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DEVELOPMENT OF AN INTEGRATED PERFORMANCE MODEL FOR TRISO-COATED GAS REACTOR PARTICLE FUEL

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ABSTRACT

The success of gas reactors depends upon the safety and quality of the coated particle fuel. The understanding and evaluation of this fuel requires development of an integrated mechanistic fuel performance model that fully describes the mechanical and physico-chemical behavior of the fuel particle under irradiation. Such a model, called PARFUME (PARticle FUel ModEl), is being developed at the Idaho National Engineering and Environmental Laboratory. PARFUME is based on multi-dimensional finite element modeling of TRISO-coated gas reactor fuel. The goal is to represent all potential failure mechanisms and to incorporate the statistical nature of the fuel. The model is currently focused on carbide, oxide and oxycarbide uranium fuel kernels, while the coating layers are the classical IPyC/SiC/OPyC. This paper reviews the current status of the mechanical aspects of the model and presents results of calculations for irradiations from the New Production Modular High Temperature Gas Reactor program.

1. Introduction

The INEEL has begun development of an integrated mechanistic fuel performance model for TRISO-coated gas-reactor particle fuel termed PARFUME (PARticle FUel ModEl). Compared to light water reactor and liquid metal reactor fuel forms, the behavior of coated-particle is inherently more multidimensional. Moreover, modeling of fuel behavior is made more difficult because of the statistical variations in fuel physical dimensions and/or component properties, from particle to particle due to the nature of the fabrication process.

Our objective in developing PARFUME is to physically describe both the mechanical and physico-chemical behavior of the fuel particle under irradiation, with the proper dimensionality, and still capture the statistical nature of the fuel. The statistical variation of key properties of the particle associated with the production process requires Monte Carlo analysis of a very large number of particles to understand the aggregate behavior. Thus, state-of-the-art statistical techniques are being used to incorporate the results of the detailed multi-dimensional stress calculations and the fission product chemical interactions into PARFUME. Furthermore, we want to verify PARFUME using data from historical TRISO-coated particle irradiations so that the code can be used to design advanced coated-particle fuel with greater confidence for the gas reactor and other particle fuel applications (Pu and minor actinide burning, gas-cooled fast reactors).

2. Key Phenomena

Our mechanistic model for coated-particle fuel will consider both the structural and physico-chemical behavior of a particle-coated fuel system during irradiation. The following important phenomena will be included:

- Fission gas release from the kernel as a function of burnup, temperature and kernel type (oxide, carbide, oxycarbide);
- Anisotropic response of the pyrolytic carbon layers to irradiation (shrinkage, swelling, and creep that are functions of temperature, fluence, and orientation/direction in the carbon);
- Failure of the pyrolytic carbon and SiC layers based on the classic Weibull formulation for a brittle material either by traditional pressure vessel failure criteria or by mechanisms such as asphericity, layer debonding, or cracking;

- Fission product inventory generation as a function of burnup and enrichment of the particle;
- Chemical changes of the fuel kernel during irradiation (changes in carbon/oxygen, carbon/metal and/or oxygen/metal ratio depending on the kernel fuel type, production of CO/CO_2 gas) and its influence on fission product and/or kernel attack on the particle coatings;
- Kernel migration;
- Fission product diffusion, migration and segregation;
- Statistical variations of key properties of the particle associated with the production process, requiring Monte Carlo analysis of a very large number of particles to understand the aggregate behavior.

Due to space limitations, this paper will focus only on the structural aspects of the model.

3. Material Properties

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 during irradiation of the particle while the SiC exhibits only elastic response. A portion of the gas pressure is transmitted through the IPyC layer to the SiC. This pressure continually 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 anywhere 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.

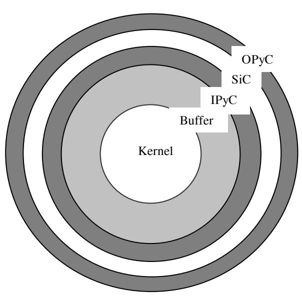

Figure 1. Typical TRISO-coated fuel particle geometry.

