

Improvements to the Predictive Capability of FCM Fuel Performance Modeling

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Abstract

A proposed fuel type for improved accident performance in LWRs (Light Water Reactors) involves TRISO (Tristructural-Isotropic) particles embedded in a NITE (Nano Infiltrated Eutectic) silicon carbide matrix. TRISO fuel particles contain a spherical fuel kernel of about 500 to in excess of 800 microns in diameter. The kernel and buffer layer are then coated with three isotropic layers consisting of a dense inner pyrolytic carbon (IPyC), a silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer. These layers are about 40 microns thick. The TRISO particle packing fraction in the NITE-SiC matrix is expected to be about 40 vol percent.

The release of radioactivity into the coolant is dependent on the integrity of the silicon carbide layer of the TRISO particles and the NITE-SiC matrix. Currently BISON is a code being used to simulate the thermo-mechanical behavior of this fuel type. BISON, a code under development by Idaho National Laboratory, is built on the Multi-physics Object Oriented Simulation Environment (MOOSE). MOOSE is a massively parallel, finite element computational system that uses a Jacobian-free, Newton-Krylov (JFNK) method to solve coupled systems and non-linear partial differential equations.

Due to the anisotropic geometry of the FCM pellet, the capability to model a large and random arrangement of discrete TRISO particles was developed. Additional work has been performed to develop models for the fracture of the FCM materials and transport of silver and cesium. This combination allows sufficient predictive capability to perform preliminary analysis of FCM fuel performance.

TRISO FCM is predicted to perform well for linear powers less than 45 kW per meter in light water reactor environments and 15 kW per meter in high temperature gas reactors. The silicon carbide pellet is expected to limit the cesium inventory release to less than one percent in the first two days following a major accident.

Future work would focus on the coupling of PyC volume change and irradiation creep effects. Coupling these effects may prevent the large stresses predicted due to rapid volume expansion. An additional objective is to design and perform experiments that show the PyC behavior at high neutron fluence.

Keywords: FCM, TRISO, thermo, mechanical, BISON, fracture

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CHAPTER 1: INTRODUCTION

1.1 Background

This dissertation is focused on the improvements made to finite element based thermal mechanical fuel performance modeling of the FCM fuel concept for commercial light water reactors (LWRs). The Fully Ceramic Microencapsulated (FCM) fuel concept is a proposed replacement for conventional uranium dioxide fuel pellets [1]. The potential benefit is reduced economic impact and decreased radioactive contamination from accident scenarios such as station blackout and loss of coolant.

The FCM concept for LWR applications consists of a standard zircaloy cladding surrounding a silicon carbide (SiC) pellet, also referred to as the “matrix.” This matrix has been embedded with TRISO fuel bearing particles that are approximately 1 mm in diameter. A schematic of the geometry is shown in Figure 1. The matrix provides a means to contain the TRISO particles with minimal damage, low centerline temperatures due to the high thermal conductivity, and long diffusion distances to limit radioactivity release to the environment [1,2]. The matrix is produced by the Nano Infiltration Transient Eutectic process, which produces NITE-SiC. In brief, the NITE process uses cold pressing to consolidate the SiC nanopowder with aluminum and yttrium oxides. This “green” pellet is then sintered to form the NITE-SiC matrix. A paper by Terrani et al. discusses the process in detail [3].

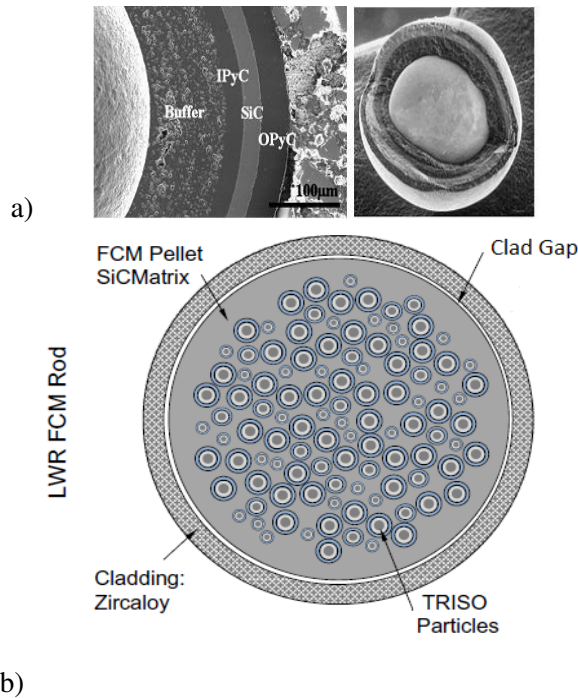


Figure 1. a) Photomicrographs showing a TRISO particle with its individual layers of porous carbon buffer, inner pyrolytic carbon, silicon carbide, and outer pyrolytic carbon [4]. **b)** Schematic illustration of the geometrical model for an FCM particle containing 40% packing fraction of TRISO particles [5].

The following is a general description of a TRISO particle, which contains the fuel and is embedded in the NITE-SiC matrix. Each TRISO particle has five distinct layers. At the core of the particle is the fuel

kernel. The fuel kernel is spherical and ranges from 500 to in excess of 800 μm in diameter. A range of fuel materials can be used such as uranium dioxide, uranium oxycarbide, and uranium nitride. The second layer is the “buffer.” This buffer layer is a low density isotropic pyrolytic carbon ($\sim 1\text{ g cm}^{-3}$), typically about 50-100 μm thick, and reduces its volume under irradiation by $\sim 25\text{-}35\%$. The shrinkage of the buffer layer provides additional volume for the swelling of the fuel kernel and accumulation of fission gases. The third layer is the Inner Pyrolytic Carbon (IPyC) layer. This is a 90% dense ($\sim 1.9\text{-}2.1\text{ g cm}^{-3}$) isotropic pyrolytic carbon layer that is about 30 to 40 μm thick [5]. This layer provides a suitable substrate and corrosion protection for the fourth layer that is a Chemical Vapor Deposited silicon carbide (CVD-SiC) layer. There are many variations to the CVD process, but in general the SiC carrier gas methyltrichlorosilane (MTS) and argon cover gas flow over a heated carbon substrate. The increase in temperature causes the MTS to decompose which deposits the SiC onto the carbon substrate [6]. This produces a high purity and monolithic SiC that is typically about 40 μm thick. This allows the SiC layer in the TRISO particle to act as a pressure vessel and barrier to fission product release into the coolant [7]. The fifth layer is the outer pyrolytic carbon (OPyC) layer, which is similar to the IPyC and is a 90% dense isotropic pyrolytic carbon that is about 30 μm thick. The OPyC layer prevents cracks in the SiC pellet from propagating into the CVD-SiC TRISO particle layer and vice versa [5].

1.2 Summary of TRISO Fuel Performance Modeling

Current established TRISO fuel performance codes are one dimensional models that use either a closed form analytical solution or finite elements. The closed form solution solves the stresses radially outwards from the center of the particle. This method allows for a rapid set of solutions but does not capture three dimensional effects. The finite element models have the potential to be expanded to three dimensions but require extensive computational resources and are not designed for statistical variations of parameters [8]. PARFUME is a TRISO fuel performance model (FPM) that employs the closed form solution with ABAQUS finite element code to provide the solutions for three dimensional effects [8,9,10]. This allows a wide range of effects and parameters to be simulated for a single particle while maintaining a reasonable computational requirement. The PARFUME code has been verified through comparison with the IAEA TRISO benchmarks [10,11] and validated through predicted coating layer failure fractions [9,11]. However, there is still significant uncertainty in TRISO fuel performance models.

However, the lack of symmetry in the TRISO particle arrangement within the NITE-SiC matrix generates the need for three dimensional modeling capabilities of a large system. Hence, the goal is to develop a finite element based thermal-mechanical fuel performance model to predict the behavior and performance of TRISO-based FCM fuel. This requires the development of accurate and predictive models for heat transfer, fission product release from the fuel kernel, and thermal-mechanical evolution with neutron irradiation and burnup. In addition, possible gaps or interfacial debonding may develop between the TRISO buffer and inner pyrolytic carbon layer, or between the outer pyrolytic carbon layer and the silicon carbide matrix. Thus, predictive models must be available for thermal expansion, thermal conductivity, density changes, and irradiation creep phenomena as a function of fluence and temperature for LWR conditions. Also of importance, is the potential for release of fission products from failed TRISO particles and their subsequent diffusional transport in the NITE-SiC matrix. This work is being performed using the BISON code developed at Idaho National Laboratory [12].

The BISON code is under development by Idaho National Laboratory, which is built upon the Multi-physics Object Oriented Simulation Environment (MOOSE) [12,13,14]. MOOSE is a massively parallel, finite element computational system that uses a Preconditioned Jacobian-free, Newton-Krylov (PJFNK) method with an implicit Euler solver to provide solutions to coupled systems and non-linear partial differential equations. The partial differential equations are contained in kernels stored within the BISON program. MOOSE is built on LIBMESH and PETSc programs that provide the numerical solutions [12]. This configuration allows highly coupled physics to be solved simultaneously. Also, additional equations can be added or modified with minimal disruption to the other kernels [15].

1.3 Review of Irradiation Effects

1.3.1 Structure

Due to the limited data available for isotropic pyrolytic carbon behavior under neutron irradiation, it is insightful to examine the irradiation behavior of graphite and highly ordered pyrolytic graphite despite the differences in structure. Graphite has two general structures: hexagonal and rhombohedral. Figure 2 shows representations of these structures and compares them to the turbostratic structure seen in Highly Ordered Pyrolytic Graphite (HOPG) [16,17]. The basal planes are oriented along the a-axis (horizontal direction) while the c-axis refers to the vertical direction displayed in Figure 2. The turbostratic structure has planes that are randomly rotated and translated. It should also be noted that the turbostratic structure has greater distances on average between planes ($3.44\text{\AA}$) than the hexagonal or rhombohedral structures ($3.35\text{\AA}$) [18]. Highly Ordered Pyrolytic Graphite (HOPG) has a turbostratic structure with a mosaic spread of about $0.1\text{--}3.0$ degrees, while isotropic pyrolytic carbon (PyC) appears to have amorphous pockets and growth features on the order of $0.5\text{ }\mu\text{m}$ in diameter which are composed of small domains ranging from $2\text{--}5\text{ nm}$ [19].

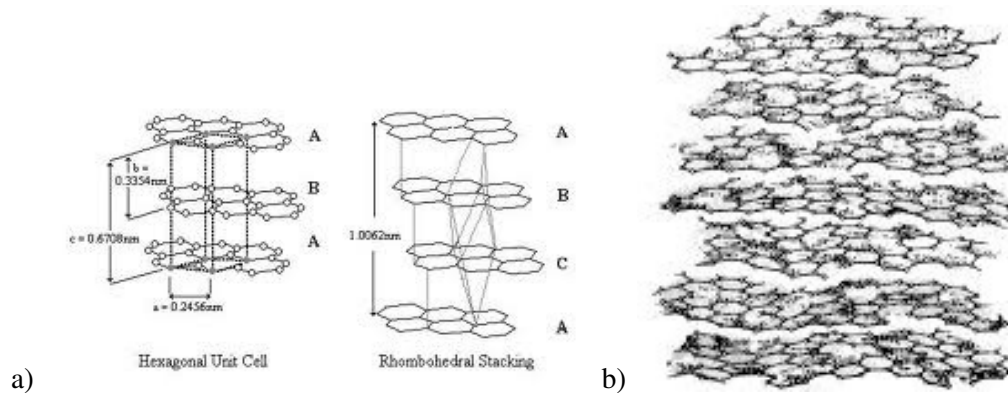


Figure 2. a) A representation for the hexagonal and rhombohedral stacking sequences in graphite. C-axis is in the vertical direction and A-axis is horizontal. Adapted from University of Strathclyde [16]. **b)** Representation of the turbostratic structure observed in HOPG. Adapted from a paper by B. Claub [17].

The atoms in the basal plane are covalently bonded while Van der Waals bonding occurs between layers (C-axis). This difference in bond type produces significant anisotropy in the bulk properties. In graphite, the thermal expansion coefficient in the C-axis is far higher than parallel to the basal plane (A-axis).

Mrozowski cracks parallel to the basal plane are caused by this thermal contraction [20]. The graphitization process occurs at 2600-3000 °C. Upon cooling, the Van der Waals bonding between the graphene planes may allow fracture. It has been estimated that a change in temperature of about 1000 °C is required to generate these cracks [18,20]. Figure 3 shows a Transmission Electron Microscope (TEM) image of several Mrozowski cracks observed in graphite. In the TEM image, the basal planes are aligned mostly vertically and slightly to the right. The scale is 100 nm, which suggests that the crack concentration is quite large.

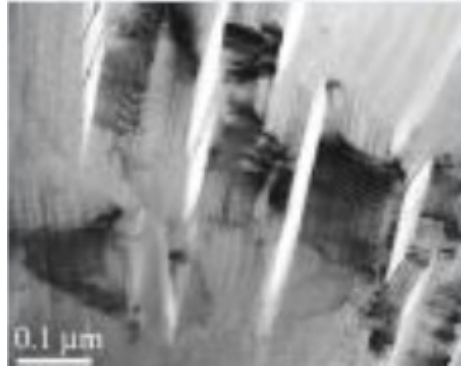


Figure 3. A TEM image of the cracks running parallel to the basal plane caused by thermal contraction. Adapted from Tongxiang Liang at Tsinghua University [20].

According to Bokros et al., these thermal contraction cracks do not occur in pyrolytic carbon [21]. Given the lower temperatures of the chemical vapor deposition (CVD) process (1450 °C) and the disordered structure, it seems reasonable that such cracks would not be plentiful or as large. However, both graphite and highly ordered pyrolytic graphite appear to have greater temperature dependence than the isotropic pyrolytic carbon. Figure 4 shows TEM images of HOPG and isotropic pyrolytic carbon [22,23]. The planes of the HOPG are oriented diagonally, and two cracks can be seen in the TEM image. The PyC close up TEM image of a growth feature shows the disordered domain structure and three isotropic pockets.

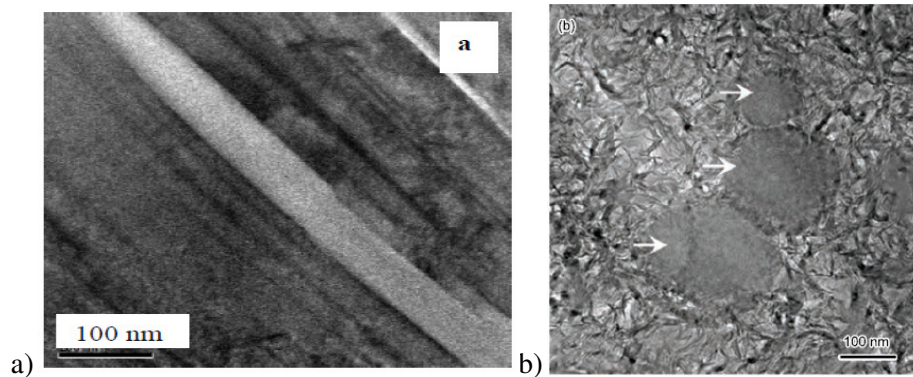


Figure 4. a) A micrograph of the turbostratic structure seen in HOPG [22]. The C-axis orientation is diagonal to the top right. Two thermal contraction cracks can be seen oriented parallel to the basal planes. **b)** A TEM image of as deposited PyC with a density of about 1.3 g cm⁻³ [24]. Note both images are similar in scale.

1.3.2 Graphite Dimensional Change

Under high temperature neutron irradiation, graphite has been observed to experience a volumetric turnaround behavior. The fluence for the turnaround from volumetric shrinkage to swelling is accelerated and the maximum shrinkage for graphite is reduced by increasing temperature [25]. Figure 5 plots experimental results for a small sample of H-451 graphite irradiated at 900 and 600 °C, respectively. The experiments were performed in the High Flux Isotope Reactor (HFIR). Initial density was 1.75 g cm^{-3} . The mechanisms for the dimensional change behavior are not very well understood. However, it is interesting to note that the Irradiation Induced Dimensional Change (IIDC) in the parallel direction to the basal planes follows the perpendicular direction but in a delayed manner. The figures show that graphite experiences initial shrinkage in both directions followed by a turnaround. After the turnaround, the perpendicular direction expands more rapidly than the parallel direction. It is unknown if the graphite dimensional change will saturate at some level or how sensitive the dimensional change is to stress.

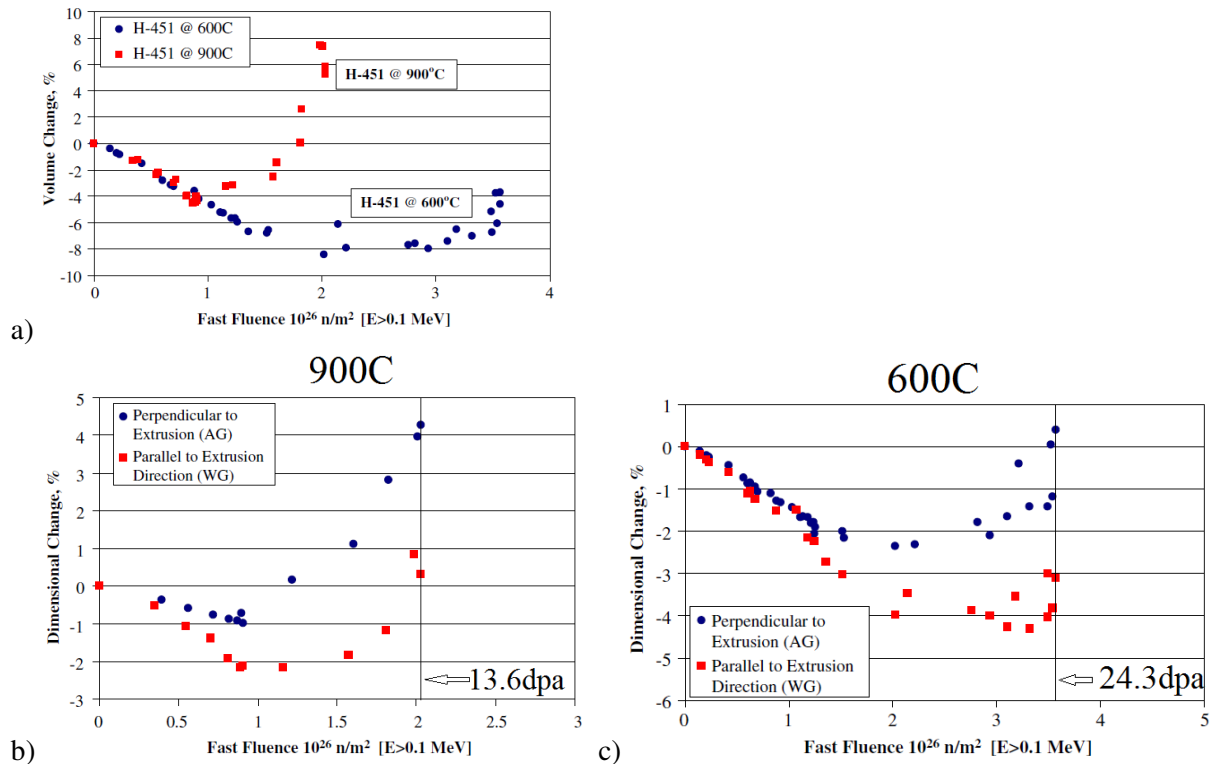


Figure 5. a) Plot of the volumetric change for graphite irradiated at 900 and 600 °C. b) Plot of the dimensional change for graphite irradiated at 900 °C. c) Plot of the dimensional change for graphite irradiated at 600 °C. The estimated conversion for fluence to dpa for these experiments is $0.148 \times 10^{26} \text{ n m}^{-2} \text{ dpa}^{-1}$. This produces a maximum dose of about 13.6, and 24.3 dpa for the 900 and 600 °C irradiations, respectively [25].

