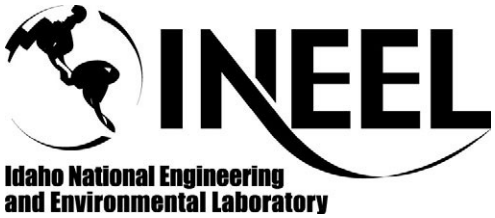

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Current Capabilities of the Fuel Performance Modeling Code PARFUME

G. K. Miller
J. T. Maki
D. L. Knudson
D. A. Petti

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CURRENT CAPABILITIES OF THE FUEL PERFORMANCE MODELING CODE PARFUME

G. K. MILLER, J. T. MAKI, D. L. KNUDSON, AND D. A. PETTI
Idaho National Engineering and Environmental Laboratory
P. O. Box 1625
Idaho Falls, Idaho, USA 83415

ABSTRACT

The success of gas reactors depends upon the safety and quality of the coated particle fuel. A fuel performance modeling code (called PARFUME), which simulates the mechanical and physico-chemical behavior of fuel particles during irradiation, is under development at the Idaho National Engineering and Environmental Laboratory. Among current capabilities in the code are: 1) various options for calculating CO production and fission product gas release, 2) a thermal model that calculates a time-dependent temperature profile through a pebble bed sphere or a prismatic block core, as well as through the layers of each analyzed particle, 3) simulation of multi-dimensional particle behavior associated with cracking in the IPyC layer, partial debonding of the IPyC from the SiC, particle asphericity, kernel migration, and thinning of the SiC caused by interaction of fission products with the SiC, 4) two independent methods for determining particle failure probabilities, 5) a model for calculating release-to-birth (R/B) ratios of gaseous fission products, that accounts for particle failures and uranium contamination in the fuel matrix, and 6) the evaluation of an accident condition, where a particle experiences a sudden change in temperature following a period of normal irradiation. This paper presents an overview of the code.

1. Introduction

The INEEL is developing an integrated mechanistic fuel performance model for TRISO-coated gas-reactor particle fuel termed PARFUME (PARticle Fuel ModEl). Coated particle fuel exhibits statistical variations in physical dimensions and material properties from particle to particle due to the nature of its fabrication process. Its behavior is also inherently multidimensional, further complicating development of the model. 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. This paper describes current capabilities of the code that are used ultimately to determine particle failure probabilities and release-to-birth ratios of gaseous fission products.

2. Basic Fuel Particle Behavior

A typical TRISO-coated particle is shown in Figure 1. 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. The basic behavior modeled in PARFUME is shown schematically in Figure 2. 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. Countering the effect of the pressure load is the shrinkage of the IPyC during irradiation, which pulls inward on the SiC. Likewise, shrinkage of the OPyC causes it to push inward on the SiC. 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 pyrocarbon layers.

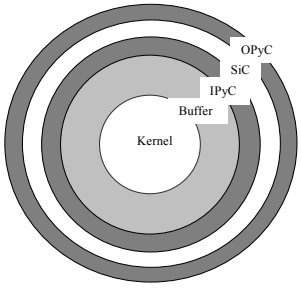

FIGURE 1. Typical TRISO-coated fuel particle geometry.

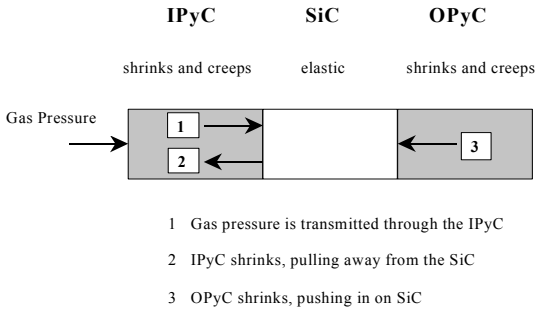

FIGURE 2. Behavior of coating layers in fuel particle.

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 [1]. Irradiation-induced creep in the pyrocarbon layers is treated as secondary creep, i.e. the creep strain rate is proportional to the level of stress in the pyrocarbon. The creep coefficient increases significantly with increases in the irradiation temperature. Swelling in the pyrocarbon layers is anisotropic and a function of four variables, i.e. fluence level, pyrocarbon density, degree of anisotropy (as measured by the Bacon Anisotropy Factor, BAF), and irradiation temperature. The magnitude of the shrinkage increases as BAF increases or as the irradiation temperature increases. Thermal expansion of the pyrocarbons is also anisotropic, and is a function of the BAF and temperature. The SiC layer has an elastic modulus (stiffness) that is an order of magnitude higher than that for the pyrocarbons.