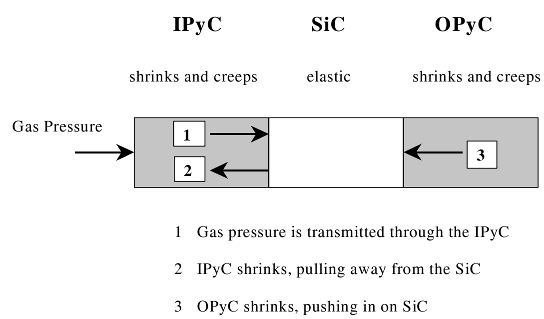

Figure 2. Behavior of coating layers in fuel particle.

Numerous material properties are needed to represent fuel particle behavior in the performance model. These include irradiation-induced strain rates to account for shrinkage (or swelling) of the pyrocarbon layers, creep coefficients to represent irradiation-induced creep in the pyrocarbon layers, and elastic properties to represent elastic behavior for the pyrocarbons and silicon carbide. The properties used in the model were obtained from data that was compiled in a report by the CEGA Corporation in July 1993. This data was based on a review and evaluation of material properties published in the literature to that date [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. Due to anisotropy in the swelling behavior of the pyrocarbon layers, the strains are different for the radial and tangential directions. The swelling strains are functions of four variables, i.e. fluence level, pyrocarbon density, degree of anisotropy (as measured by the Bacon Anisotropy Factor, BAF), and irradiation temperature. In the radial direction, the pyrocarbon generally shrinks at low fluences but swells at higher fluences. In the tangential direction, the pyrocarbon shrinks at all levels of fluence. The magnitude of the shrinkage increases as

BAF increases or as the irradiation temperature increases. The silicon carbide is a much stiffer material than the pyrocarbons, with a Young's modulus that is an order of magnitude larger.

4. Models

4.1 Structural

The ABAQUS program [2] is used in the performance model to perform finite element stress analysis on coated fuel particles. This program is capable of simulating the complex behavior of the coating layers, and can be used to evaluate multidimensional effects, such as shrinkage cracks in the IPyC, partial debonding between layers, and asphericity. We have shown [3] that radial shrinkage cracks in the IPyC could make a significant contribution to fuel particle failures, and such cracks have been observed in post-irradiation examinations. We have, therefore, devoted significant effort toward including this failure mechanism in PARFUME (in addition to the traditional pressure vessel failure associated with buildup of internal fission gas pressure).

ABAQUS models for both normal and cracked three-layer geometries are shown in Figure 3. These are axisymmetric models that allow for nonsymmetry in the plane of the model, thus enabling an evaluation of multidimensional effects on stress behavior of the coating layers. The model of the normal spherical particle has no cracks or defects in the layers of the particle. The IPyC and OPyC layers are assumed to remain fully bonded to the SiC layer throughout irradiation. This model is used to demonstrate behavior of a normal particle in expected reactor conditions, as well as to determine stresses in the various layers throughout irradiation. The model consists of quadrilateral axisymmetric elements, giving the effect of a full sphere. Only the three structural layers (i.e. the IPyC, SiC, and OPyC) of the particle are included in the model. The layer thicknesses for the IPyC, SiC, and OPyC are nominally set at 40, 35, and 43 μm, respectively, but these can be varied as desired. An internal pressure is applied in the analysis to simulate the buildup of fission gas pressure, and an external pressure is applied to represent either reactor or test conditions. Particles are analyzed in a viscoelastic time-integration analysis that progresses until the fluence reaches 3×10^{25} n/m^2, occurring at a time of 1.2×10^7 s in the analysis. These are representative conditions that can be varied as desired.

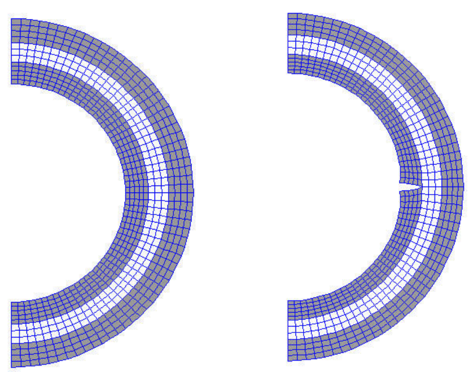

Figure 3. Finite element models for normal and cracked configurations.