One of the proposed mechanisms for graphite dimensional change is that irradiation damage generates interstitial loops which become additional planes in the C-axis. However, the Mrozowski cracks accommodate these atoms, and the resulting vacancies in the A-axis collapse to generate net shrinkage. After the cracks are filled, the C-axis begins to swell. Figure 6 illustrates this concept.

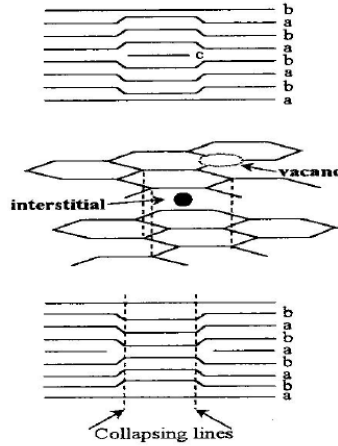


Figure 6. A schematic of the proposed interstitial loop driven dimensional change in graphite. The interstitial loop is thought to cause expansion in the perpendicular direction and contraction in the parallel axis [25].

An alternate proposed mechanism is vacancy loop dissociation and positive dislocation climb [26]. Graphite was electron beam irradiated at room temperature and dose rates 10^{-4} to 10^{-3} dpa s^{-1} . The noise filtered High Resolution Transmission Electron Microscopy (HRTEM) images indicate that additional lattice planes can be generated by vacancy loops. Figure 7 shows the HREM images for vacancy loop and interstitial loops. Vacancy loops were observed more frequently than interstitial loops. However, there was also a molecular dynamics article suggesting that these observed features could be ramp type defects and vacancy lines [27].

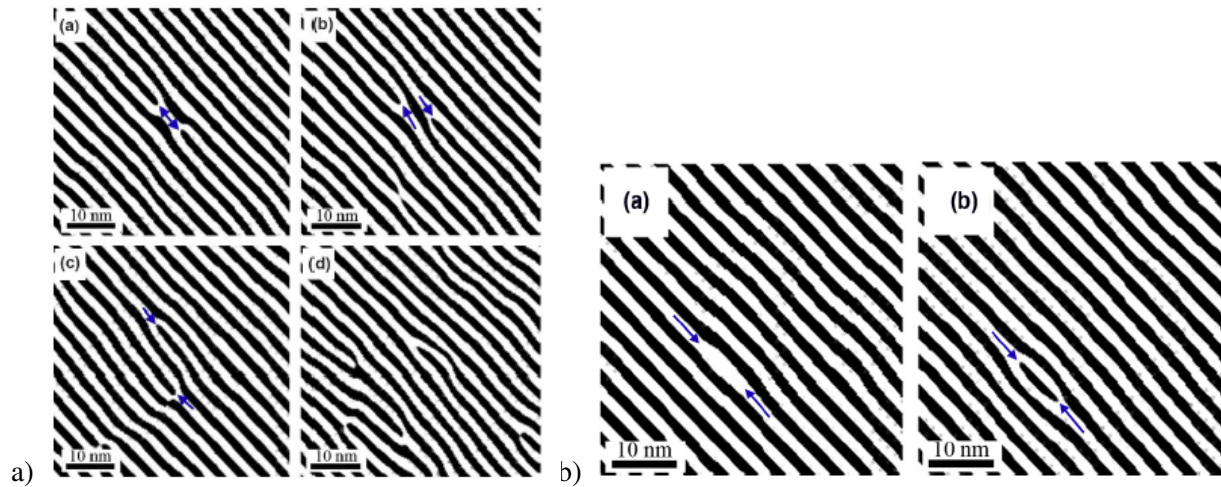


Figure 7. HRTEM images for room temperature electron irradiated graphite [26]. **a)** On the left are the images of vacancy loop formation and positive climb [26]. **b)** On the right are the images for interstitial loop formation.

1.3.3 Pyrolytic Carbon Microstructural Changes Under Irradiation

As previously mentioned, PyC is composed of micro crystallite features about 500 nm in diameter. At low density, these features are roughly spherical, but as density increases, the pores around each feature are filled. Each of these features contains domains or crystallites that are initially about 2-3 nm across in the C-axis. These domains will increase in size under both heat and irradiation. Heat treatments by Zhang et al. saw an increase in the domain C-axis size from about 2 to 5 nm at a temperature of 1800 °C [28]. Figure 8 shows as deposited TEM images of low density ($\sim 1.3 \text{ g cm}^{-3}$) PyC [24]. Low temperature HFIR irradiations of high density ($\sim 2.0 \text{ g cm}^{-3}$) PyC at about $\sim 320 \text{ }^{\circ}\text{C}$ and fluence of $7.25 \times 10^{25} \text{ n m}^{-2}$ have produced domain sizes of about 15-25 nm [29].

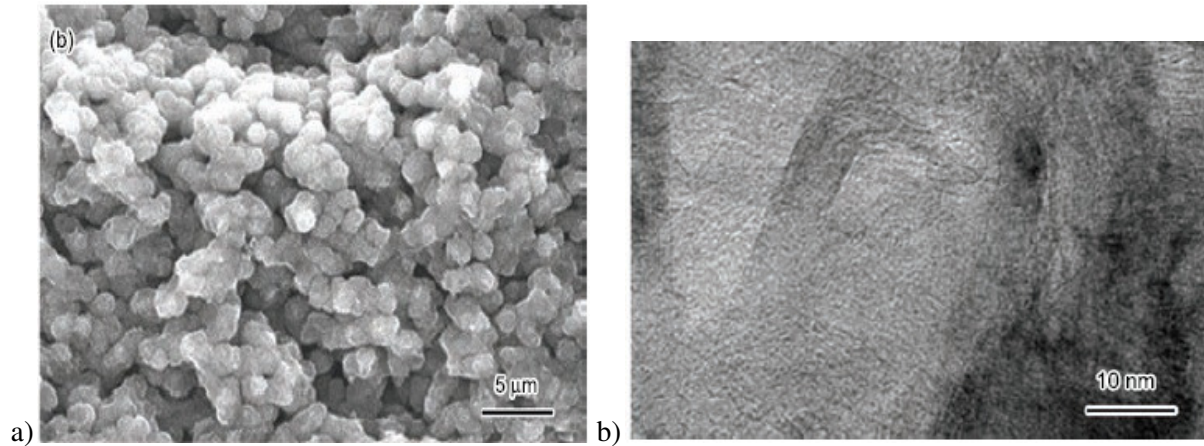


Figure 8. TEM images of as deposited low density PyC [24]. **a)** Image of the growth features. **b)** A magnified image of the domains contained within each growth feature.

Irradiations by Kaae revealed the densification of the micro crystallite features. It was estimated that most of the densification came primarily from within the micro crystallite features rather than the closure of intra-feature pores. It was also observed that the domains on the surface of micro crystallite features have the basal planes oriented parallel to the surface [19].

1.3.4 Isotropic Pyrolytic Carbon Irradiation Induced Dimensional Change

The available data for PyC dimensional change is limited to about $4\text{-}8 \times 10^{25} \text{ n m}^{-2}$ and intended for high temperature applications. Fast neutron fluences ranging up to $30 \times 10^{25} \text{ n m}^{-2}$ are expected in the FCM fuel concept. There is considerable scatter in the available data, and the lack of a mechanistic understanding prevents the ability to extrapolate to higher fluences with any degree of confidence.

There are two notable published correlations available. The first is the German FZJ correlation [9], which assumes an essentially constant volume IIDC with radial expansion and tangential shrinkage. The second is the Lawrence Livermore National Laboratory (LLNL) correlation [30], which assumes a turnaround similar to the graphite dimensional change. Figure 9a and b display the available experimental data as points and then overlays the FZJ and LLNL IIDC correlations [31,32,21,30]. Figure 9c displays the curve fits to the data used in extrapolating/interpolating the LLNL correlation [30].

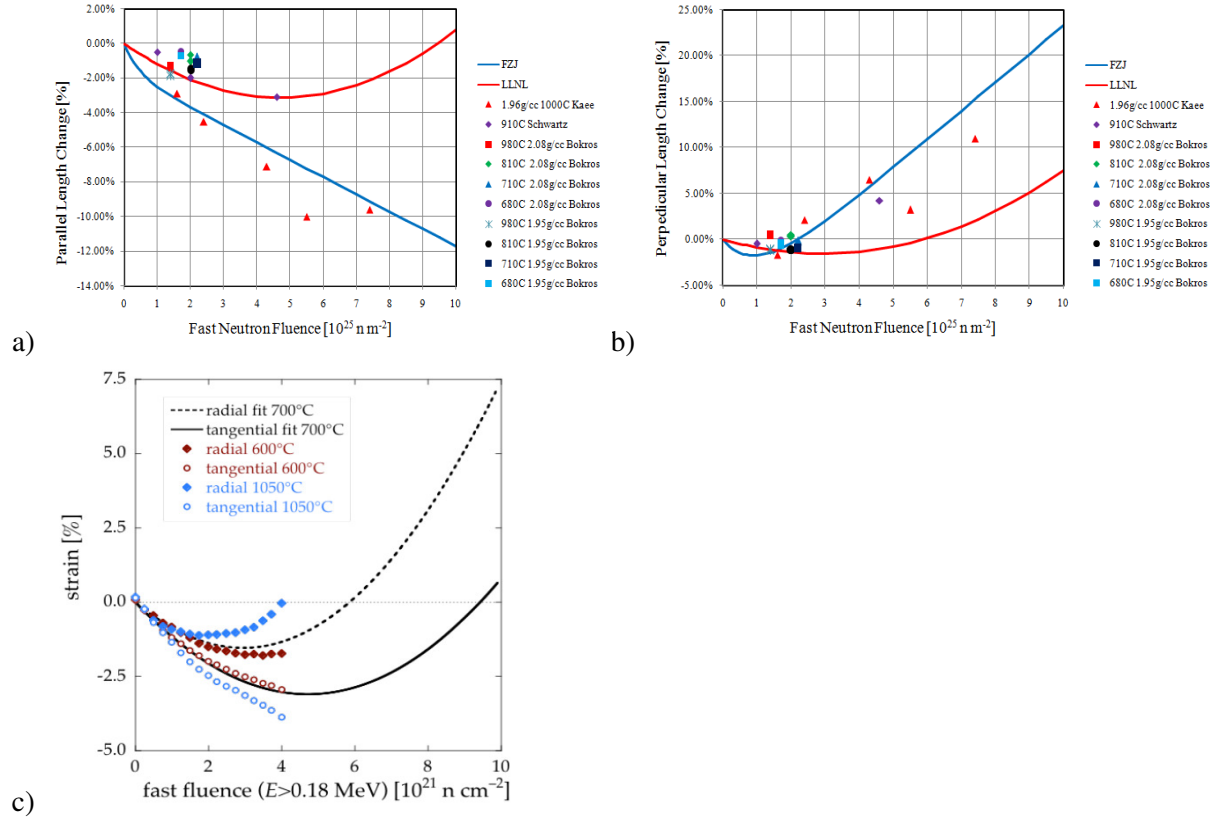


Figure 9. a) A plot of the parallel dimensional change data overlaid by the FZJ and LLNL correlations. b) A plot of the perpendicular dimensional change data overlaid by the FZJ and LLNL correlations. c) Curve fits to data from Ballinger et al. with the 700 °C interpolation and extrapolation also displayed [30].

1.3.5 Thermal Creep

Graphite thermal creep has been noted to be a strong function of the angle between the applied stress and the C-axis. In compression, the thermal creep rate varies by a factor of four with the maximum occurring at 45° to the C-axis. In tension, the thermal creep rate varies by about five orders of magnitude with the maximum occurring parallel to the C-axis [18]. This suggests a constant volume slip mechanism between the basal planes in compression. In tension, it seems likely that the mechanism is micro cracking, which allows volume expansion. If this latter mechanism is accurate, then after tensile stresses are applied in the C-axis resulting in micro cracking, a compressive stress in the same direction should decrease the net volume. Whereas initially applying a compressive stress should result in a slip mechanism, which could be approximated as a constant volume creep. As a result, the effective Poisson ratio in creep may change under irradiation and applied conditions. In addition, it should be noted that irradiation creep is far greater in magnitude than thermal creep. However, the mechanisms of thermal and irradiation creep may be related.

1.3.6 Irradiation Creep

There is significant scatter in the information available for the irradiation creep rate of isotropic pyrolytic carbon. A factor of five spread is shown in Table 1, and the disagreement in low temperature trends is shown in Figure 10. The extensive uncertainty has not yet been resolved.

Table 1. List of the prominent measured irradiation creep constants for isotropic pyrolytic carbon at 1200 °C. Table reproduced from Petti et al [9].

Author	Creep Constant $10^{-29} (\text{MPa n m}^{-2})^{-1}$
Kaae et al. (1972)	1.0
Price and Bokros (1967)	1.3
Buckley et al. (1975)	4.9
Buckley et al. (1975)	4.0
Brocklehurst and Gilchrist (1976)	3.3
Brocklehurst and Gilchrist (1976)	1.7
Morgand (1975)	13.3

Low temperature irradiation creep data for graphite from Kennedy and Platonov indicated an increase in creep rate at temperature below 500 °C while graphite data from Kelly and Brocklehurst indicated a constant creep rate at low temperatures [33]. Figure 10 plots the discrepancy. A constant creep rate below 600 °C is more defensible at this time since a mechanism for a low temperature increase has not been suggested. However, carbon materials are known for their unique behaviors.

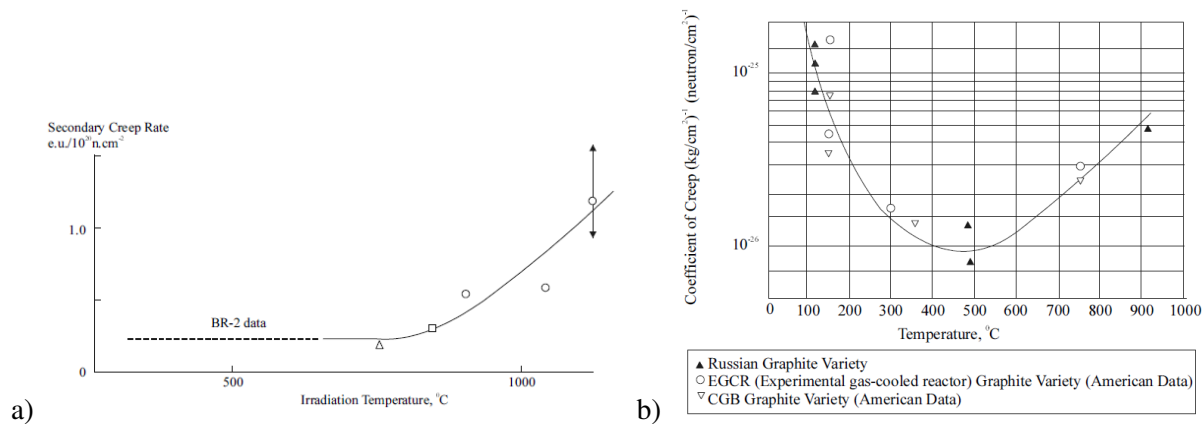


Figure 10. The different creep trends observed at low temperatures from British and American-Russian sources [33]. **a)** A plot of the trend from Kelly and Brocklehurst [33]. **b)** A plot of the data from Kennedy and Platonov. Figures adapted from IAEA-Tecdoc-1154 Figure 5.2 [33].

1.3.7 Poisson Ratio in Creep

Data from Kaae indicates that the Poisson ratio in creep for isotropic pyrolytic carbon may change with creep strain [32]. Figure 11 plots the results.

Due to the low bond strength between graphene layers, pyrolytic carbon may experience what is essentially micro cracking. As a result, a change in volume may occur and could be approximated as low Poisson ratio in creep. A Poisson ratio in creep of 0.4 is used in the STRESS3 TRISO fuel performance code [9].

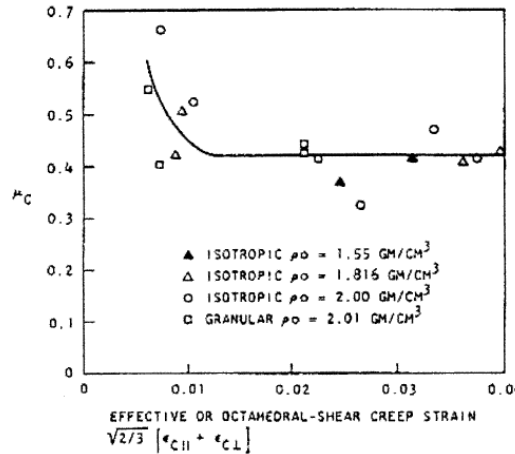


Figure 11. A plot of the Poisson ratio in creep data from Kaae for pyrolytic carbon [32].

