., and D. A. Knoll, 2009, "Enhancing the ABAQUS Thermomechanics Code to Simulate Steady and Transient Fuel Rod Behavior," *Proceedings of Top Fuel 2009, Paris, France, September 6–10, 2009.*
4. Liu, B., T. Liang, and C. Tang, 2006, "A review of TRISO-coated particle nuclear fuel performance models," *Rare Metals*, Spec. Issue, Vol. 25, p. 337.
5. Lee, Y., et. al, 2008, "Development of HTGR-coated particle fuel technology in Korea," *Nuclear Engineering and Design*, Vol. 238, p. 2850.
6. Maki, J. T., D. A. Petti, D. L. Knudson, G. K. Miller, 2007, "The challenges associated with high burnup, high temperature and accelerated irradiation for TRISO-coated particle fuel," *Journal of Nuclear Materials*, Vol. 371, No. 1–3, pp. 270–280.
7. IAEA, "Safety related design and economic aspects of HTGRs," IAEA-TECDOC-1210, International Atomic Energy Agency, p. 187, 2001.
8. Petti, D. A. (Lead Principal Investigator), et al., 2004, *Development of Improved Models and Designs for Coated-Particle Gas Reactor Fuels*, INEEL/EXT-05-02615, Idaho National Laboratory, December 2004.
9. CEGA Corporation, *NP-MHTGR Material Models of Pyrocarbon and Pyrolytic Silicon Carbide*, CEGA-002820, Rev. 1, July 1993.
10. IAEA, "Fuel Performance and Fission Product Behavior in Gas-Cooled Reactors," IAEA-TECDOC-978, International Atomic Energy Agency, 1997.
11. AIAA, *Guide for the Verification and Validation of Computational Fluid Dynamics Simulations,* AIAA G-077-1998, American Institute of Aeronautics and Astronautics, 2002.
12. ASME, *Guide for Verification and Validation in Computational Solid Mechanics*, ASME V&V 10-2006, American Society of Mechanical Engineers, 2006.
13. ASME, *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer*, ASME V&V 20-2008, American Society of Mechanical Engineers, 2008.

Appendix A

Input Parameter Summary

Appendix A

Input Parameter Summary

Table A-1. Input data deck parameter summary.

Card Number	Parameter	Description	Units	Options/Notes	Default
RUN PARAMETERS					
100001	title	simulation description	-	60 characters (max)	-
101001	pfss	solution scheme	-	0 = Monte Carlo 1 = full integ. 2 = fast integ.	Monte Carlo
101001	ncases	CFP number	-	pfss = 0 (only)	0
101001	nburp	runtime updates	-	-	1000
101001	sample	includes std. deviation in analyses	-	<0 or ≥0 (≥0 std. dev. analyses included)	0
101001	dtf	design to fail flag analysis	-	0 = no analysis 1 = analysis	0
101001	iseed	random number seed	-	pfss = 0 (only)	305
101002	idebondp	activates debonding model	-	off = 0 on = 1	0
101002	ifacet	activates faceting model	-	off = 0 on = 1	0
101002	rbvalue	activates R/B model	-	off = ≤ 0 Kr-85m = 1 12 nuclides >1	1
101002	comodel	activates CO production model	-	1 = off, 2 = GA 3 = HSC 4 = German	3
101002	fgmodel	activates fission gas Kr&Xe model	-	100% release = 1 Booth model = 2	2
101002	idebug	activates “h” function output data	-	off = 0 on = 1	0
FUEL CHARACTERISTICS					
102001	u235enr(%)	kernel enrichment	%	values ≤0 (user warning)	user input values >0
102001	ourat	oxygen to uranium atom ratio	-	values ≤0 (user warning)	user input values >0
102001	curat	carbon to uranium atom ratio	-	values ≤0 (user warning)	user input values >0