The model for a cracked particle is identical to that of the normal particle except that it has a radial crack through the thickness of the IPyC layer. Such a crack is typical of those observed in post-irradiation examinations of the New Production Modular High Temperature Gas Reactor (NP-MHTGR) fuel particles. During irradiation, shrinkage of the initially intact IPyC layer induces a significant tensile stress in that layer. If the tensile strength of the IPyC layer is exceeded, then a radial crack develops in the IPyC layer. This crack is included in the model from the beginning of the solution since it is not feasible to initiate the crack later in the ABAQUS analysis. Because the shrinkage in the pyrocarbons dominates the particle behavior early during irradiation, large tensile stresses in the IPyC occur early. Therefore, the assumption of the presence of a crack at the beginning of the solution should be a reasonable approximation. The analysis does not include dynamic effects associated with a sudden failure of the IPyC, which could increase the magnitude of the stresses calculated.

Figure 4 plots the calculated tangential stress history for the SiC layer of a normal (uncracked) particle. As shown, the SiC remains in compression largely because of the shrinkage in the pyrocarbon layers (the IPyC pulls while the OPyC pushes on the SiC). Figure 4 also plots the maximum principal stress in the SiC layer near the crack tip of a particle with a cracked IPyC. In the particle analyzed, the crack leads to a calculated tensile stress in the SiC layer of about 440 MPa. It can be seen that a cracked IPyC greatly changes the stress condition in the SiC, which significantly increases the probability of SiC failure.

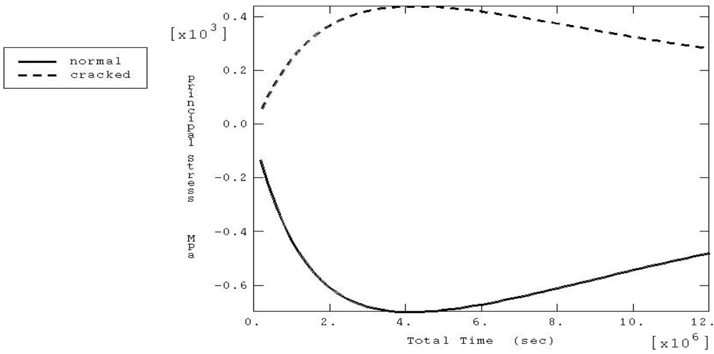

Figure 4. Time histories for stress in the SiC layer for normal and cracked particles.

4.2 Statistical

We have also investigated the effect of statistical variations in fuel particle design parameters on the structural response of the fuel particle. In the case of a normal (uncracked) particle, statistical variations in design parameters are treated with simplified solutions built into the PARFUME code, rendering finite element analysis unnecessary. In the case of a cracked particle, however, finite element analyses are performed to capture the multidimensional behavior and thereby characterize the effects of variations in these parameters. Based on the results of analyses on cracked particles, there are a number of parameters that are important in describing the behavior of the cracked particle and thus merit a detailed statistical evaluation. These include the IPyC thickness, SiC thickness, OPyC thickness, the densities of the pyrocarbon layers, BAF of the pyrocarbon layers, irradiation temperature, particle diameter, and the creep coefficient for the pyrocarbon layers. For example, Figure 5 shows the maximum calculated stress in the SiC layer as a function of the irradiation temperature (when all other parameters are held constant). The stress decreases with temperature because the higher creep in the pyrocarbons at higher temperatures tends to relax stresses in the coating layers earlier during irradiation.