1.3.8 Irradiation Behavior of SiC

Based on a combination of data from Snead et al. and Price et al. [34,35,36,37], the irradiation induced swelling of silicon carbide appears to saturate for temperatures less than 1000 °C and is inversely proportional to temperature. This is thought to be caused by greater interstitial and vacancy recombination at higher temperatures. However, at temperatures between 1000 and 1250 °C data from Price et al. suggests there is a transition to cavity formation [37]. The expected result is a linear swelling that is only fluence dependent for temperatures above 1250 °C. Also based on Oak Ridge data, the thermal conductivity and irradiation creep are modeled as dependent on the irradiation swelling. This produces a stable material under irradiation.

The effect of these behaviors on an FCM pellet in a light water reactor is to generate more swelling on the perimeter of the pellet due to its lower temperature, which causes compressive hoop stresses at the surface. This is expected to reduce the probability of cracks reaching the surface of the pellet. However, the high temperature SiC swelling can eventually reach the same amount as the saturated perimeter of the pellet. When this occurs, the hoop stress profile inverts and tensile stresses are predicted at the surface of the pellet.

Other material properties of SiC are well understood and will be discussed in Chapter 2. A publication by Snead et al. [34] is an excellent reference for SiC elastic properties under irradiation. However, most of these properties vary less than 10% and are considered constant in the model.

1.4 Summary

In summary, the FCM fuel concept has the potential to reduce economic impact, provide additional coping time, and energy storage in the event of an accident. However, there is considerable uncertainty in the material properties of the pyrolytic carbon. The shrinkage of this material could cause interface debonding which can increase the probability of through wall fracture of the CVD-SiC layer within the TRISO particles leading to increased radioactivity release. Also, there is the possibility of significant volumetric increase from PyC dimensional change which has the potential to cause very large stresses in

the matrix. Additional factors such as Poisson ratio in creep and hydrostatic stress may substantially reduce the stress and thereby improve the fuel performance.

The effect of low temperature SiC swelling is beneficial to FCM fuel. The greater swelling at low temperatures compared to 1000 °C produces compressive stress in the perimeter of the pellet. However, operating the fuel type in mixed saturated/continuous swelling regimes for long durations has the potential to cause tensile hoop stresses in the perimeter of the pellet. This profile inversion would occur when the interior swelling exceeds that of the perimeter. The remaining operating condition is the high temperature regime where the pellet perimeter is above 1250 °C. Operating at this high of a temperature should be possible, however, substantial fission gas pressures may occur at high burnups. The fission gas pressure will also depend on the porosity of the kernel and volume of the buffer.

1.5 Dissertation Overview

Chapter 2 introduces the material models used in the BISON simulations. These materials are uranium nitride, low density pyrolytic carbon, high density pyrolytic carbon, CVD silicon carbide, NITE silicon carbide, graphite, and Zircaloy-4. In some cases, uranium dioxide properties have been substituted for uranium nitride due to lack of data.

Chapter 3 describes the BISON code and the methods used to progress from a two dimensional single particle to a three dimensional single particle. This chapter also includes the implementation of debonding.

Chapter 4 discusses the difficulty in predicting both high and low temperature TRISO experiments with the same material correlations. As a result, an empirical correlation for PyC dimensional change that depends on initial density, Bacon Anisotropy Factor (BAF), temperature, and fluence was developed.

Chapter 5 presents the results of the HTGR FCM sensitivity study simulations. The parameters of interest are PyC dimensional change, hydrostatic stress, linear power, coolant temperature, and binder.

Chapter 6 presents the results of the LWR FCM sensitivity study simulations. Variables include Poisson ratio in creep, creep rate, and linear power with the resulting high temperature silicon carbide swelling.

Chapter 7 introduces matrix cracking and diffusional based transport of silver and cesium fission products.

Chapter 8 summarizes the conclusions reached in the dissertation and topics for future work.

CHAPTER 2: MATERIAL MODELS

2.1 Property Summary and Assumptions

There are several materials used in the FCM fuel type that exhibit different behaviors under irradiation. This combination of effects can interact to generate unexpected results. Hence, a review of the material properties is essential to understanding the simulation results and uncertainties. The elastic modulus, Poisson ratio, and coefficient of linear thermal expansion (CTE) were modeled as constants (the effect of dose and temperature on these properties was neglected) for all materials including the kernel.

In the case of silicon carbide, ignoring dose effects for these properties is reasonable since <10% change is detected [34]. The temperature trend for CTE saturates at about 1000 K. The CTE at 500 K is about 16% below its saturation value. The specific heat increases from about 1050 J kg⁻¹ K⁻¹ at 500 K to about 1300 J kg⁻¹ K⁻¹ at 1500 K [34]. The constant SiC specific heat assumption is the most questionable. However, in this application the power levels and temperatures change slowly. During accident modeling, this assumption will need to be improved.

Data used in the CEGA model [38] for PyC shows that the bulk average coefficient of thermal expansion varies with temperature from about 4.5x10⁻⁶ K⁻¹ at 350 K to about 5.6x10⁻⁶ K⁻¹ at 850 K [9]. Data for thermal expansion dependence on fluence is limited, and no recommendations are provided by the German, British or American sources [9]. Elastic Poisson ratio values in literature vary from 0.3 to 0.21 and are constant with fluence and temperature. In this model, the CEGA recommendation of 0.21 is used for dense PyC while a value of 0.3 is used for porous buffer PyC [9,38]. The Young's modulus is a different situation. FZJ recommends a constant 29 GPa, but BNFL suggests that it saturates at 1.5x10²⁵ n m⁻² with a value of 33 GPa. The CEGA recommendation is a linear increase from 29 GPa for unirradiated PyC to a value of 55 GPa at a fluence of 4x10²⁵ n m⁻² [9]. Due to different trends, a constant value of 47 GPa is used in this model which is also the default value used by the BISON team at INL [4].

Table 2 provides the constant properties for the uranium nitride kernel, ~50% dense carbon buffer, dense pyrolytic carbon, graphite, and Zircaloy-4 cladding. UO₂ data was used for the UN elastic modulus and thermal conductivity degradation with burnup due to the limited data available. These values were obtained from the available literature [9,4,39,40,41].

Table 2. The constant properties used for UN, low and high density pyrolytic carbon, and Zr-4 cladding. The NITE and CVD SiC use the same mechanical properties. At this time, BISON did not allow for anisotropic properties with the exception of dimensional change. Hence, the properties listed in the table are applied isotropically [9,4,39,40,41].

	CVD-SiC	NITE-SiC	Kernel	Buffer	Dense PYC	Graphite	Cladding
Elastic Modulus [GPa]	450	400	250	20	47	12	100
Elastic Poisson Ratio [-]	0.21	0.2	0.35	0.30	0.21	0.15	0.37
Thermal Expansion [1x10 ⁻⁶]	4.5	4.5	8.6	3.5	5.6	5.6	5.0
Specific Heat [J kg ⁻¹ K ⁻¹]	1200	1200	250	500	500	500	330

Table 3 lists the data used to assess the diffusional transport of silver and cesium release model. Transport in graphite was not considered due to its anisotropic nature, the limitations of BISON, and the available data sets. Soret thermal gradient diffusion was also considered and included in the transport term, but due to a lack of data the effect remains disabled.

Table 3. Below are the diffusion properties for the modeled fission products. Data was lacking for palladium and cadmium. Data is taken from reputable sources as much as possible, but considerable gaps in knowledge exist.

	SiC	SiC	PYC	PYC	UN	UN	Source
	D_0 [$m^2 s^{-1}$]	Q [$kJ mol^{-1}$]	D_0 [$m^2 s^{-1}$]	Q [$kJ mol^{-1}$]	D_0 [$m^2 s^{-1}$]	Q [$kJ mol^{-1}$]	
Ag	3.6×10^{-9}	220	5.3×10^{-9}	154	6.7×10^{-9}	165	[42]/[42]/[43]- -UO ₂
Cs	5.5×10^{-8}	222	6.8×10^{-8}	222	5.6×10^{-8}	209	[4]/[4]/[4]- UO ₂
Pd	3.6×10^{-10}	220	5.3×10^{-10}	154	6.7×10^{-10}	165	0.1 of Ag
Cd	3.6×10^{-11}	220	5.3×10^{-11}	154	6.7×10^{-11}	165	0.01 of Ag
Ba	2.2×10^{-10}	200	5.1×10^{-6}	180	4.6×10^{-8}	209	[44]/[44]/0.8x Cs
Xe	1×10^{-20}	0	1.12×10^{-5}	284	4×10^{-10}	271	Approx/[44]/[45]

However, there is considerable data available for silver and cesium transport in silicon carbide, which is the primary material that resists the release of these elements. As a result, it is possible to provide insight into the potential effects of cracking in the NITE-SiC matrix and CVD-SiC TRISO layers. It should be noted that as the diffusion coefficient increases, the time step size must also decrease to allow for convergence of the solution. As a result, simulations involving high temperature require a large amount of computational resources. The implementation of the silver and cesium transport will be discussed in the following chapter.

2.2 Uranium Nitride

2.2.1 Thermal Conductivity

Figure 12a plots the parabolic curve fit for un-irradiated UN thermal conductivity from 500 to 2000 K [39]. The curve fit is based on experimental data using a laser flash method performed by Arai et al. [41]. The curve was extrapolated to 3000 K to ensure reasonable numbers if temperatures above 2000 K are encountered in the simulation. Figure 12b plots the predicted UN thermal conductivity trends versus burnup. These trends are based on the known thermal conductivity degradation in UO₂ [46]. At high temperature, the net reduction in thermal conductivity becomes less after irradiation. Equation 1 provides the UN thermal conductivity equation.

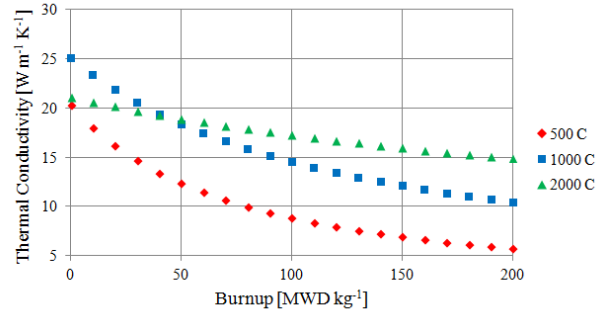
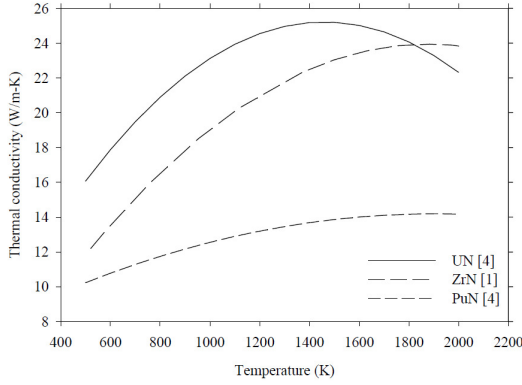


Figure 12. a) Plot of the unirradiated uranium nitride thermal conductivity fit. The figure indicates that the unirradiated UN reaches a maximum thermal conductivity around 1500 K. Measurements were done with the flash laser method [41]. Adapted from Kim and Hoffman Figure 5-3 [39]. **b)** Plot of the modeled UN thermal conductivity versus burnup. This is a combination of the unirradiated UN data from Kim and Hoffman and the UO_2 thermal conductivity degradation data from Lucuta et al. [46]. The trend predicts less degradation at higher temperatures.

$$k_{UN} = k_{UN}^{initial} \frac{k_{\text{UO}_2}}{k_{\text{UO}_2}^{initial}} \quad (\text{Eq. 1})$$

$$k_{UN}^{initial} = 3.7 \times 10^{-9} (T + 273)^3 - 2.1877 \times 10^{-5} (T + 273)^2 + 3.5747 \times 10^{-2} (T + 273) + 7.51 \quad (\text{Eq. 1a})$$

$$k_{\text{UO}_2} = \frac{1}{0.1148 + 0.0035B + 2.475 \times 10^{-4} (1 - 0.003B)T} + 0.0132 \exp(0.00188T) \quad (\text{Eq. 1b})$$

Equation 1. B is the burnup in MWD per kg UN and T is the temperature in $^{\circ}\text{C}$.

2.2.2 Swelling and Fission Gas Release

Figure 13 plots the irradiation swelling of UO_2 , which is based on correlations from the RELAP5 library [40]. This correlation has been adapted to model UN kernel swelling. Initially, the fuel densifies and then swells due to solid and gaseous fission products. At high burnups, the swelling rate is modeled at about 0.7% volumetric swelling per at% burnup. The gaseous fission product swelling increases with temperature as does the amount of fission gas released. The fission gas release was modeled using the Simple Integrated Fission Gas Release and Swelling (SIFGRS) model [47] which at low temperatures predicts an incubation period preceding quadratic release. The net effect is that the early life UN swelling is temperature dependent. However, the swelling rate at high burnups is nearly temperature independent. Due to the dominating nature of the irradiation swelling, it was assumed that uranium nitride creep would be negligible in comparison and thus is not included in the model.

Figure 14 plots an example of the fractional fission gas release fraction from a spherical kernel at temperatures from 1500 to 900 $^{\circ}\text{C}$. At low temperatures, there is an incubation period, but at high temperatures the gas release begins almost immediately.

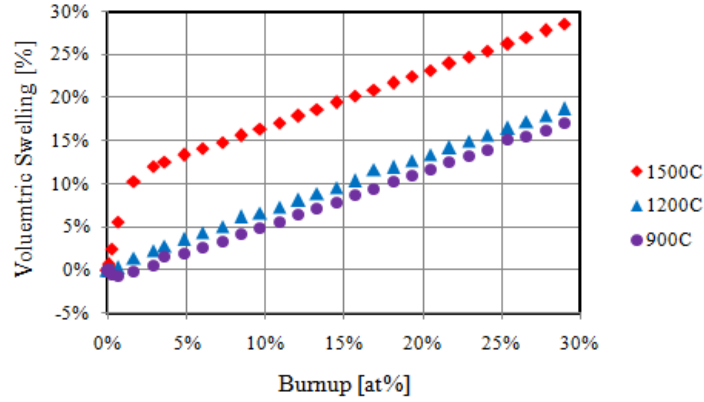


Figure 13. The uranium nitride swelling is plotted as a function of burnup at three different temperatures. The swelling is based on the MATPRO library used in the SCDAP/RELAP5 program [40]. The densification and gaseous fission product swelling are temperature dependent, but the solid fission product swelling is not. Also, the fission gas release increases with temperature which allows the long term swelling slopes to be similar as a function of temperature at high burnups.

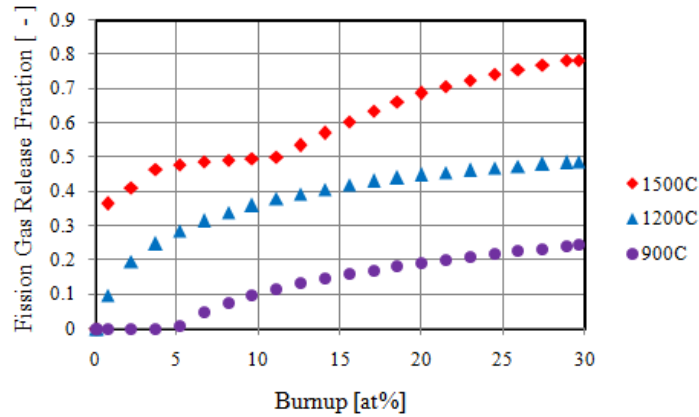


Figure 14. The fission gas release plotted as a function of burnup at three different temperatures obtained from with the SIFGRS model [47]. Kernel density was set to 11.3 g cm^{-3} . Changing the density of the kernel had no impact on the predicted fission gas release.

2.3 High Density Pyrolytic Carbon

2.3.1 Irradiation Induced Dimensional Change and Thermal Conductivity

LLNL correlations were used, which rely on experimental data out to about $4 \times 10^{25} \text{ n m}^{-2}$. The curve fits are extrapolated and interpolated for fluences beyond $4 \times 10^{25} \text{ n m}^{-2}$. The experimental data indicates that the dense pyrolytic carbon will initially shrink [30]. However, the PyC may experience volumetric swelling at high fluence. The maximum swelling is expected to be limited by the increasing brittleness of the material and external stress. Hence, the LLNL correlations with a 30% maximum volumetric swelling recommendation were used in the model [30]. Equation 2a and Equation 2b provide the LLNL relationship for the anisotropic swelling. Equation 2c and Equation 2d provide the FZJ IIDC trend [9].

Equation 2e provides the conversion from radial and tangential strain to volumetric change [30]. Figure 15a plots Equations 2c and 2d. The radial strain continues in a linear fashion reaching about 85% at $30 \times 10^{25} \text{ n m}^{-2}$. The pyrolytic carbon thermal conductivity trend is solely driven by volumetric swelling [8]. Equation 3 provides the relationship between porosity and thermal conductivity.

$$S_{\text{tan gential}}^{LLNL} = -0.013\Phi + 0.0014\Phi^2 \quad (\text{Eq. 2a})$$

$$S_{\text{radial}}^{LLNL} = -0.017\Phi + 0.0018\Phi^2 \quad (\text{Eq. 2b})$$

$$S_{\text{tan gential}}^{FZJ} = 0.017143 \exp(-2.1\Phi) - 0.01\Phi - 0.017143 \quad (\text{Eq. 2c})$$

$$S_{\text{radial}}^{FZJ} = 0.077 \exp(-\Phi) + 0.031\Phi - 0.077 \quad (\text{Eq. 2d})$$

$$S_{\text{vol}} = 2S_{\text{rad}} + S_{\text{tan}} + 2S_{\text{rad}}S_{\text{tan}} + 2S_{\text{rad}}^2S_{\text{tan}} \quad (\text{Eq. 2e})$$

Equation 2. S indicates the swelling fraction and Φ is the fast neutron fluence with $E > 0.1 \text{ MeV}$. a plots Equation 2a and Equation 2b with the maximum swelling limited to 30% by volume. This limit is reached at about $13 \times 10^{25} \text{ n/m}^2$ ($E > 0.1 \text{ MeV}$).

$$k_{\text{pyc}} = \frac{10.9866(1 - \text{porosity})}{(1 + 9\text{porosity})} \quad (\text{Eq. 3})$$

Equation 3. The equation used for the PyC thermal conductivity [8].