3. Thermal Model

The PARFUME thermal model is based on a finite difference heat conduction approach with internal heat generation capabilities. It is used to calculate temperatures that are required for determining internal pressures, fission product release, and stresses in the coating layers. Temperatures from the model are also used to evaluate migration of the kernel toward the SiC layer in the direction of the global temperature gradient (the amoeba effect).

Thermal modeling in PARFUME begins with calculation of temperature profiles through either a pebble bed sphere or a prismatic block, depending on the reactor type specified by the user. These profiles are based on a number of other user inputs including the fuel element geometry, the number of fuel particles within the element, burnup specifications for the irradiation of interest, and the fuel element boundary temperature (i.e., the surface temperature for a pebble bed sphere or the coolant channel surface temperature for a prismatic block). Time-dependent burnup and/or boundary temperature specifications are allowed. The boundary temperature can be provided by the user or can be read from results of a reactor system analysis. The fuel element profiles can be calculated for both steady state and transient conditions. In either case, material property dependence on temperature and/or fluence is considered as appropriate.

The resulting time-dependent fuel element temperature profiles, or the 'macro' gradients, are then used to calculate time-dependent fuel particle temperature profiles, or 'micro' gradients, for each particle analyzed. Each micro gradient is based on a particle surface temperature, which is derived from the macro gradients at statistically determined particle positions. Because fuel particles are very small, the micro gradients are calculated using a quasi-steady state approach. However, material property dependencies on temperature, pressure, and/or fluence are treated as appropriate.

The capability to predict the potential development of a gap between the buffer and the IPyC is an important feature of the thermal model because such a gap can significantly affect the micro temperature gradients. Accordingly, the thermal model simulates all of the major factors in gap development including the net effects of kernel swelling; shrinkage and creep in the buffer, IPyC, and OPyC layers; and the associated kernel/buffer contact pressure. Furthermore, the model accounts for changes in gap conductivity with changes in particle geometry and gap gas composition, pressure, and temperature.

An example of results from the thermal model are shown in Figure 3, where kernel centerline temperatures were calculated as functions of particle power and burnup. In this case, fuel particles with a diameter of 780 μm were assumed to contain UCO kernels with a diameter of 350 μm. A volume average irradiation temperature of 1250 °C was also assumed. This effectively sets the temperature on the outer surface of each particle. The increase in kernel centerline temperatures as shown was due primarily to increases in the gap between the buffer and the IPyC as a result of buffer shrinkage with increasing fast fluence and power being generated in the particle. At high particle powers that might be expected in very accelerated irradiations, the model predicts that the kernel centerline temperature can be as much as 200 °C higher even though the average temperature is 1250 °C.

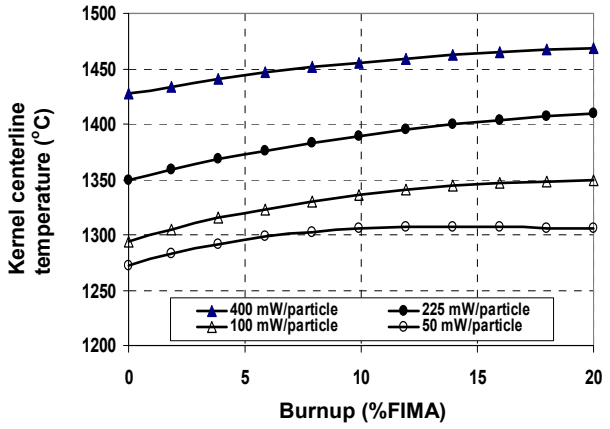

FIGURE 3. Kernel centerline temperatures as functions of particle power and burnup.

4. Physico-Chemical Models

Particle internal gas pressures are calculated according to the Redlich-Kwong equation of state [2]. Parameters utilized by this equation of state are derived from the critical temperature and pressure of each gas specie [3] occupying void volume within the particle. PARFUME considers the generation of CO and the release of the noble fission product gases, xenon and krypton, in this pressure calculation.

Either of two algorithms may be chosen for calculating CO production. A simple temperature dependent General Atomics (GA) correlation [4] is used primarily for comparison to historic evaluations. The other

algorithm is a detailed model derived from thermochemical free energy minimization calculations performed by the HSC code [5]. Input to the HSC code consisted of elemental fission product inventories generated by the MOCUP [6] code which couples the MCNP [7] and ORIGEN2 [8] codes. This CO production model considers burnup, temperature, uranium enrichment, and fuel composition in the calculation.