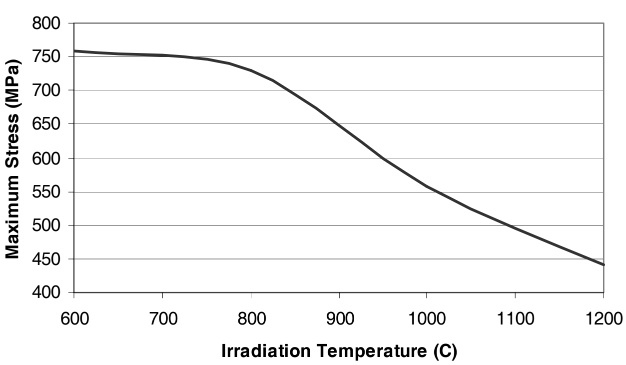

Figure 5. Calculated SiC stress as a function of irradiation temperature.

Initially, regression analyses were performed using the Design Expert program [4] to produce an algorithm that can be used to predict the stress level in the SiC layer of particles having a cracked IPyC. The program used response surface analysis to develop a sixth-order polynomial that statistically fit stress data to a high level of accuracy when variations in six parameters were considered. A full-factorial analysis required results from a total of 972 finite element analyses to successfully develop the algorithm. The problem with this statistical treatment is that it becomes impractical to consider further parametric variations or to redo the analysis if basic assumptions (such as the pyrocarbon shrinkage properties used) are changed. Therefore, an alternative method has been developed that greatly reduces the number of finite element analyses needed. In this approach, finite element analyses are performed on just enough cases to determine the effects of varying each parameter individually. We then analyze the same cases using a closed-form solution that solves for stresses in a normal (uncracked) TRISO fuel particle [5]. Finally, we perform statistical fits on the results of the analyses and draw a correlation between the stress in an uncracked particle with the stress in a cracked particle for the same parametric variations. In the PARFUME code, then, the stress in the SiC layer of a particle having a cracked IPyC is determined by first computing the stress for the same particle having an intact IPyC. This stress is then converted to a stress for a cracked particle by applying the correlations. With this approach, there is little effort involved in adding more parameters to the statistical base, and there is no limit to the number of parameters that can be considered. The number of finite element analyses needed for statistical analysis of six parameters was reduced from 972 to 14. Thus, even if assumptions change or a new failure mechanism is introduced, the effort required to perform a new statistical analysis is easily manageable. The accuracy of this statistical approach was verified by comparing results with those obtained from the Design Expert algorithm. The two methods showed close agreement when used to calculate particle failure probabilities.

5. Approach for Determining the Particle Failure Probability

To treat the statistical variations in material properties and other parameters for the fuel particle, PARFUME uses Monte Carlo sampling on a batch of fuel particles in determining the particle failure probability. In these samplings, the code performs statistical variations on any number of parameters (such as IPyC, SiC, OPyC thicknesses, IPyC BAF, etc.) by applying Gaussian distributions to these parameters. When the code samples a particle, it first uses a closed form solution [5] to calculate the stress in the IPyC layer. Because of the brittle nature of pyrolytic carbon, the IPyC is expected to fail in a probabilistic manner according to the Weibull statistical theory [6]. As such, the calculated stress for the IPyC is compared to a Weibull strength for the IPyC to determine whether it cracks. This strength is obtained by sampling from a Weibull distribution having a mean strength σ_{mc} and a modulus *m*. The mean strength σ_{mc} is defined to be the stress level at which 63.2% of the IPyC layers would fail if all were stressed equally. It is derived from a volumetric integration of stresses in the IPyC, and is based on CEGA's data for the characteristic strength σ_0.

If it is determined that the IPyC layer of the particle cracks, then the statistical correlation equations described in Section 4.2 are used to calculate the stress in the SiC layer. As with the IPyC, the SiC layer is expected to fail according to a Weibull statistical distribution, having a mean strength σ_{mc} and a modulus *m*. The mean strength is derived from an integration of SiC stresses in the vicinity of the crack, and again is based on CEGA's data for the characteristic strength σ_0. If it is determined that the IPyC layer of the particle does not crack, then the code uses the closed form solution to calculate the SiC stress. In this case, the Weibull mean strength σ_{mc} is derived from an integration of the more uniform stresses of an uncracked particle.