Figure 15c and Figure 15d shows a plot of the dense pyrolytic carbon thermal conductivity for LLNL and FZJ respectively. It is essentially the inverse of the volumetric swelling, which reaches a maximum about $4 \times 10^{25} \text{ n m}^{-2}$ then decreases until the swelling saturates at about $13 \times 10^{25} \text{ n m}^{-2}$.

Pyrolytic carbon creep was modeled as a function of fluence and initial density. The CEGA correlations with a 2x creep constant multiplier and a Poisson ratio of 0.5 were used for both the dense and buffer creep rates [9]. Equation 4 provides the creep constant correlation. The creep rate of the pyrolytic carbon increases with temperature, but decreases with initial density and is from the CEGA corporation [38].

$$K = 2K_o [1 + 2.38(1.9 - \rho_o)]$$

$$K_o = 1.996 \times 10^{-29} - 4.415 \times 10^{-32}T + 3.6544 \times 10^{-35}T^2 \quad (\text{Eq. 4})$$

$$\dot{\epsilon}_1 = K[\sigma_1 - \nu_c(\sigma_2 + \sigma_3)]\phi$$

Equation 4. K is the creep constant [$\text{m}^2 \text{ n}^{-1} \text{ MPa}^{-1} \text{ s}^{-1}$], T is the temperature in $^{\circ}\text{C}$, ρ_o is the initial density [g cm^{-3}], σ is the principal stresses, ϕ is the fast neutron flux, and ν_c is the Poisson ratio in creep.

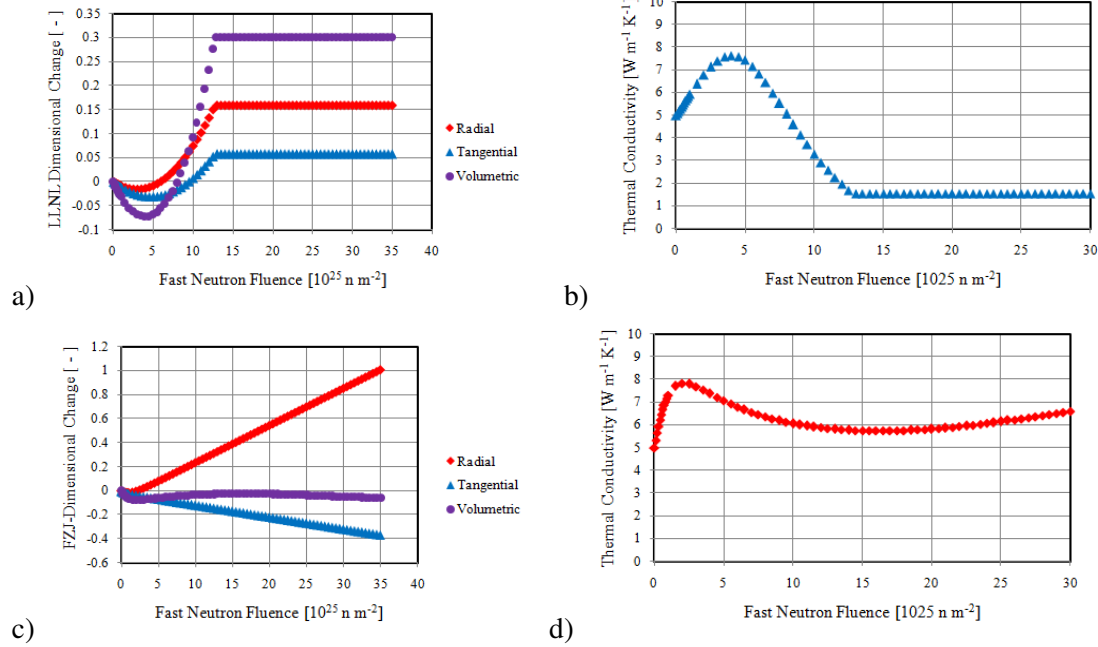


Figure 15. **a)** Plot of the irradiation dimensional change of the dense pyrolytic carbon using the LLNL correlation [30]. At 30% volumetric swelling, the pyrolytic carbon is assumed to be too brittle to continue swelling. However, under load the pyrolytic carbon may stabilize at a considerably lower swelling amount. **b)** Plot of the predicted thermal conductivity using the LLNL IIDC correlations plotted in Figure 5a. Due to the dependence on density, the thermal conductivity is the inverse of the volumetric dimensional change. **c)** Plot of the FZJ IIDC. The FZJ correlation was originally intended for a maximum fluence of $5 \times 10^{25} \text{ n m}^{-2}$ however, it extrapolates very well [9]. **d)** Plot of the PyC thermal conductivity using the FZJ IIDC correlation.

Data obtained in zirconium alloys suggests that hydrostatic stress may limit the amount of dimensional change. The recommendation of a linear dependence on hydrostatic stress was used [48]. Equation 5 provides the relationship between the hydrostatic stress and dimensional change. The swelling rate refers to the volumetric change. It was assumed that a tensile or positive hydrostatic stress would accelerate an increase in volume, but reduce a reduction in volume. The reverse of this was also assumed for a compressive hydrostatic stress. Thus the “ $\pm$ ” in Equation 5 takes the same sign as the volumetric change.

$$\dot{S} = \dot{S}_0 \left(1 \pm \left(\frac{\sigma_{\text{hydrostatic}}}{A} \right)^n \right) \quad (\text{Eq. 5})$$

Equation 5. The parameter A sets the stress value that gives a 100% change in IIDC. The IIDC multiplier is limited to a range from zero to two. $\sigma_{\text{hydrostatic}}$ is the average of the three principal stresses. When the volumetric dimensional change is increasing the term is additive, but when there is volumetric shrinkage the stress term is subtracted.

2.4 Low Density (Buffer) Pyrolytic Carbon

2.4.1 Irradiation Induced Dimensional Change and Thermal Conductivity

The buffer is a 50% dense pyrolytic carbon material intended to accommodate fuel kernel swelling and fission gas release. Figure 16a plots the irradiation swelling for the buffer material. The German swelling correlations are used for the buffer, which predicts a rapid shrinkage and then saturation at about $3 \times 10^{25} \text{ n m}^{-2}$. Due to the highly porous nature of the buffer, it is expected to shrink isotropically.

The thermal conductivity of the buffer is likewise based solely on the material swelling. The German correlations indicate that the buffer would shrink and then saturate at about -25% volumetric swelling. Figure 16b plots the resulting thermal conductivity, which indicates a rapid increase and then saturation.

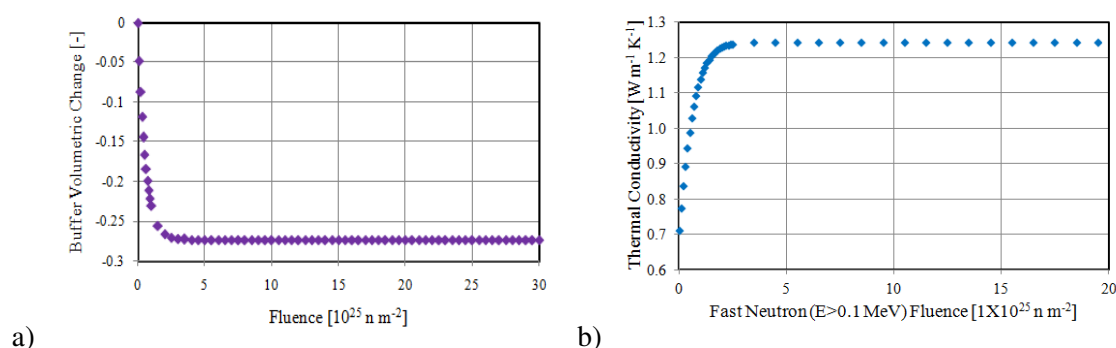


Figure 16. a) The swelling of the 50% dense pyrolytic carbon buffer, based on the German FZJ correlations [9]. The buffer is predicted to shrink isotropically. **b)** Thermal conductivity versus fluence assuming a saturation dimensional change as plotted in Figure 16a. As with dense PyC, the buffer thermal conductivity is expected to be solely dependent on density.

2.5 Chemical Vapor Deposited and Nano Infiltrated Transient Eutectic Silicon Carbide

2.5.1 Swelling and Thermal Conductivity

Prior experimental data [34,35,36] indicates that the thermal conductivity and creep of silicon carbide is dependent on the swelling of the material. Constant temperature irradiations indicate that SiC swells and rapidly saturates by about $1 \times 10^{25} \text{ n m}^{-2}$ for temperatures less than 800 °C. In this temperature range, the swelling of the material decreases as the temperature rises. This trend is important to the thermo mechanical stress evolution of FCM pellets. Increased swelling at low temperature produces compressive stresses in the pellet perimeter. Data from Price [9,37] indicates that at temperatures above 1000 °C the SiC swells continuously with fluence. This is also included in the model. Figure 17a plots the volumetric swelling for SiC at temperatures of 400 to 800 °C.

CVD-SiC is predicted to have the same trends as NITE-SiC but greater degradation with swelling. Silicon carbide irradiation creep appears to be dependent on swelling, and therefore it shows the same

trend with fluence and temperature which is a rapid increase between $0.1-1 \times 10^{25} \text{ n m}^{-2}$ and then saturation [36]. Thermal creep is not considered here since it is essentially absent at $T < 1400^\circ\text{C}$ [49]. Equation 6 shows the relationship between stress, swelling, and irradiation creep for SiC. Figure 17 shows the predicted dependence of silicon carbide creep on irradiation swelling.

$$\dot{\bar{\epsilon}} = 0.55 \times 10^{-10} [Pa^{-1}] \dot{S} \bar{\sigma} \quad (\text{Eq. 6})$$

Equation 6. This gives the relationship between creep rate, swelling, and stress for silicon carbide [50].

Figure 17b and Figure 17c plot the thermal conductivity of CVD [34] and NITE SiC [3] respectively which is dependent on swelling and temperature. Unirradiated SiC thermal conductivity decreases with temperature due to the increase in phonon-phonon (Umklapp) scattering. Thermal conductivity of irradiated SiC in the swelling saturation regime is inversely proportional to the temperature due to higher defect mobility and annealing mechanisms [51].

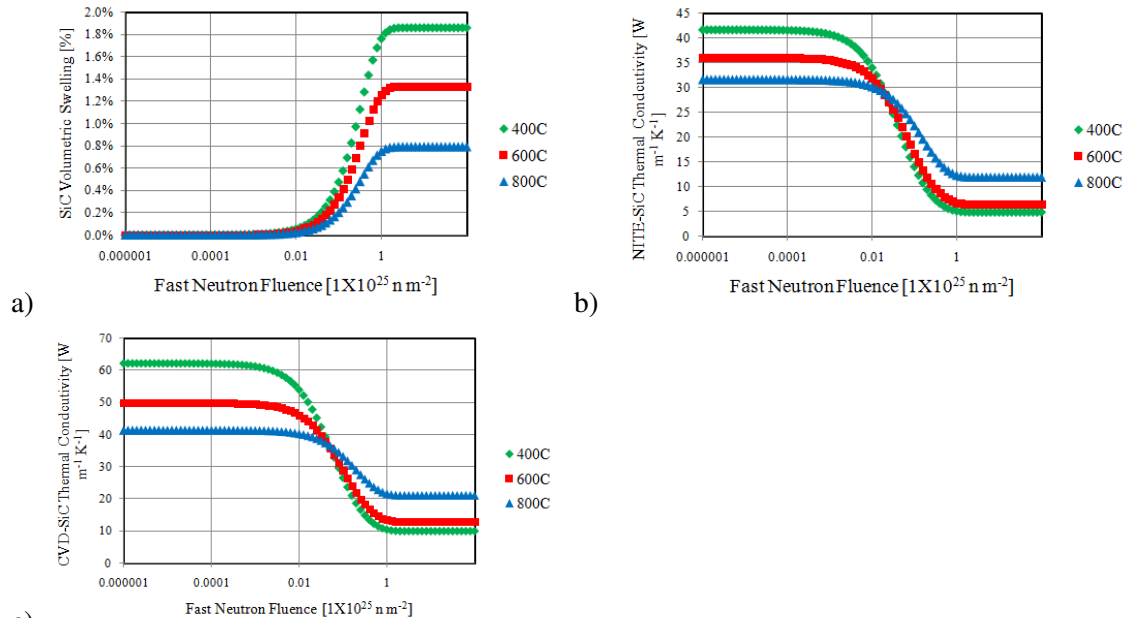


Figure 17. a) The swelling of NITE SiC as a function of fast neutron fluence [$E > 0.1 \text{ MeV}$]. The SiC swells due to the combined effects of dislocation loops and annealing. The resulting effect is greater swelling at low temperatures. This swelling gradient generates the compressive hoop stress in the perimeter of the matrix and is expected to provide an effective barrier to fission product release. b) Plot of the thermal conductivity for NITE-SiC. Thermal conductivity of SiC is a function of both volumetric swelling and temperature. c) Thermal conductivity behavior for CVD-SiC with fast neutron fluence ($E > 0.1 \text{ MeV}$).

2.6 Graphite

2.6.1 Dimensional Change

Graphite is considered for use as the “matrix” in high temperature gas reactors. Graphite is predicted to have a higher thermal conductivity at high temperatures and fluences than NITE-SiC. Graphite also creeps rapidly and is comparatively soft to the materials used in the TRISO particles. This would reduce the stresses that pellets can induce on each other. The disadvantage is that graphite is far less resistant to the diffusion of fission products than NITE-SiC.

Figure 18 shows the IIDC data and correlations used for graphite. The IIDC is based on Oak Ridge irradiations [25]. In the HTGR simulation, the perpendicular direction (C-axis which is perpendicular to the basal planes) was set to the vertical Z-axis of the pellet. The IIDC is implemented in the same fashion as the Zircaloy growth which employs cylindrical rather than the spherical coordinates which are used for the PyC IIDC within each TRISO particle. Due to lack of data, the initial shrinkage rate is independent of temperature. However, the amount of shrinkage is determined by the temperature difference from graphitization. As a result, the fluence at which the turnaround occurs is temperature dependent. The swelling is capped at 30% volumetric, following the approach from the PyC recommendation by Lawrence Livermore National Laboratory [30]. The swelling cap is an estimate for the limitation that the material is expected to encounter for additional expansion under any appreciable stress. Later in this paper, a stress limited dimensional change relationship will be introduced as an attempt to provide a more justifiable limit to the possible volume expansion of the PyC.

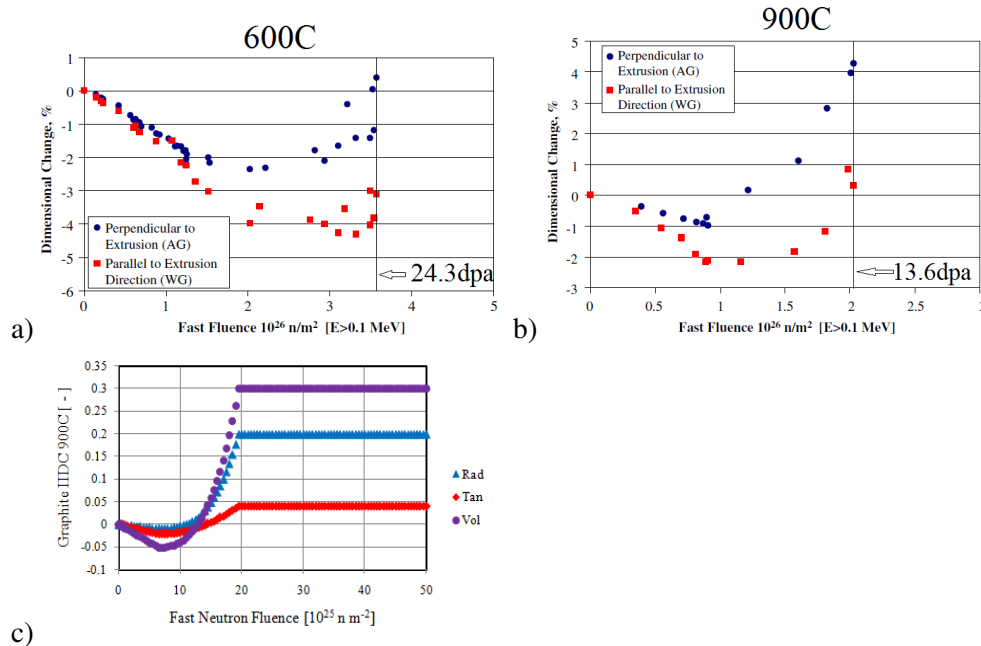


Figure 18. a) The H-451 graphite dimensional change from HFIR irradiations at 600 °C [25]. b) A plot of the H-451 graphite dimensional change from HFIR irradiations at 900 °C [25]. c) The resulting correlations from the graphite IIDC data for 900 °C.

2.6.2 Thermal Conductivity

Figure 19 shows the thermal conductivity data and resulting correlations for graphite. The thermal conductivity data is from Li, Mohokov, Bell et al., and Kelly et al.[52,53]. The behavior is a rapid decrease in the thermal conductivity followed a saturated trend with fluence and limited temperature dependence. Figure 19a and c plot the experimental data while b and d show the modeled behavior of the graphite thermal conductivity.