Card Number	Parameter	Description	Units	Options/Notes	Default
103001	kernd	kernel density	Mg/m^3	values ≤0 (user warning)	user input values >0
103001	kernt	theoretical kernel density	Mg/m^3	values ≤0 (user warning)	11.03
103002	buffd	buffer density	Mg/m^3	values ≤0 (user warning)	user input values >0
103002	bufft	theoretical buffer density	Mg/m^3	values ≤0 (user warning)	2.25
103003	ipycdn	mean IPyC density	Mg/m^3	values ≤0 (user warning)	user input values >0
103003	ipycdvar	IPyC density standard deviation	Mg/m^3	user input values ≤0, (default to 0)	user input values >0
103005	opycdn	mean OPyC density	Mg/m^3	values ≤0 (user warning)	user input values >0
103005	opycdvar	OPyC density standard deviation	Mg/m^3	user input values ≤0, (default to 0)	user input values >0
103013	ibafn	IPyC mean BAF	-	values ≤0 (user warning)	user input values >0
103013	ibafvar	IPyC mean BAF standard deviation	-	user input values ≤0, (default to 0)	user input values >0
103015	obafn	OPyC mean BAF	-	values ≤0 (user warning)	user input values > 0
103015	obafvar	OPyC mean BAF standard deviation	-	user input values ≤0, (default to 0)	user input values >0
103023	ipycm	IPyC Weibull modulus	-	user input values ≤0, (default to 9.5)	9.5
103024	sigm	SiC Weibull modulus	-	user input values ≤0, (default to 6.0)	6.0
103025	opycm	OPyC Weibull modulus	-	user input values ≤0, (default to 9.5)	9.5
103033	cnu	Poisson's creep ratio pyrocarbons	-	user input values ≤0, (default to 0.5)	0.5
103033	cnub	Poisson's creep ratio buffer	-	user input values ≤0, (default to 0.5)	0.5
103043	creepampn	mean creep amplification factor	-	user input values ≤0, (default to 2.0)	2.0
103043	creepvar	mean creep amplification factor std. deviation	-	user input values ≤0, (default to 0.0)	0.0
103054	zrc	ZrC indicator		If zrc = 1, SiC material properties are replaced; geometry remains the same as specified for SiC	0

Card Number	Parameter	Description	Units	Options/Notes	Default
103054	zrcp	fraction of ZrC theoretical density		options: 1,2,3,4 1 = 0.96 2 = 0.85 3 = 0.80 4 = 0.77	1
103061	fdef	fraction of initial defective SiC layers	-	not yet used by code	0
PARTICLE GEOMETRY					
104001	kerndia	mean kernel diameter	µm	values ≤0 (user warning)	user input values >0
104001	kernvar	mean kernel diameter std. deviation	µm	user input values ≤0, (default to 0.0)	0
104002	buffthk	mean buffer thickness	µm	values ≤0 (user warning)	user input values >0
104002	buffvar	mean buffer thickness std. deviation	µm	user input values ≤0, (default to 0.0)	0
104003	ipycthk	mean IPyC thickness	µm	values ≤0 (user warning)	user input values >0
104003	ipycvar	mean IPyC thickness std. deviation	µm	user input values ≤0, (default to 0.0)	0
104004	sicthk	mean SiC thickness	µm	values ≤0 (user warning)	user input values >0
104004	sicvar	mean SiC thickness std. deviation	µm	user input values ≤0, (default to 0.0)	0
104005	opycthk	mean OPyC thickness	µm	values ≤0 (user warning)	user input values >0
104005	opycvar	mean OPyC thickness std. deviation	µm	user input values ≤0, (default to 0.0)	0
FUEL MATRIX DESCRIPTION					
105001	PEBBLEBED	fuel element geometry	-	geometry not specified (user warning)	none
105011	partnum	number of CFPs per pebble	-	values ≤0 (user warning)	user input values >0
105011	ngnfm	number of global nodes in fuel matrix	-	bad values result in (user warning)	3 (17 max)
105011	ngn	total number of nodes in fuel element	-	bad values result in (user warning)	6 (20 max)

Card Number	Parameter	Description	Units	Options/Notes	Default
105021	pebdia	pebble diameter	m	values ≤0 (user warning)	user input values >0
105021	pebcldtk	nonfueled region thickness	m	values ≤0 (user warning)	user input values >0
105031	fmden	fuel matrix material density	Mg/m^3	user input values ≤0, (default to 1.7)	1.7
105041	ucontam	fraction of uranium contamination in fuel matrix	-	user input values ≤0, (default 1×10^{-5})	1×10^{-5}
XXXXXXXX	XXXXXXXX	XXXXXXXX	XXXXX	XXXXXXXX	XXXXXXX
105001	PRISMATIC	fuel element geometry	-	geometry not specified (user warning)	none
105011	partnum	number of CFPs per meter of fuel element	-	values ≤0 (user warning)	user input values >0
105011	ngnfm	number of global nodes in fuel matrix	-	bad values result in (user warning)	3 (17 max)
105011	ngn	total number of nodes in fuel element	-	bad values result in (user warning)	6 (20 max)
105021	fueldia	fuel compact diameter	m	values ≤0 (user warning)	user input values >0
105021	cooldia	prismatic channel diameter	m	values ≤0 (user warning)	user input values >0
105021	fuelpitch	prismatic fuel hexagonal pitch	m	values ≤0 (user warning)	user input values >0
105021	height	fuel compact height	m	-	1.0
105031	fmden	fuel matrix material density	Mg/m^3	user input values ≤0, (default to 1.7)	1.7
105041	ucontam	fraction of uranium contamination in fuel matrix	-	user input values ≤0, (default 1×10^{-5})	1×10^{-5}
XXXXXXXX	XXXXXXXX	XXXXXXXX	XXXXX	XXXXXXXX	XXXXXXX
105001	PLANEGEOM	fuel element geometry	-	geometry not specified (user warning)	none
105011	partnum	number of CFPs per slab per m^2	CFPs per slab*m^2	values ≤0 (user warning)	user input values >0
105011	ngnfm	number of global nodes in fuel matrix	-	bad values result in (user warning)	3 (17 max)
105011	ngn	total number of nodes in fuel element	-	bad values result in (user warning)	6 (20 max)