6. Predictions for NPR Experiments

The current version of the PARFUME code has been used to analyze three irradiation experiments conducted as part of the NP-MHTGR program in the early 1990s. Fuel compacts were irradiated at the High Flux Isotope Reactor (HFIR) and the Advanced Test Reactor (ATR) in the United States. TRISO-coated particles containing high-enriched uranium were irradiated at temperatures between 750 and 1250 °C, burnups between 65 and 80% FIMA, and fluences between 2 and 3.8×10^{25} n/m^2. On-line fission gas release measurements indicated significant failures during irradiation. Post-irradiation examination (PIE) of individual fuel compacts revealed the presence of radial cracks in all layers of the TRISO coating. The irradiation conditions for the experiments are summarized in Table 1, while the levels of cracking measured during PIE are shown in Table 2. The particle dimensions, burnup, end-of-life fluence, irradiation temperature, and ^{235}U enrichment were set to appropriate values in the analysis for each experiment. Included in the results shown in Table 2 (column 5) are the percentage of particles predicted to have a cracked IPyC and the percentage of particles predicted to fail because of a cracked SiC. It is seen that PARFUME predicts that the IPyC layer cracks in 100% of the particles for every compact tested. In reality, the PIE revealed that the actual failure fractions were less than this, as shown in the table. Based on historical literature sources, it is believed that the creep coefficients currently used in the PARFUME code may be too low, which would allow the calculated shrinkage stresses to reach too high a value before creep relaxation takes effect. If the creep coefficients used in the analyses were amplified by a factor of 2, the number of failures in the IPyC and SiC decrease as shown in Table 2 (column 6). The higher creep gives significantly better correlation with the experimental results.

Table 1. Irradiation conditions for NPR experiments

Fuel Compact ID	Fast Fluence (10^{25} n/m^2)	Irradiation Temp. (°C)	Burnup (%FIMA)
NPR-2 A4	3.8	746	79
NPR-1 A5	3.8	987	79
NPR-1 A8	2.4	845	72
NPR-1A A9	1.9	1052	64

Table 2. Comparisons of ceramographic observations to PARFUME calculations for TRISO coated fissile fuel particles

IPyC Layer (a)					
Fuel Compact ID	Sample Size	% Failed	95% Conf. Interval (%)	Calc.	Calc. with 2× Creep
NPR-2 A4	83	65	54<p<76	100	99.6
NPR-1 A5	39	31	17<p<47	100	34
NPR-1 A8	53	6	2<p<16	100	94
NPR-1A A9	17	18	5<p<42	100	15
SiC Layer (a)					
	Sample Size	% Failed	95% Conf. Interval (%)	Calc.	Calc. With 2× Creep
NPR-2 A4	287	3	2<p<6	40.7	2.2
NPR-1 A5	178	0.6	0<p<3	16.1	0.2
NPR-1 A8	260	0	0<p<2	33.4	1.4
NPR-1A A9	83	1	0<p<5	10.8	0.04

a. Layer failure is considered as a through wall crack as measured by PIE.

7. Summary and Future Work

The INEEL has begun development of an integrated mechanistic fuel performance model for TRISO-coated gas reactor particle fuel named PARFUME (PARticle Fuel ModEl). The objective of PARFUME is to physically describe the behavior of the fuel particle under irradiation. Both the mechanical and physico-chemical behavior of the particle under irradiation are being considered. Statistical and modeling methods have been developed that enable prediction of the multi-dimensional behavior that is characteristic of TRISO-coated gas reactor fuel. These methods have been applied to particle failures caused by irradiation-induced shrinkage cracks in the IPyC layer. The model, with an adjustment in the creep properties for the PyC materials, makes predictions that are in reasonable agreement with the IPyC and SiC failures observed in the NP-MHTGR fuel irradiation experiments performed in the early 1990s. Future work in the code development includes:

- Completion of the fission product chemistry modules for the code
- Development of the fission product transport module
- Comparison of the code to other older gas reactor irradiations data
- Including the effects of asphericity and partial debonding between coating layers.

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