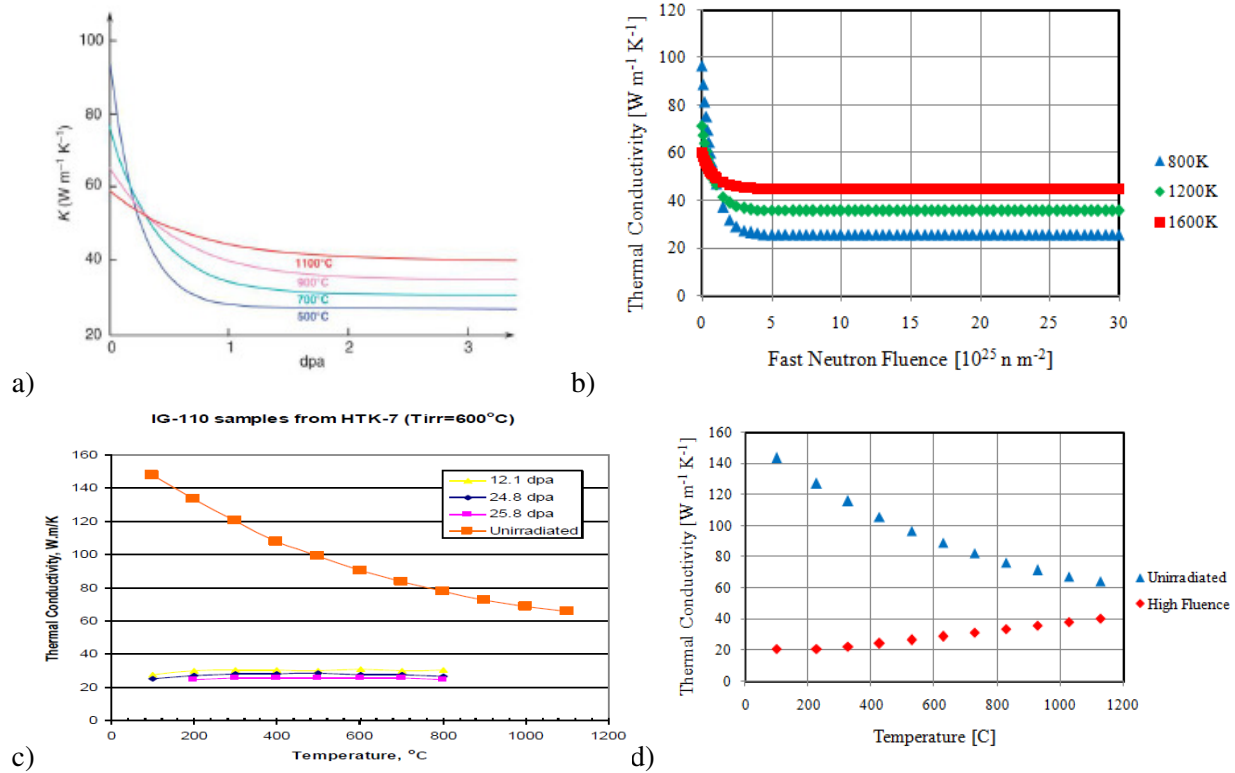


Figure 19. **a)** Curve fits to data obtained by Li and Mohokov [52]. **b)** A plot of the resulting correlations showing the fluence dependence of the thermal conductivity. **c)** Data for the thermal conductivity of graphite irradiated at 600 °C [53,54,55]. **d)** A comparison of the temperature dependence of graphite thermal conductivity when unirradiated and at 10×10^{25} n m⁻².

2.6.3 Irradiation Creep

The creep constant of graphite was assumed to have a similar trend with temperature as the PyC CECA correlation. Based on Oak Ridge data for compressive stress at 600 and 900 °C, an increased creep constant ranging from about 3.5 to 5 times higher than the PyC correlation in the model was used [56]. Figure 20 shows the data and a comparison of the graphite and PyC creep constants. Equation 7 shows the relationship for the graphite creep constant.

$$K_0 = 1.15 \times 10^{-34} T^2 [C] - 1.6227 \times 10^{-31} T [C] + 7.1898 \times 10^{-29} \quad (\text{Eq. 7a})$$

$$K = K_0 [1 + 2.38(1.9 - \rho)] \quad (\text{Eq. 7b})$$

Equation 7. K has units of [MPa n m⁻²]⁻¹, T is the temperature in °C, and ρ is the density in g cm⁻³. The correlation is based on the CECA creep equation for PyC at high temperature [38].

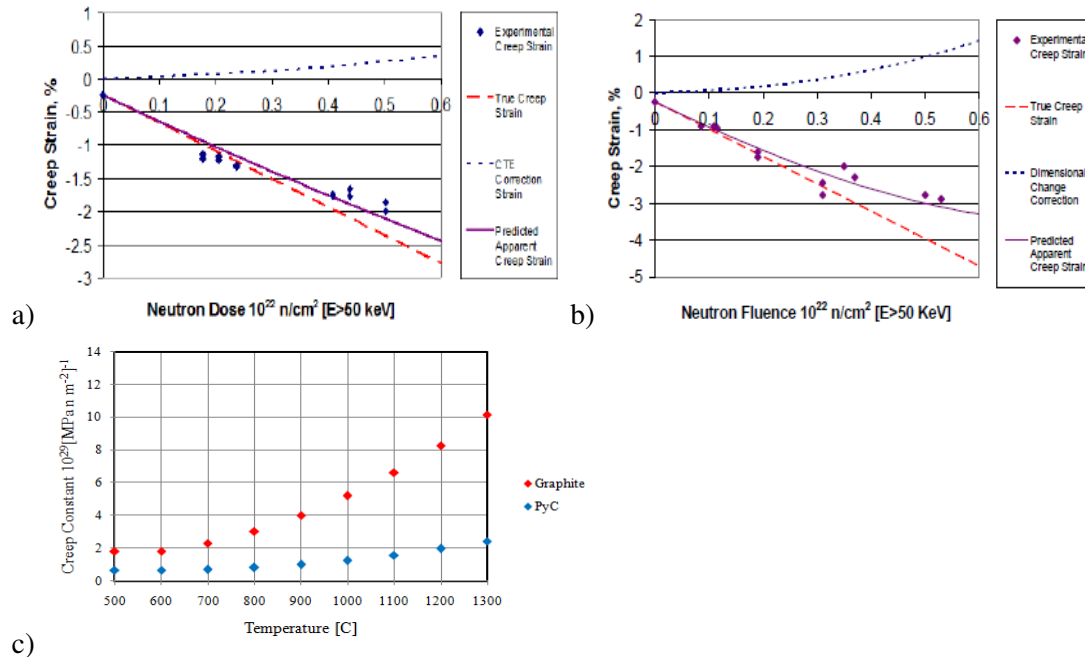


Figure 20. a) Data for graphite creep at 600 °C and -20.7MPa compressive stress [56]. b) Graphite creep data at 900°C and -20.7 MPa compressive stress [56]. c) A comparison of the graphite and PyC creep constants with temperature. Both correlations are assumed to be constant below 600 °C.

2.7 Zircaloy Cladding

A constant of $16 \text{ W m}^{-1} \text{ K}^{-1}$ was used for the thermal conductivity of Zr-4. The ESCORE fuel performance model and FRAPCON were used for the irradiation growth and irradiation creep respectively [13,57,58].

2.8 Summary

Material correlations have been selected for the necessary materials to simulate FCM fuel. There is a large amount of confidence in the SiC properties below 1000 °C. Above 1000 °C there is some question about the SiC swelling and its temperature dependence. However, the CVD and NITE silicon carbides are expected to perform well for the FCM applications.

The thermal conductivity and creep rate of the pyrocarbon materials is reasonably well understood. However, the dimensional change is highly uncertain and requires further experiments to verify its behavior.

There is substantial uncertainty in the properties of the uranium nitride, but unless this material has far greater fission gas release fractions than UO_2 it is not expected to be a limiting factor in FCM fuel performance.

CHAPTER 3: SINGLE PARTICLE SIMULATIONS

3.1 Two Dimensional Single Particle Comparison

To gain confidence in the model setup and predictive capability, a single particle comparison to other fuel performance codes was conducted. The benchmark trends were taken from IAEA Tecdoc1674 Figure 9-19 and displayed in this document as Figure 22 [11]. The geometry used in these simulations is provided in Table 4. The outer temperature was set to 1516 K, particle power was 0.263 W, the simulated duration was 351 effective full power days, 14.6 at% burnup and 7.2×10^{25} n m⁻² fast neutron fluence was reached. Figure 21 shows the 2D mesh that was used for the BISON simulation.

Conventionally, RZ coordinates refers to an infinite cylinder that is fully constrained axially. However, in MOOSE/BISON RZ meshes are revolved about the Z-axis. This allows cylindrical and spherical geometries to be simulated with a variety of axial boundary conditions. The buffer/IPyC interface was modeled as an initial gap of 5 μ m. This does increase the temperature of the kernel by about 20 °C and thereby increase the gas pressure somewhat. The other interfaces were constrained to remain in contact at all conditions, and a 0.1 MPa pressure boundary condition was applied to the outer OPyC surface.

The figures from Tecdoc 1674 show that there is a considerable uncertainty among the various TRISO fuel performance codes. Initially, the swelling of the SiC and shrinking PyC places the SiC layer in compression. Once the SiC swelling saturates and the PyC shrinkage rate lessens, the PyC creep relaxes the stress induced in the SiC layer. By about 5 at% burnup, the fission gas pressure is the dominating cause of the stress. The maximum predicted creep strain magnitude ranged between 19-22% in the OPyC and IPyC layers.

The comparison of the BISON and PARFUME results show good agreement. The BISON fission gas pressures are somewhat lower but follow the same trend as predicted by PARFUME. BISON predicts that the SiC hoop stress would reach a more compressive minimum and relax somewhat faster but the tensile stresses resulting from fission gas pressure are nearly identical. This gives confidence in the predictive capability of the BISON model.

Table 4. A list of the thicknesses and outer radii of the TRISO particle layers used in the IAEA TRISO Case 11 comparison.

Material	Outer Radius[μ m]	Thickness[μ m]
OPyC	248.5	40
CVD-SiC	342.5	36
IPyC	383.5	41
Buffer	419.5	94
Kernel	459.5	248.5

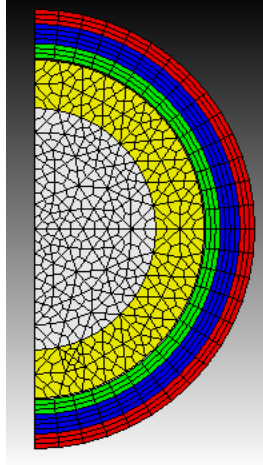


Figure 21. A representation of the mesh used on the 2D-RZ single particle comparison to PARFUME. This is a 2D-RZ mesh which is revolved about the centerline (left edge) to produce a spherical particle rather than an infinite cylinder [59].

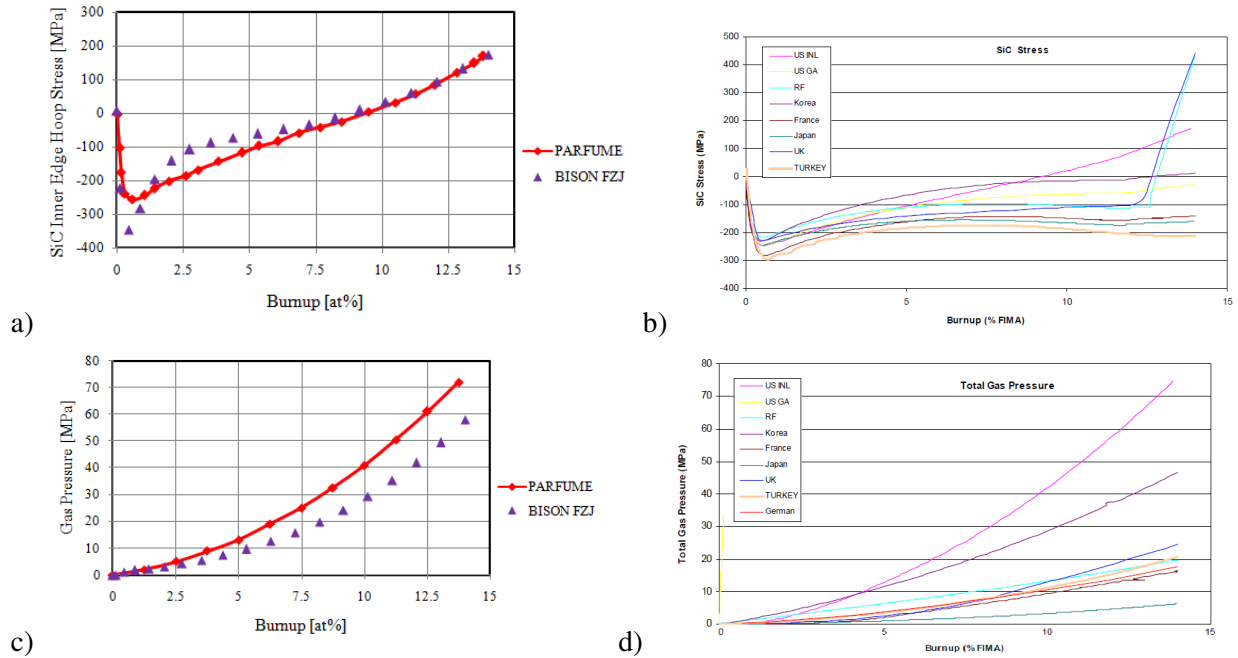


Figure 22. **a)** A comparison of the BISON and PARFUME calculations for the SiC inner edge hoop stress. **b)** The calculated hoop stress from several TRISO fuel performance code [11]. **c)** A comparison of the BISON and PARFUME calculation for the fission gas pressure applied to the Buffer/IPyC interface. **d)** The calculated gas pressures of the various codes, as reproduced from IAEA Tecdoc 1674 [11].

A mesh sensitivity study was conducted of the IPyC, SiC, and OPyC layers. However, the geometry, material properties, and simulation conditions remained the same. The mesh in the outer layers was set to 5, 10, 20, and 40 μm , and Figure 23 plots the results. All mesh sizes gave reasonable results for both gas pressure and hoop stress. The maximum difference in gas pressure due to mesh size was 0.3 MPa and the differences were not plotted. However, on closer inspection of the hoop stresses it can be seen that the

precision of the results improve considerably by reducing the mesh spacing from the 40 to 10 μm . In Figure 23b, the results are compared to the 5 μm mesh, which was considered to be the most accurate of the simulations. The fact that the results converge as the mesh size decreases gives confidence in the numerical methods used by the BISON code.

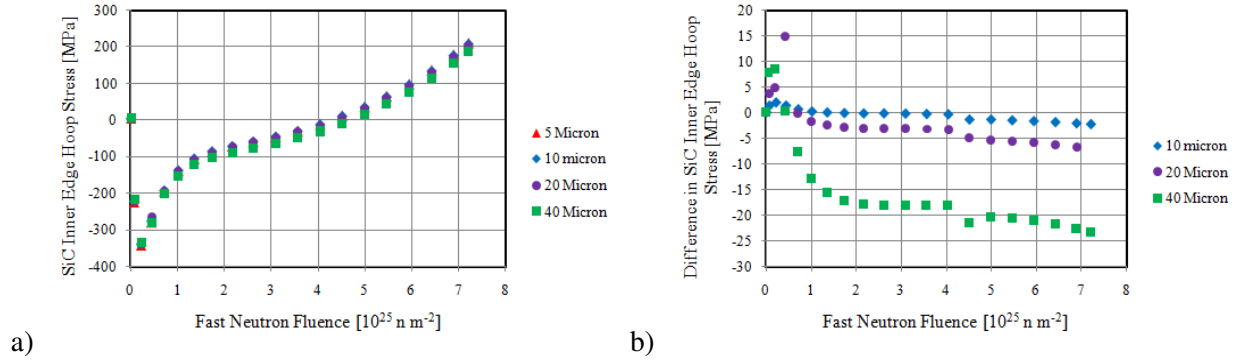


Figure 23. Mesh sensitivity for the IAEA Case 11 comparison. The mesh size was varied from 5 to 40 μm . **a)** The hoop stress at the inner edge of the SiC layer. **b)** The difference in hoop stress compared to the 5 μm mesh simulation.

The primary terms affecting the stress in the silicon carbide layer are the PyC dimensional change, irradiation creep, and fission gas pressure. The next set of simulations isolates each of these effects. Displayed is the effect of only the PyC IIDC, then PyC IIDC with creep, and then the previously seen IIDC with creep and fission gas pressure. Figure 24 shows the results. The initial PyC shrinkage places the SiC layer in compression. Once the shrinkage slows, creep relaxes the stress. Then the gas pressure begins to build in and produce tensile stresses.

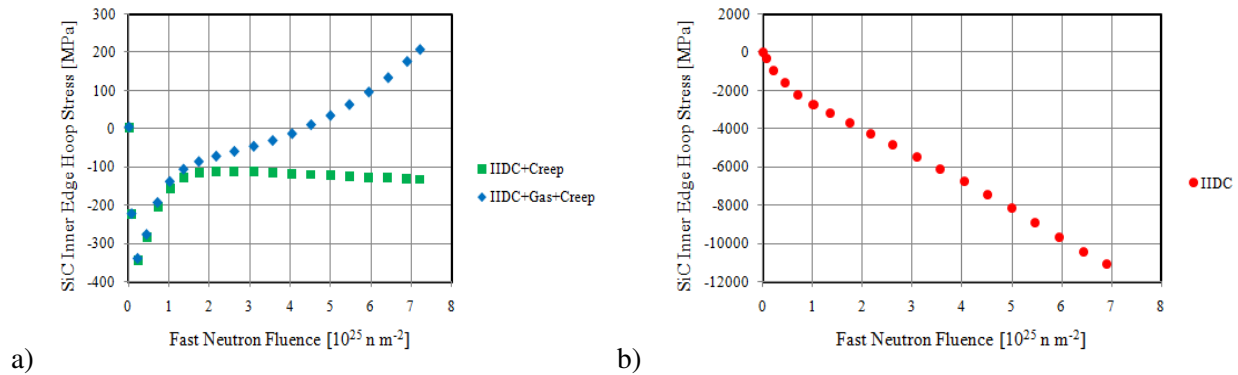


Figure 24. The effects of dimensional change, creep, and gas pressure for the Case11 comparison. **a)** Comparing the hoop stress in the SiC layer for a full physics simulation with a simulation that has the gas pressure disabled. **b)** The hoop stress in the SiC layer when the creep and gas pressure are disabled.

Additional simulations were performed to examine the potential effects of stress limited dimensional change. Two sets of simulations were performed using the FZJ and LLNL dimensional change correlations. The FZJ correlation initially predicts OPyC shrinkage. This movement is resisted by the stress limiting term in the dimensional change correlation. However, at a fluence of about $2 \times 10^{25} \text{ n m}^{-2}$ the volume behavior of the PyC begins to recover some of its volume. This change in direction causes the

hydrostatic stress limiting term to accelerate the radial expansion and tangential shrinkage due to the OPyC being in hydrostatic tension. This results in additional compressive stresses in the SiC layer despite the OPyC regaining some of its volume. Once the volume recovery slows, creep relaxes the stress and the fission gas pressure begins to induce tensile stresses in the SiC layer.