Card Number	Parameter	Description	Units	Options/Notes	Default
105021	fmthk	fuel matrix thickness	m		
105021	cldthk	clad thickness	m	values ≤0 (user warning)	user input values >0
105021	sarea	fuel plate surface area	m^2	-	1.0
105031	fmden	fuel matrix material density	Mg/m^3	user input values ≤0, (default to 1.7)	1.7
105041	ucontam	fraction of uranium contamination in fuel matrix	-	user input values ≤0, (default 1×10^{-5})	1×10^{-5}
REACTOR TEMPERATURE OPTIONS					
106001	FIFD-CALC	fully implicit finite difference	-		FIFD-CALC
106021	tgi(k)	global node temperature specification	K	FIFD-CALC must be specified	
106021	ntgi	fuel matrix node associated with temp. specification	-	FIFD-CALC must be specified (node 1 is line of symmetry)	
106001	TEMP-DATA	independent temperature input	-	ABAQUS input	FIFD-CALC
106001	VOLAVGTMP	volume average temperature heat transfer analysis	-	-	FIFD-CALC
DIFFISION MODEL					
201001	fpspecie	turns on/off diffusion	-	characters other than Ag, I, Cs, Sr, Kr, Xe (user warning)	user input required, if no input provided, diffusion off
ENVIRONMENTAL PARAMETERS					
301001	ttime	transient time	days	user input required	none
301001	flu	fluence	10^{25} n/m^2, E>0.18 MeV	user input required	none
302001	flu	fluence	10^{25} n/m^2, E>0.18 MeV	user input required	none
302001	bup	burnup	% FIMA	user input required	none
303001	flu	fluence	10^{25} n/m^2, E>0.18 MeV	user input required	none
303001	pamb	ambient pressure	MPa	user input required	none
304001	flu	fluence	10^{25} n/m^2, E>0.18 MeV	user input required	none

Card Number	Parameter	Description	Units	Options/Notes	Default
304001	ptemp	boundary temperature	K	user input required	none
306001	thus	time heatup starts	days	-	user input values >0 (values <0 1×10^6 days)
CORRELATION PARAMETERS AND COEFFICIENTS					
401001	sigcr0	SiC mean strength with IPyC cracking	MPa	values ≤0 (user warning)	user input values >0
401001	umc	SiC mean strength for cracked CFP	MPa	values ≤0 (user warning)	user input values >0
401005	c1c	IPyC thickness polynomial coefficients	-	-	0
401005	c2c	IPyC thickness polynomial coefficients	-	-	0
401006	c1c	SiC thickness polynomial coefficients	-	-	0
401006	c2c	SiC thickness polynomial coefficients	-	-	0
401007	c1c	OPyC thickness polynomial coefficients	-	-	0
401007	c2c	OPyC thickness polynomial coefficients	-	-	0
402001	siga0	SiC mean strength in faceted CFP	MPa	-	1000
402001	um	minimum SiC stress in faceted CFP	MPa	-	130
402001	delum	maximum SiC stress in faceted CFP	MPa	-	1000
402001	aration	mean aspect ratio	-	-	1.0
402001	aratvar	aspect ratio std. deviation	-	-	0.0
402001	c1a	aspericity polynomial coefficients	-	-	0
402001	c2a	aspericity polynomial coefficients	-	-	0

Card Number	Parameter	Description	Units	Options/Notes	Default
402001	d1a	aspericity polynomial coefficients	-	-	0
402001	d2a	aspericity polynomial coefficients	-	-	0
403001	sigd0	SiC mean strength in debonded CFP	MPa	-	1000
403001	umd	minimum SiC stress in debonded CFP	MPa	-	130
403001	bond0	maximum IPyC bond strength debonded CFP	MPa	-	50
403001	bond0var	IPyC bond strength std. dev.	-	-	0
403001	c1d	debonding polynomial coefficients	-	-	0
403001	c2d	debonding polynomial coefficients	-	-	0