PARFUME calculates fission product gas release due to both recoil and diffusion. Direct fission recoil from the kernel to the buffer is accounted for by geometrical considerations and fission fragment ranges derived from compiled experimental data [9]. Diffusive release is calculated according to the Booth equivalent sphere diffusion model [10] which utilizes an effective diffusion coefficient formulated by Turnbull [11]. This effective diffusion coefficient accounts for intrinsic, athermal and radiation-enhanced diffusion.

A model accounting for release of short-lived fission product gases from failed particles and from uranium contamination in the fuel matrix material is incorporated into PARFUME. This correlation calculates release rate to birth rate (R/B) ratios for several prominent fission product nuclides. Also based upon the Booth equivalent sphere gas release model [12], this correlation uses different reduced diffusion coefficients for release from failed particles [13] and from uranium contamination [14].

Kernel migration (amoeba effect) occurs within the presence of a macroscopic temperature gradient and is calculated according to a standard formulation [15]. This algorithm utilizes kernel migration coefficients derived from experimental data. For UCO fuel where kernel migration is expected to be miniscule, a General Atomics derived correlation [15] is used. For UO_2 fuel where kernel migration can be significant, recent data (from the last 20 years) [16,17] were fitted to an Arrhenius function to derive a kernel migration coefficient correlation. Particle failure is assumed to occur when the kernel comes into contact with the SiC layer.

A Pd-SiC interaction model is nearing completion. To date, all available in-reactor data for Pd penetration in SiC [18-21] have been fitted to an Arrhenius function. The resulting penetration depth correlation will be folded with finite element stress analyses of corroded, or thinned, SiC to develop a failure algorithm.

5. Simulation of Multi-dimensional Behavior

A key element of the PARFUME program is a closed form solution that calculates stresses in the coating layers of a one-dimensional (symmetrical) spherical particle [22]. This solution accounts for the irradiation-induced creep and swelling in the pyrocarbon layers in addition to the elastic behavior of the three layers of a TRISO-coated particle. To treat situations where the particle temperature varies throughout irradiation, the solution has been enhanced to include the effect of differential expansion among the layers. Failure of a one-dimensional particle occurs if the internal pressure is high enough that the tangential stress in the SiC layer reaches the SiC strength for that particle. PARFUME also considers multi-dimensional behavior that has been observed in post-irradiation examination (PIE) of US fuel particles and 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, 4) kernel migration, and 5) thinning of the SiC due to interaction with fission products.

To model the first three of these multi-dimensional effects, PARFUME utilizes the results of detailed finite element (FE) analysis on cracked, debonded, or aspherical particles in conjunction with results from the closed form solution for a one-dimensional particle to make a statistical approximation of the stress levels in any particle. Using this approach [23], numerous parameters can be varied statistically (about a mean value) such as thicknesses of the three coating layers, densities and BAF values for the pyrocarbons, kernel diameter, buffer thickness, etc.

Treatment of a cracked IPyC is presented in References [24] and [25], while debonding and asphericity are described in Reference [26]. Early during irradiation of a particle, shrinkage of the IPyC layer induces a significant tensile stress in that layer. If the stress exceeds the tensile strength of the IPyC layer, then a radial crack develops in the IPyC. For a through-thickness crack, a stress concentration occurs in the SiC layer at the tip of the crack containing tensile stress components that can contribute to particle failures. Shrinkage of the IPyC layer also induces a radial tensile stress at the interface between the IPyC and SiC layers. Debonding of the IPyC from the SiC layer occurs if the stress exceeds the bond strength between layers. The debonding process begins at an initiation point from which the layers progressively unzip during irradiation. A stress concentration occurs in the SiC layer at the tip of the debonded region, which moves with the crack tip as debonding progresses. The area of stress concentration contains tensile stress components that can contribute to particle failures.

PARFUME incorporates the effects of asphericity for particles that have a flat facet but that are otherwise spherical, which is typical of what has been observed in some fabricated particles. During irradiation, the faceted portion of the particle acts as a flat plate that restrains the internal gas pressure. If the pressure reaches a high enough value, a local region of tensile stress develops in the central portion of the plate that can contribute to particle failures. Unlike failures caused by cracking or debonding of the IPyC, which are governed by shrinkage of the pyrocarbons, failures caused by asphericity are controlled by the internal pressure.

Failures due to the amoeba effect are evaluated by determining the distance that the fuel kernel migrates as a function of the temperature gradient at the particle location. The gradient is calculated using the thermal model contained in PARFUME. Particle failure is assumed to occur when the kernel comes into contact with the SiC layer. Failure due to thinning of the SiC caused by SiC/fission product interaction is under investigation. The intent is to establish a failure criterion that is based on the size of the thinned area.