In the case of the LLNL simulation, a volume direction change from shrinkage to expansion is predicted at a fluence of about $4.5 \times 10^{25} \text{ n m}^{-2}$. However, the radial and tangential expansion generates compressive and tensile stresses in the SiC layer respectively. When the volume change of LLNL I IDC correlation is accelerated by the hydrostatic stress term, these effects maintain their proportions and a continuous SiC hoop stress trend is predicted when using the LLNL I IDC correlation. Figure 25 plots the results.

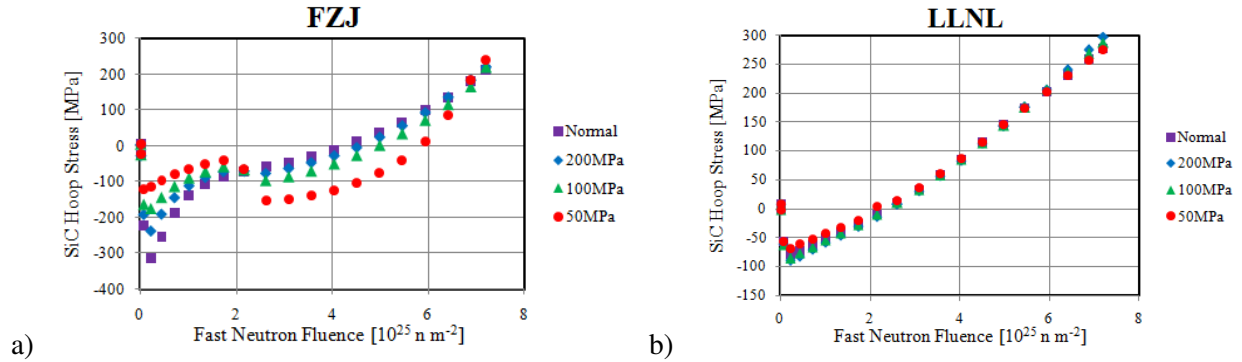


Figure 25. The effects of stress limited dimensional change for the IAEA TRISO Case11 comparison. The stress threshold for preventing further expansion was varied from infinite to 50 MPa. **a)** The variation in the SiC hoop stress with changes to the hydrostatic stress threshold when using the FZJ pyrolytic carbon correlation. **b)** The variation in the SiC hoop stress with changes to the hydrostatic stress threshold when using the LLNL correlation.

3.2 Two Dimensional RZ Five TRISO Particles in a FCM Matrix

Previous simulations have focused on the behavior of a single isolated particle. The next simulations are of five TRISO particles placed in a SiC matrix. This simulation uses the mesh shown in Figure 26, and the purpose was to investigate inter particle effects. The particles were placed along the Z-axis centerline which when revolved produces spherical geometry for the particle. Likewise, the NITE-SiC matrix when revolved produces a cylinder that is constrained on the bottom edge but free to move upward in the Z-axis. The particle spacing is 200, 100, 50, and 25 μm from top to bottom in the Z-direction. This setup shows the effect of particle spacing on the matrix. The particles are 900 μm in diameter with the OPyC, SiC, and IPyC being 30, 40, and 30 μm thick respectively. This is different from the geometry used in the Case 11 benchmark discussed previously but still useful for investigating the potential effects of embedded particles on the NITE-SiC matrix.

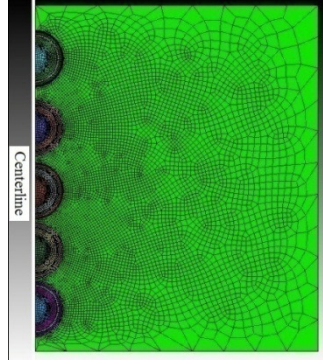


Figure 26. This is the mesh used for the five particles embedded in a matrix. Particles are spaced at 200, 100, 50, and 25 μm increments top to bottom in the Z-direction.

The outer matrix edge was set to a temperature of 1000 K. However, due to the presence of only five particles there is not a substantial temperature gradient across the matrix. Due to the lack of temperature gradient in the matrix, the effects of matrix swelling cannot be investigated with this simulation. The LLNL correlation is used in this simulation for the PyC in the TRISO particles. This correlation assumes that the PyC will encounter a volumetric turnaround from shrinkage to swelling at high fluence in a similar fashion as graphite [60]. This assumption has not been confirmed by experimental data [9,30]. However, it is a conservative assumption that can have significant potential effects.

Figure 27b plots the matrix hoop stress for the maximum stress concentration generated by the bottom particle, which follows the PyC volumetric dimensional change trend. This strongly indicates that the OPyC is the dominate source of these large stresses. In this simulation, all interfaces are constrained to remain in contact. The result is that the initial PyC shrinkage generates a compressive stress on the matrix, and the subsequent PyC swelling causes large tensile stresses in the matrix. It should be noted, that these particle effects have a maximum range in the matrix of about 300–400 μm , and the stress in the CVD-SiC layer is the opposite of the matrix. The existence of these large stresses suggests at least the possibility of debonding at fluences around $5 \times 10^{25} \text{ n m}^{-2}$.

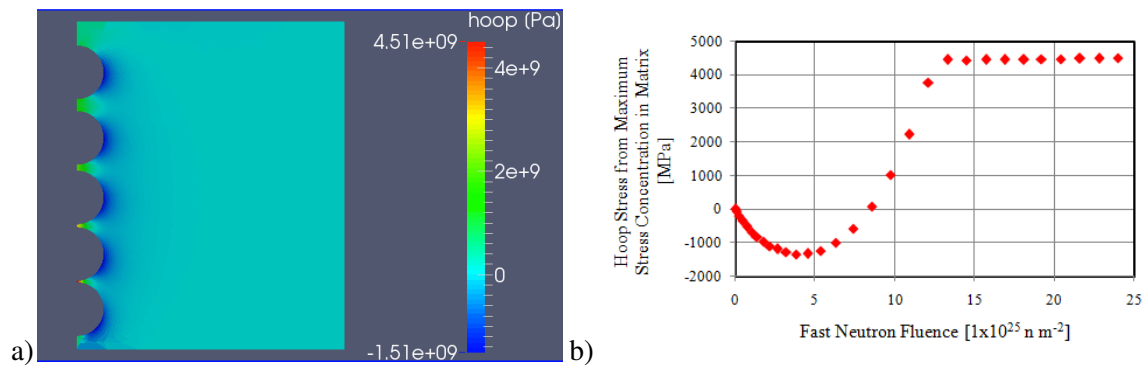


Figure 27. a) Image of the matrix hoop stress profile at $24 \times 10^{25} \text{ n m}^{-2}$. As expected, the largest stress occurs at the closest particle spacing. **b)** The hoop stress as a function of fluence from the smallest particle spacing of 25 μm which is a probable event in a prototypic FCM pellet.

3.3 Shell Simulations

The previous simulations predicted very large stresses induced on the matrix by the OPyC layer. The next simulations are aimed at identifying the property behaviors that cause these predictions. Three spherical regions were meshed to illustrate the effects of Poisson ratio in creep and free volume. These layers are each 50 μm thick with an outer diameter of 1 mm. In these simulations, the LLNL pyrolytic carbon dimensional change correlations were used. The “IPyC” simulation condition consisted of an inner PyC shell with the outer two layers being SiC. The “OPyC” condition was where the middle layer is PyC, while the outer and inner shells were SiC. In the first simulation, the “IPyC” condition is simulated with constant volume creep and displayed as the red line in Figure 28b. There are some stresses induced in the SiC by the PyC. However, the free volume within the shells accommodates the IPyC expansion and avoids excessive stress levels. In the next two simulations, the “OPyC” condition is simulated with a Poisson ratio of 0.5 and 0.4 as the green and blue lines respectively. The resulting stress from the constant volume green line in Figure 28b has the same trend as the volumetric behavior predicted by the IIDC correlation. This is due to the lack of free volume available to the OPyC and the inability to reduce volume without elastic strain. The blue line in Figure 28b with a Poisson ratio in creep of 0.4 has the ability to reduce volume in creep. As a result, the stress is relaxed after the IIDC saturates. Figure 28c plots the predicted effect of creep rate for the “OPyC” condition with a Poisson ratio in creep of 0.4. As expected, larger creep rates reduce the maximum stress and recovery time after PyC saturation.

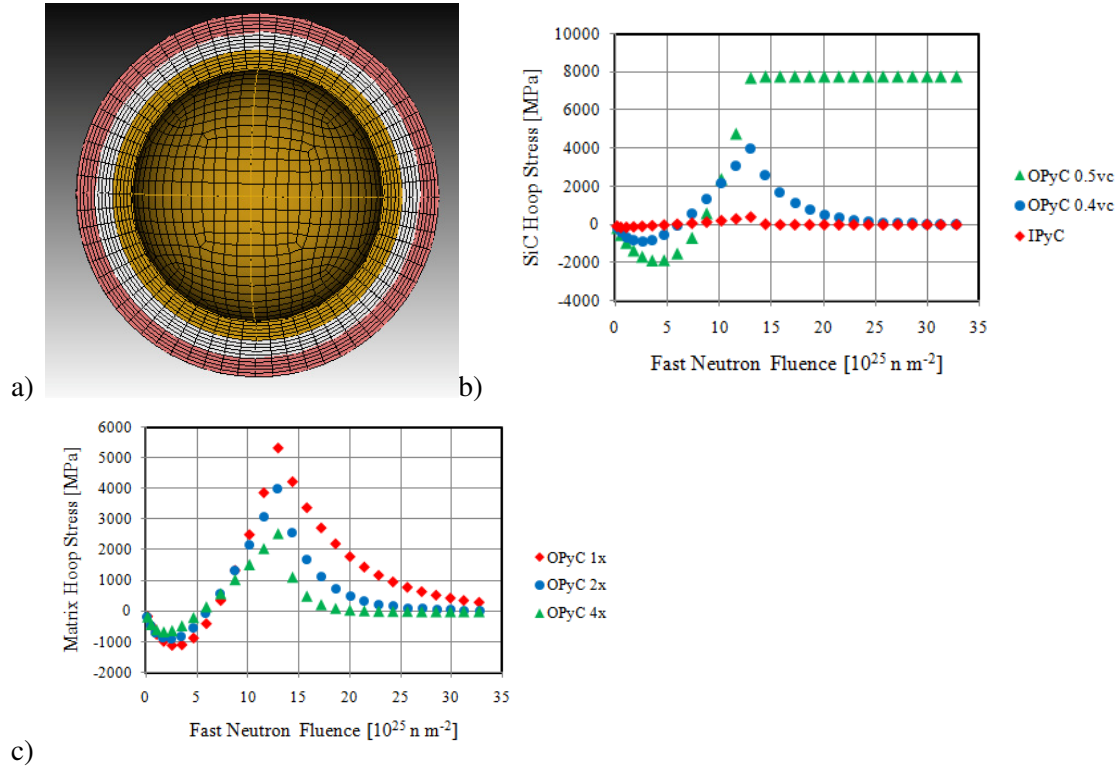


Figure 28. a) The mesh used in the shell simulations. b) A plot showing the importance of the Poisson ratio in creep if the PyC is fully constrained and the lack of importance if the PyC is free or only partially constrained. c) A plot showing the effect of creep rate for 1x, 2x, and 4x multipliers of the recommended CECA creep constant [9].

3.4 Interface Debonding and Through Wall Fracture

3.4.1 Crack Propagation Methods

Due to the different irradiation behaviors of pyrolytic carbon and silicon carbide, it is possible for a TRISO particle to experience interface debonding and through wall fracture. The following section discusses the numerical methods used to predict these occurrences. At the beginning of the simulation, each element is assigned a random failure probability between approximately zero and less than one. If that value is exceeded, then the element is considered to be cracked. These assigned probabilities were given a normal distribution with a mean of 0.5 and standard deviation of 0.2. This assigned failure probability could be referred to as “failure probability at fracture” to distinguish it from the Weibull failure probability which is a function of stress, element volume and material properties. In the event that an element cracks, the time step is greatly reduced. This decouples crack propagation from other effects such as creep and swelling. Once the propagation is complete, normal simulation time steps resume, and the cracking process is entirely explicit. To approximate the behavior of a crack, a cracked element has a reduced modulus and thermal conductivity. Also, to prevent heat from disappearing from the simulation the specific heat is set to zero. This effectively sets the time derivative to zero.

To prevent the cracks from resembling stress concentrations, it was necessary to limit the number of elements that are allowed to crack each time step. Selecting elements that have the highest stresses and exceed their failure probability at fracture has worked well. Using the exponential term from Equation 8 with a Weibull modulus of about 20 provides a wide spread in the resulting values which creates a reliable selection process even at high stresses. The result is that a large crack modulus of 1-10 GPa instead of a much lower 1 kPa can be used and still obtain a satisfactory crack propagation pattern. This allows larger and more unstable systems to be simulated.

Equation 8 was derived from Weibull statistics and was used to calculate the failure probability per element. The integral has been dropped since the volume averaged stress is reported in each element.

$$F_p = 1 - \exp\left[\frac{-V_e}{V_c \sigma_c^m} (\sigma_r^m + 2\sigma_h^m)\right] \quad (\text{Eq. 8a})$$

$$F_{cumulative} = 1 - \exp\left(\frac{1}{V_c} \int_V \left(\frac{\sigma_r}{\sigma_c}\right)^m + 2\left(\frac{\sigma_h}{\sigma_c}\right)^m dV\right) \quad (\text{Eq. 8b})$$

Equation 8. F_p is the failure probability per element, $F_{cumulative}$ is the cumulative failure probability over the layer, σ_c and V_c are the characteristic stress and volume obtained experimentally, V_e is the mesh element volume used in simulation, σ_h is the hoop stress, σ_r is the radial stress, σ_a is the axial stress, and m is the scale parameter.

Crack closure is determined by comparing the element's density to what it an intact element's density ought to be considering initial density, volumetric swelling, and thermal expansion. If the crack closes, element's modulus and thermal conductivity are restored to allow for the transfer of stresses across the crack. Contact thermal conductivity was not implemented in this model. To allow crack re-opening, the failure probability at fracture is reduced to approximately zero. This allows “closed” cracks to re-open

without having to fail the material again. Inevitably, this introduces the possibility for elements to infinitely cycle between open and closed configurations. As a result, elements that oscillate in such fashion are considered permanently cracked open.

3.4.2 Debonding

Interface fracture can occur from shear and normal forces. Normal stress dominates the debonding mechanism, but both are considered in the model. Debonding is modeled similarly to brittle fracture with a few modifications. Equation 9 shows the modifications to the failure probability equation, which allows different characteristic shear and normal stresses.

$$F_p = 1 - EXP \left\{ \frac{-V_e}{V_c} \left[\left(\frac{\sigma_r}{\sigma_c^{normal}} \right)^m + 2 \left(\frac{\sigma_h}{\sigma_c^{shear}} \right)^m \right] \right\} \quad (\text{Eq. 9})$$

Equation 9. As before, F_p is the failure probability per element, σ_c and V_c are the characteristic stress and volume obtained experimentally, V_e is the mesh element volume used in simulation, σ_h is the hoop stress, σ_r is the radial stress, and m is the scale parameter.

If the failure probability exceeds the assigned failure probability at fracture then the element is considered fractured. However, a tensile radial stress is required to predict an open gap since an interface gap cannot occur when it is compressed in the radial direction. The gap width is calculated by the change in element volume from the initial value at simulation start. Volumetric changes from swelling and thermal expansion are accounted for in the calculation. Table 5 lists the material properties used for pyrolytic carbon and silicon carbide interface debonding.

Table 5. A list of the parameters used for the fracture of the silicon carbide and high density PyC fracture and PyC debonding [61,3,62].

Parameter	Value
SiC Characteristic Volume [m ³]	1.57x10 ⁻⁹
SiC Characteristic Stress [MPa]	426
SiC Scale Parameter [-]	8.0
PyC Characteristic Through Wall Fracture Volume [m ³]	1.0x10 ⁻¹⁸
PyC Characteristic Debonding Volume [m ³]	2.25x10 ⁻¹²
PyC Characteristic Shear Stress [MPa]	240
PyC Characteristic Normal Stress [MPa]	100
PyC Characteristic Through Wall Fracture [MPa]	1316
PyC Scale parameter [-]	9.5

3.4.3 Crack Thermal Conductivity

Crack thermal conductivity is essentially an order of magnitude estimate. Due to underlying assumption of heat conduction in a solid material, the cracked elements are considered gas filled. Equation 10 is derived from 1D Cartesian heat resistance and provides an element average thermal conductivity. Equation 10 makes the conservative assumption that all the heat must pass through the crack. The modeled gases released to the buffer are Nitrogen, Krypton and Xenon. The initial gas was modeled as a small quantity (10⁻¹⁵ mol) of Argon. The thermal conductivity of these gases was determined using

MATPRO equations in BISON material files The crack volume is estimated during the simulation using density, swelling, and thermal expansion to estimate the increase in volume that resulted from stress. This assumes that volume is conserved in creep or that creep with low Poisson ratio in creep is negligible.

$$\bar{k} = \left(\frac{1 + crackVolum\ e}{\frac{1}{k_{PyC}} + \frac{crackVolum\ e}{k_{crack}}} \right) \quad (\text{Eq. 10})$$

Equation 10. The element average thermal conductivity. The k_{crack} is the gas conductivity.

A set of simulations was conducted to estimate the accuracy of the predicted gap width. The geometry consists of an IPyC, debondable interface layer, and buffer regions. The outer IPyC surface was constrained to remain stationary. The Poisson ratio in creep was 0.5 or constant volume for all layers. In the first simulation, dimensional change and thermal expansion was disabled for the debondable layer while the buffer shrinks by about 30% volumetric. This allows a direct comparison of the calculated displacements and the gap width predictor. The second simulation enables the dimensional change and thermal expansion in the debondable layer, and the third simulation is to compare the results for very large gaps and show the limitations of the predictor. Figure 29 and Figure 30 plot the results. The results show that the gap width predictor under predicts the calculated displacement. However, the predictor follows the same trend as the calculated displacements and shows good agreement for gap widths up to about 150% radial strain. This is deemed acceptable for FCM fuel performance modeling. Additionally, the width of the debondable layer can be increased to give greater accuracy if necessary. In these simulations, the predictor is about 12% low compared to the calculated displacements. However, this discrepancy is not necessarily constant during gap closure and partial contact.

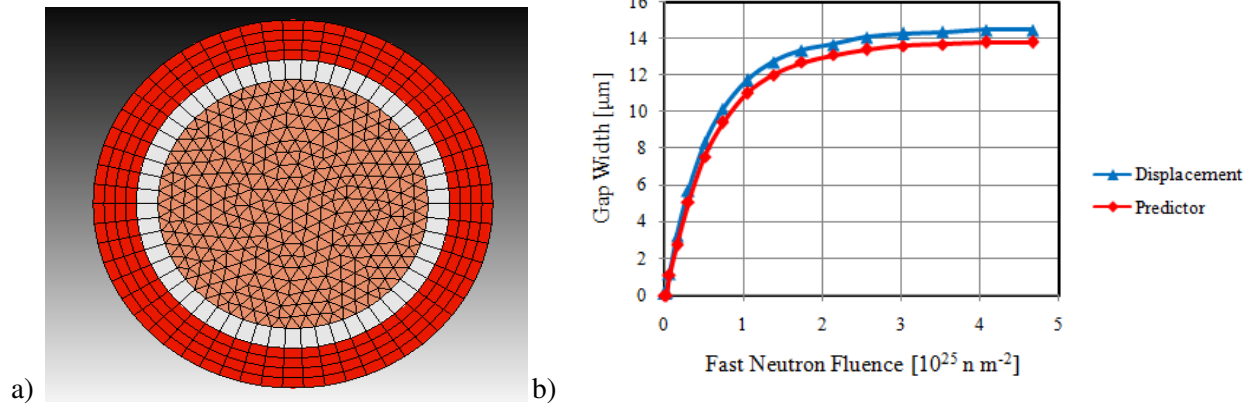


Figure 29. A comparison of the gap width predictor with the actual gap size. **a)** Representation of the mesh used to estimate the effectiveness of the gap width predictor. **b)** The gap width when the debondable layer has IIDC and thermal expansion disabled as compared to the actual gap width.

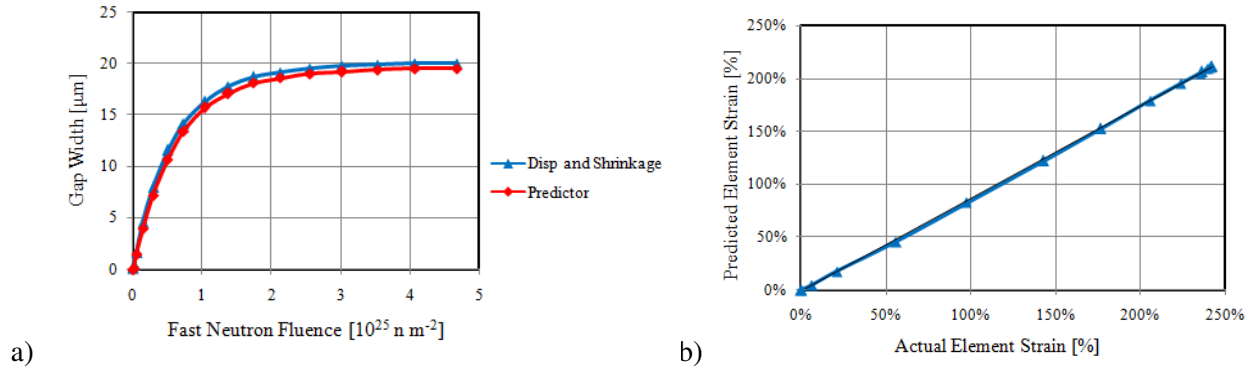


Figure 30. a) The predicted and expected gap widths when dimensional change is enabled in the debondable layer. **b)** A comparison of the predicted to actual element strain. The predictor is about 12% low.

3.5 Single TRISO Particle with NITE-SiC Shell

A simulation of a single particle surrounded by a 500 μm thick SiC shell was developed to examine the potential effects of interface debonding and layer interactions. The modulus of elements considered cracked at the Buffer/IPyC interface was set to 1 kPa, while a modulus of 1 GPa was used for the IPyC/SiC and OPyC/matrix interfaces. The 1 kPa buffer/IPyC modulus was necessary to prevent an increase in the probability of the IPyC debonding from the SiC layer. The thermal conductivity reduction at the buffer/IPyC interface includes the fission gas contributions. This typically results in an order of magnitude lower conductivity than the IPyC/SiC and OPyC/matrix gaps, which are approximated as residual Argon gas from the manufacturing process. Figure 31a shows the mesh used in the simulation. Figure 31b compares the maximum hoop stress in the NITE-SiC shell when the PyC IIDC is modeled with the LLNL and FZJ correlations. Figure 31c and d plot the buffer/IPyC gap width and the maximum kernel temperature for different dimensional change behaviors.

Due to the volume expansion of the OPyC, the LLNL correlation predicts large stresses in the matrix peaking at about $13 \times 10^{25} \text{ n m}^{-2}$. Once 30% increase in volume is reached, the swelling is arbitrarily capped and the 0.4 Poisson ratio in creep relaxes the stresses. The FZJ correlation predicts radial expansion and tangential shrinkage at nearly constant volume. This behavior results in partial contact beginning at about $13 \times 10^{25} \text{ n m}^{-2}$ and continuing to the end of the simulation. The buffer/IPyC gap widths are a combination of the volume behavior of the IPyC, buffer and kernel. In these simulations, the particle temperature is driven by the gap width behavior since it is the primary change in thermal resistance. It should also be noted that due to the symmetry of the simulation, the maximum temperature is found at the kernel center point. This is vastly different from a FCM pellet.

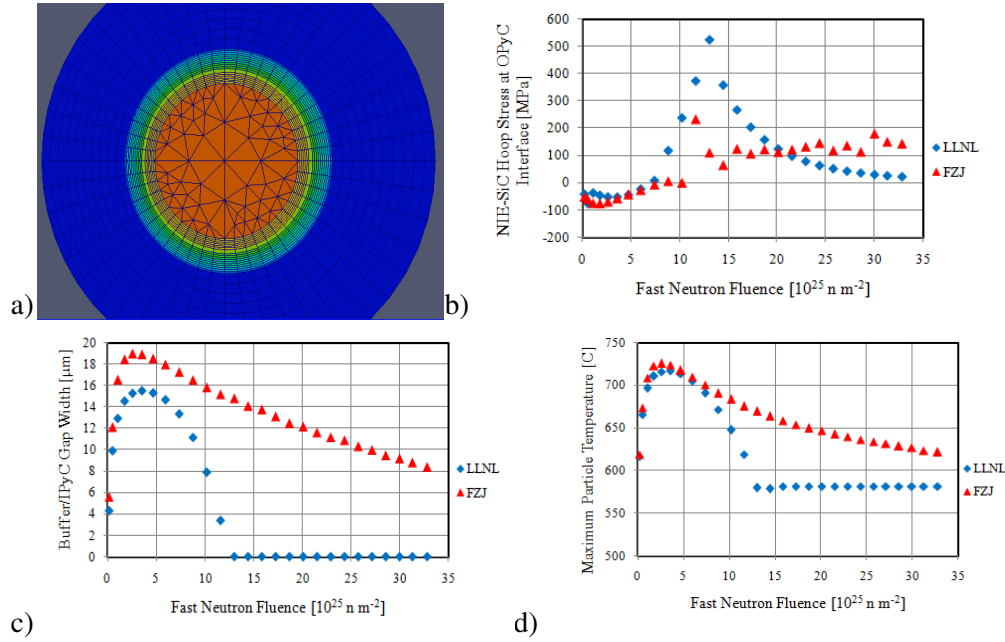


Figure 31. a) The mesh used in the single TRISO particle surrounded by a 500 μm thick NITE-SiC shell. b) A plot of the hoop stress at the OPyC/NITE-SiC interface. c) A plot of the buffer/IPyC interface gap. The gap forms due to the rapid and large buffer shrinkage, and then closes due to the kernel and IPyC expansion. d) A plot of the maximum particle temperature.

To date, the model has used the assumption of constant elastic properties. However, it has been observed that the elastic modulus of graphite increases as the material shrinks, and it has also been inferred that it should deteriorate after the turnaround is reached and volumetric swelling begins [25]. A set of simulations were performed to investigate the potential effect in single TRISO particles should the elastic modulus decrease with volumetric swelling. The elastic modulus was set to deteriorate to 0.1 GPa at volumetric swelling levels ranging from 5% to 50%. Also, debonding at the OPyC/matrix interface was disabled for these simulations to provide a readable plot of the hoop stresses. Figure 32a and b plot the results for the variable elastic modulus. The larger sensitivity of the PyC modulus to swelling produces a greater stresses during the initial shrinkage, but a faster reduction after the turnaround. The minimum modulus was set to 0.1 GPa and was found to be sufficiently small to negate the effects of 30% volumetric swelling. The prediction of nearly identical stresses during the initial shrinkage, despite a factor of two differences in elastic modulus, was unexpected since the creep magnitude in these simulations was within 1% of each other. When the same simulations were rerun without creep, the resulting stresses were about a factor of two different, which indicates that the ability of the creep to reduce stress is proportional to the modulus. This relationship between creep stress relaxation and modulus maintains its proportionality until the modulus is reduced below about 1 GPa.

The potential effect of hydrostatic stress limiting the dimensional change was considered and included in a separate set of simulations. Figure 32c plots the results of using a linear dependence and varying the 100% stress level from 100 to 25 MPa. The 100% level refers to the amount of hydrostatic stress required to prevent further PyC dimensional change. The small spike in the 100 MPa trend occurred when the buffer made contact with the IPyC. Both the variable modulus and stress limited dimensional change have the potential to produce major effects on the SiC stress level and thereby the FCM fuel performance.

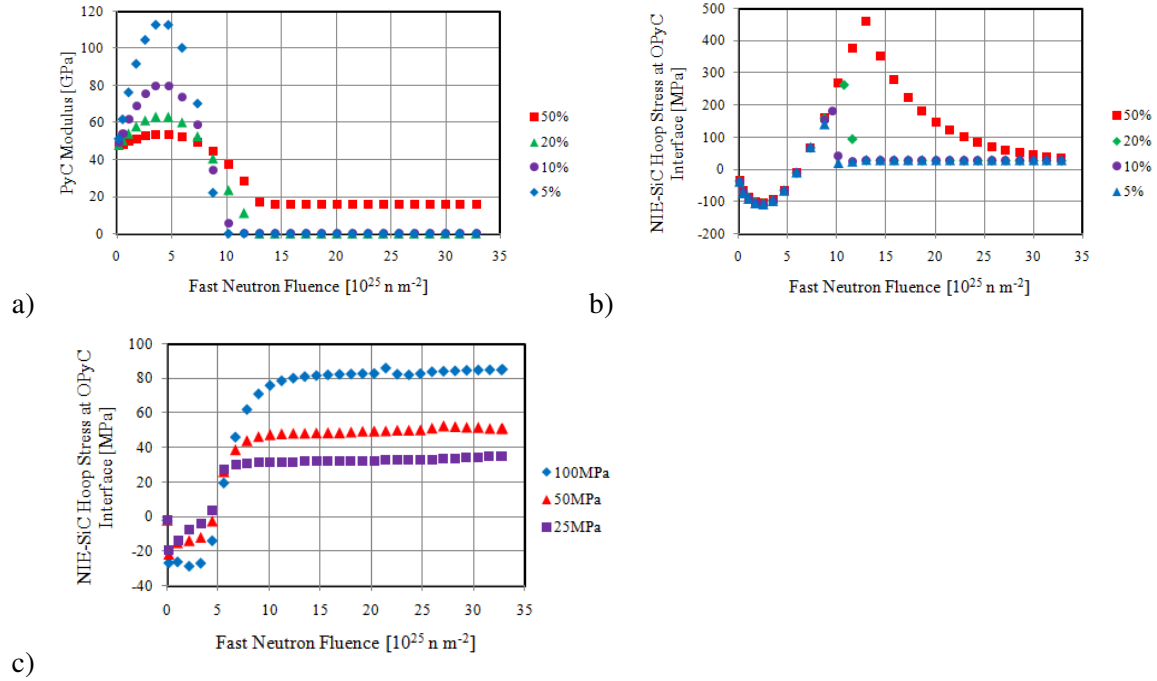


Figure 32. Plots illustrating the potential effects of variable elastic modulus and stress limited dimensional change in a single TRISO particle. **a)** The predicted elastic modulus for different sensitivities to volumetric swelling. **b)** The hoop stresses at the NITE-SiC/OPyC interface as a function of fluence and PyC swelling. **c)** The hoop stresses resulting from stress limited dimensional change.

The effects of stress limited dimensional change on the debonding and gap widths of a single particle were considered. Two sets of simulations were performed with FZJ and LLNL dimensional change correlations respectively. Figure 33 and Figure 34 plot the results. The model predicts that the width of the interface gaps will reduce as the stress threshold becomes smaller, but the point of re-contact is mostly unchanged. It should be noted that even a threshold of 50 MPa was unable to prevent debonding.

It is important to note that the stress independent FZJ correlation predicts a change from shrinkage to swelling at $2 \times 10^{25} \text{ n m}^{-2}$ and the reverse at $14 \times 10^{25} \text{ n m}^{-2}$. This behavior will influence the gap widths when stress limited dimensional change is included. Due to the initial shrinkage, the IPyC is in hydrostatic tension and recovering volume for fluences of about $2\text{--}7 \times 10^{25} \text{ n m}^{-2}$. This causes an accelerated volume expansion and the second volume direction change occurs more quickly. Once the IPyC is predicted to begin shrinking for a second time, the hydrostatic stress limiting term resists this movement and the creep pulls the IPyC closer to the SiC layer thereby reducing the gap width.

In the case of the OPyC, the accelerated volume recovery can force the OPyC/matrix interface into re-contact. When the PyC is modeled as largely insensitive to hydrostatic stress the OPyC/matrix interface is predicted to re-open at high fluence due to the volume shrinkage of the PyC. However, at stress sensitivities the hydrostatic stress is expected to resist this movement and prevent a re-opening of the OPyC/matrix gap.

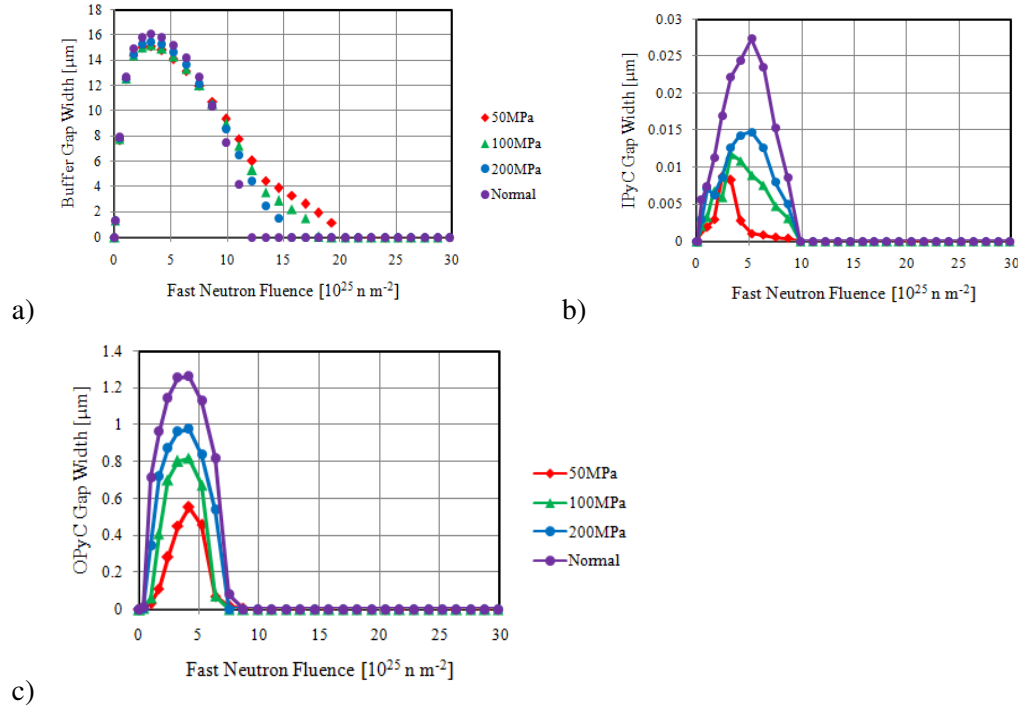


Figure 33. Plots showing the effects of stress limited dimensional change on interface gap widths using the LLNL dimensional change correlation. **a)** Buffer/IPyC interface gap widths for various stress thresholds. **b)** IPyC/SiC interface gap width. **c)** OPyC/Matrix gap width interface.

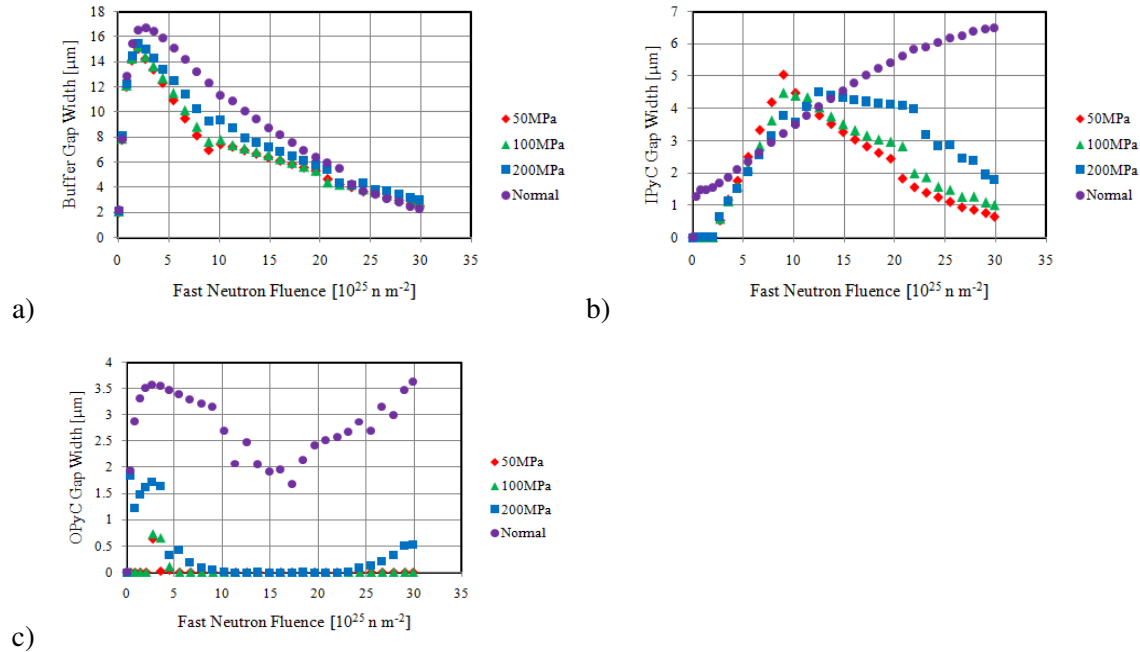


Figure 34. Effects of stress limited dimensional change using the FZJ dimensional change correlation. **a)** Buffer/IPyC interface gap widths. **b)** IPyC/SiC interface gap width. **c)** OPyC/Matrix gap width interface.