The various failure modes are implemented in PARFUME such that a particle fails only in the mode of failure that would occur first for that particle. The code uses the Weibull statistical theory to determine whether particles fail, using a mean strength for the SiC layer that is based on a stress distribution corresponding to the failure mechanism under consideration. PARFUME retains the time at which failures occur, allowing for the construction of a time evolution of the failure probability for a batch of particles. Figure 4 shows a time history calculated for a representative experiment. The failure probability reaches 2.5×10^{-5} early during irradiation due to cracking of the IPyC, then levels off for a period of time. After the neutron fluence reaches 3×10^{25} n/m^2 (E>0.18 MeV), particles progressively fail due to the buildup of internal pressure until the failure probability reaches 1.8×10^{-2} at the end of irradiation.

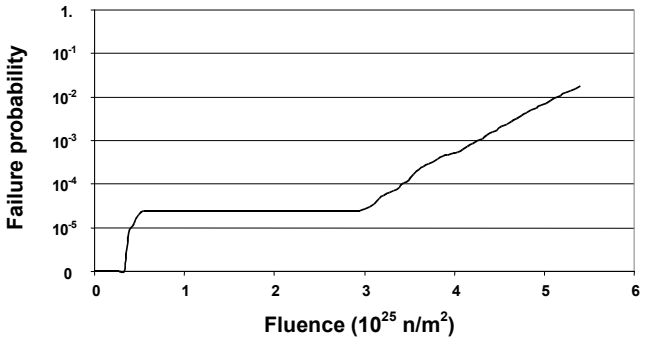

FIGURE 4. Calculated failure probability time history.

6. Failure Probability Determination

The failure probability for a batch of fuel particles generally depends on statistical variations in a number of input parameters and on a Weibull statistical variation in the strength of the SiC layer among particles in the batch. The probability can be calculated in PARFUME using the traditional Monte Carlo method wherein a large number of particles are statistically sampled to account for these variations. The lower the failure probability, the larger this sample of particles must be to produce an accurate estimate of the probability. Because sampling a large number of particles to calculate small failure probabilities can be a time consuming effort, PARFUME offers an alternate approach using an integral formulation to calculate failure probabilities. The integration treats each statistically varying parameter as a dimension in parameter space. The integral convolves density functions representing the statistical distributions for the varying parameters with the failure probability as it varies over the parameter space. Among advantages of the integration method are that it calculates a very small failure probability as quickly as a large failure probability, and can be much faster than the Monte Carlo method. Furthermore, the integration method can be used to verify failure probabilities calculated by the Monte Carlo method and vice versa. Because this is a multiple integration, the speed of the probability calculation depends largely on how many parameters are given a statistical variation.

7. Accident Condition

The PARFUME Code has the capability to analyze for stresses in a TRISO-coated particle during an accidental heatup condition. In this analysis, the particle is irradiated for a period of time at the normal irradiation temperature, and then suddenly heated to a much higher temperature due to the accident. This sudden heatup induces differential thermal expansion stresses in the coating layers and significantly increases the internal gas pressure. PARFUME solves (in its closed-form solution) for differential thermal expansion among the three coating layers concurrently with irradiation-induced creep and swelling of the pyrocarbon layers, and the buildup of internal pressure. Thus, the program can treat any varying temperature history, such as the suddenly increasing temperature of an accident condition or the cyclic temperature that may be experienced in a pebble-bed reactor.

8. Conclusions

Many of the key phenomena of TRISO-coated fuel particle behavior have been or are in the process of being incorporated into INEEL's fuel performance model called PARFUME. These include:

- CO production and fission product gas release that affect the internal gas pressure,
- fission product generation and migration and its influence on the particle coatings,
- temperature profiles across the fuel matrix and across the particle layers,
- kernel migration (amoeba effect),
- other multi-dimensional mechanisms that affect the particle failure probability, e.g., partial debonding of the IPyC layer, cracking of the IPyC layer, an aspherical geometry, and thinning of the SiC layer due to interaction with fission products,
- statistical variations of key properties of the particle associated with the production process, which are treated with either Monte Carlo sampling or with an integral formulation,
- an accident condition, where a normal period of irradiation is followed by a sudden change in temperature.

The INEEL is participating in the International Atomic Energy Agency (IAEA) Coordinated Research Program (CRP) benchmark program, which is designed to compare coated fuel particle performance codes around the world. Many of PARFUME's capabilities are being exercised in these benchmark activities.

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