3.6 Summary

A comparison between BISON and PARFUME was performed and good agreement in stress and gas pressure was obtained. This provided confidence in the setup of the BISON model. The mesh size was varied and it was found that 10 μm elements produce satisfactory results.

Interface debonding was added using a reduction in modulus and thermal conductivity. This approach avoids the convergence issues of using an unmeshed gap and allows for recontact. However, friction and thermal contact resistance are not included in the model. In the event of partial recontact, this can lead to elements with higher stress concentrations than is realistic. In addition, for convergence it was necessary to debond all elements that exceeded their stress threshold for debonding in each timestep. As a result, the predicted patches during partial interface debonding are most likely larger than what would be experimentally observed.

Single particles were simulated inside of thick NITE-SiC shells and it was found that the model predicted very large stresses induced in the NITE-SiC by the OPyC layer. It was determined that this prediction is due to the modeled volume expansion combined with the lack of free volume to accommodate the OPyC layer expansion.

CHAPTER 4: EXPERIMENTAL COMPARISONS

4.1 Experiments

The correlations available for PyC IIDC are the FZJ and LLNL correlations. The FZJ was intended for high temperatures between 900-1300 °C while the LLNL correlation was intended for irradiation at 700 °C [9,30]. TRISO based FCM is expected to experience temperatures from about 400 to 1100 °C depending on the reactor environment. Additionally, initial densities and BAF may vary. Thus, it is desirable to develop a correlation that considers these factors and provides reasonable predictions when compared to the available experimental data.

4.1.1 NPR Experiments

Previously, TRISO irradiation experiments have been performed in the Advanced Test Reactor (ATR) as part of the New Production Reactor initiative (NPR), which is a modular high temperature gas cooled reactor. Average irradiation temperatures ranged from 746 to 1052 °C with fast neutron fluences of 1.9 to $3.8 \times 10^{25} \text{ n m}^{-2}$ [9]. The reported burnups were very high ranging from 64-79 at%. However, the fission gas pressures were not reported. The geometry of the TRISO particles is listed in Table 6, and the irradiation parameters are listed in Table 7 [9,63]. Table 8 provides the NPR coating layer failure fractions and compares them to previous PARFUME calculations [9]. The NPR data set gives a good comparison for the FZJ dimensional change correlations in the BISON model since that relationship is based on high temperature irradiation data with a similar initial density for the pyrolytic carbon [19].

Table 6. List of the TRISO geometry for the NPR experiments [63].

Layer	Outer Radius [μm]	Thickness [μm]
OPyC	328.5	43
SiC	285.5	35
IPyC	250.5	53
Buffer	197.5	100
Kernel	97.5	97.5

Table 7. NPR irradiation parameters [9].

	NPR-A4	NPR-A5	NPR-A8	NPR-A9
Time [EFPD]	170	170	170	170
Fast Neutron Fluence [10^{25} n m^{-2}]	3.8	3.8	2.4	1.9
Average Irradiation Temperature [C]	746	987	845	1052
Burnup [at%]	79	79	72	64
Particle Power [W]	0.18	0.18	0.164	0.146

The PyC was given an initial density of 1880 kg m^{-3} with a mean fracture stress of $1316 \text{ MPa } \mu\text{m}^{3/m}$ and Weibull parameter (m) of 9.5 [63,62]. The characteristic shear and normal debond stresses were reduced from 240 and 100 MPa to 190 and 80 MPa respectively due to the lower density. Fission gas pressure was applied at the buffer/IPyC interface and the outer OPyC surface was given a 0.1 MPa pressure boundary condition. The particle power was modeled as constant for the duration of the simulation.

Table 8. List of the TRISO layer failure fractions from the NPR experiments [9,63].

	Failed [%]	95% Confidence Interval [%]	Sample Size	PARFUME [%]	PARUFME with 1.8x Creep Rate [%]
NPR-A4 IPyC	65	54 - 76	83	100	99.8
NPR-A5 IPyC	31	17 - 47	39	100	34.8
NPR-A8 IPyC	6	2 - 16	53	100	94.0
NPR-A9 IPyC	18	5 - 42	17	100	14.5
NPR-A4 SiC	3	2 - 6	287	9.2	3.4
NPR-A5 SiC	0.6	0 - 3	178	1.8	0.22
NPR-A8 SiC	0	0 - 2	260	5.9	1.8
NPR-A9 SiC	1	0 - 5	83	1.1	0.044

4.1.2 High Flux Isotope Reactor

Surrogate TRISO particles in a NITE-SiC matrix were irradiated in the High Flux Isotope Reactor (HFIR) [29]. The irradiation temperature was about 320 °C and a neutron fluence of $7.7 \times 10^{25} \text{ n m}^{-2}$ was reached in the irradiation. The gamma heating was estimated at 32 W g^{-1} with an irradiation time 88 days [29]. The geometry of the TRISO particles is listed in Table 9 [64], and Table 10 lists the irradiation parameters [29]. The initial density of the PyC was estimated at 2012 kg m^{-3} with a Bacon Anisotropy Factors (BAF) of 1.009 and 1.029 for the OPyC and IPyC respectively [29,64]. The debonding, shear, and normal characteristic stresses were set to 240 and 100 MPa respectively due to the higher density than in the NPR experiments.

Post irradiation inspection did not find any evidence of debonding, or through-wall fracture with the exception of debonding at the kernel/buffer interfaces. This is a significant difference compared to the NPR experiments which found substantial fractions of failed IPyC layers and a few failed SiC layers [9,29]. Although, the irradiated samples were surrogate TRISO particles irradiated at low temperatures and experienced minimal internal gas pressures.

Table 9. List of the TRISO geometry used in the HFIR irradiations [64].

Layer	Outer Radius [μm]	Thickness [μm]
Matrix	950	492
OPyC	458	36
SiC	422	31
IPyC	391	41
Buffer	350	85
Kernel	265	265

Table 10. List of the irradiation parameters for the HFIR irradiations [29].

	HFIR
Time [Days]	88
Fast Neutron Fluence [10^{25} n m^{-2}]	7.7
Average Irradiation Temperature [C]	320
Gamma Heating [W]	0.05

4.2 Simulations

4.2.1 Setup and Initial Results

Figure 35 shows the meshes used in BISON to simulate the NPR and HFIR irradiation conditions respectively. The NPR mesh consists of a single TRISO particle with debondable IPyC/SiC and Buffer/IPyC interfaces. The external pressure was set to 0.1 MPa. The HFIR mesh includes a 500 μm thick NITE-SiC shell surrounding the single TRISO particle with an additional debondable OPyC/NITE-SiC interface.

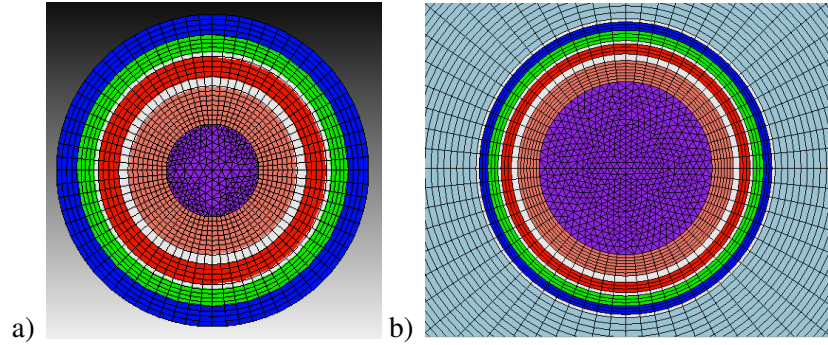


Figure 35. a) Representation of the mesh used to simulate the NPR experiments. Debondable layers are represented with the white regions. b) The mesh used in the BISON model for HFIR simulations. The TRISO particle is embedded in a NITE-SiC matrix (gray region) which is approximated as a 500 μm thick shell of NITE-SiC. Debondable layers at the OPyC/matrix, IPyC/SiC, and Buffer/IPyC interfaces were added.

Table 11 lists the results for the NPR simulations and compares them to the experimental values, and Figure 36 plots the predicted OPyC and IPyC gap widths for the HFIR irradiations. The FZJ correlations over predicted the results for the NPR simulations. While there are considerable differences between predictions and observations in typical TRISO fuel performance codes, it is hoped that greater accuracy can be achieved. However, the LLNL dimensional change correlations did not produce reasonable agreement with the NPR observations and severely under predicted the failure fractions as shown in **Table 11**. This is due to a mixture of a 0.4 Poisson ratio in creep that does not require volume to be conserved during creep and a slower initial PyC shrinkage.

For the HFIR simulations, it was found that neither the FZJ nor the LLNL dimensional change correlations were able to predict the lack of observed OPyC and IPyC interface debonding. This implies that the dimensional change is a function of density, temperature. There is also a possibility of hydrostatic stress, variable Poisson ratio in creep, and an increase in creep rate below 500-600 $^{\circ}\text{C}$ which may produce significant effects [33]. It should be noted that the OPyC was predicted to completely debond, while a partial debond was predicted for the IPyC when using the LLNL correlations. Whereas when using the FZJ correlation both layers were predicted to completely debond.

In these simulations, the failure probability of the SiC is highly dependent on the through wall fracture of the IPyC layer. As a result, the SiC failure probabilities are not included in this table. Both the FZJ and LLNL correlations produce results that are significantly different from the observations.

Table 11. Comparison of the NPR results with BISON calculations.

	Failed [%]	95% Interval [%]	BISON FZJ [%]	BISON LLNL [%]
NPR-A4 IPyC	65	54 - 76	100.0	1.79
NPR-A5 IPyC	31	17 - 47	99.96	8.6×10^{-3}
NPR-A8 IPyC	6	2 - 16	100.0	0.26
NPR-A9 IPyC	18	5 - 42	97.15	2.21×10^{-3}

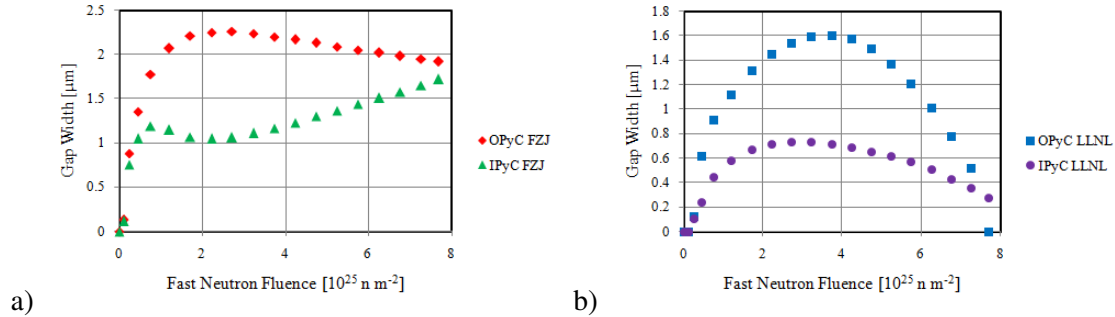


Figure 36. Plots showing the predicted OPyC/matrix and IPyC/SiC interface gap widths using FZJ and LLNL dimensional change correlations with 0.5 and 0.4 Poisson ratios in creep respectively. **a)** Global maximum gap widths using FZJ correlations with a 0.5 Poisson ratio in creep. **b)** Global maximum gap widths using LLNL correlations with a 0.4 Poisson ratio in creep. The same creep correlation was used in all cases.

4.2.2 Effect of Hydrostatic Stress

The effect of hydrostatic stress was considered. It was found that reasonable agreement with the NPR simulations can be obtained using a stress limited FZJ dimensional change correlation. However, stress limited dimensional change was not able to prevent the prediction of interface debonding in the HFIR simulations. In addition, a power of five for the hydrostatic stress ratio (n) was required to obtain agreement with experiments instead of the recommended linear dependence [48]. The stress sensitivity was set to 155 MPa for the NPR simulations while far lower values of 50-25 MPa were considered for the HFIR simulations. The volumetric swelling multiplier equation is shown in Equation 11, and Table 12 provides the stress limited predictions then compares them to the previous FZJ predictions and NPR experimental results.

Table 12. List of the NPR failure fractions using hydrostatic stress limited dimensional change.

	Failed [%]	95% Interval [%]	BISON FZJ [%]	BISON FZJ Stress Limited [%]
NPR-A4 IPyC	65	54 - 76	100.0	69.80
NPR-A5 IPyC	31	17 - 47	99.96	33.08
NPR-A8 IPyC	6	2 - 16	100.0	57.57
NPR-A9 IPyC	18	5 - 42	97.15	23.03

$$\dot{S} = \dot{S}_0 \left(1 \pm \left(\frac{\sigma_{hydrostatic}}{A} \right)^n \right) \quad (\text{Eq. 11})$$

Equation 11. The adjusted volumetric change due to hydrostatic stress. In this expression, A sets the stress value that gives a 100% change in IIDC. The IIDC multiplier is limited to a range from zero to two. $\sigma_{hydrostatic}$ is the average of the three principal stresses. When the volumetric dimensional change is increasing the term is additive, but when there is volumetric shrinkage the stress term is subtracted. Five was the value used for n.

The stress limited dimensional change was active in the HFIR simulation. However, once the FZJ volumetric trend began to recover some of its initial shrinkage, the IPyC/SiC and the OPyC/matrix interfaces began to debond. In the case of the OPyC, it was possible to prevent complete debonding except for a short duration from about 1.6 to $1.8 \times 10^{25} \text{ n m}^{-2}$. The duration of this total debonding period increases with larger hydrostatic stress thresholds. However, the IPyC interface completely debonded in all simulations. These results suggest that hydrostatic stress may be present in the experiments but it is not the only significant factor causing the difference seen at high and low temperatures.

4.2.3 Effect of Poisson Ratio in Creep

The FZJ correlation assumes a constant volume in creep, which corresponds to a 0.5 Poisson ratio in creep. However, the LLNL correlation assumes a volume change in creep and a value of 0.4 for the Poisson ratio in creep. A set of simulations was performed where the Poisson ratios in creep for the FZJ and LLNL correlations were reversed and set to 0.4 and 0.5 respectively. Table 13 lists the results. The results indicate that using a value of 0.4 for the Poisson ratio in creep for the FZJ and 0.5 for the LLNL correlations did improve the accuracy somewhat. However, the agreement is not very good in either case.

Table 13. Predicted failure probabilities for the IPyC layer in NPR simulations. The FZJ correlation used a Poisson ratio in creep of 0.4 and the LLNL use a value of 0.5 that is the reverse of the recommended values.

	Failed [%]	95% Interval [%]	FZJ 0.4 v_c [%]	LLNL 0.5 v_c [%]
NPR-A4 IPyC	65	54 - 76	99.92	13.55
NPR-A5 IPyC	31	17 - 47	44.05	0.21
NPR-A8 IPyC	6	2 - 16	99.73	5.12
NPR-A9 IPyC	18	5 - 42	16.47	5.2×10^{-2}

4.2.4 Effect of Accelerated Low Temperature Creep

Graphite data from Russian and American sources [33] suggest an increase in creep rate below 500 °C. However, data from British sources indicates a constant creep rate at low temperature as shown in Figure 37 [33]. In the BISON model, the constant creep behavior at low temperatures is used since it provides a conservative and more defensible assumption. However, the following HFIR simulations were conducted to investigate the potential effect of accelerated low temperature creep. A creep multiplier of 1.45 was used (2.9x CEQA) and Figure 38 shows the resulting OPyC/NITE-SiC gap widths for FZJ and LLNL dimensional change correlations. The results show only minor differences in the predicted gap widths. As a result, it is clear the dimensional change behavior must be different in the NPR case versus the HFIR environment.

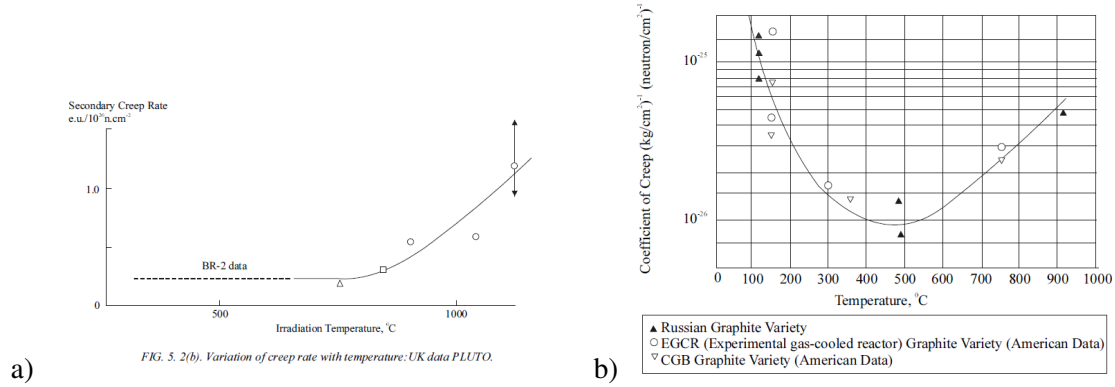


Figure 37. The above figures plot the different creep trends at low temperatures from British and American-Russian sources. Adapted from IAEA-Tecd-1154. **a)** A plot of the trend from Kelly and Brocklehurst [33]. **b)** A plot of the data from Kennedy and Platonov [33].

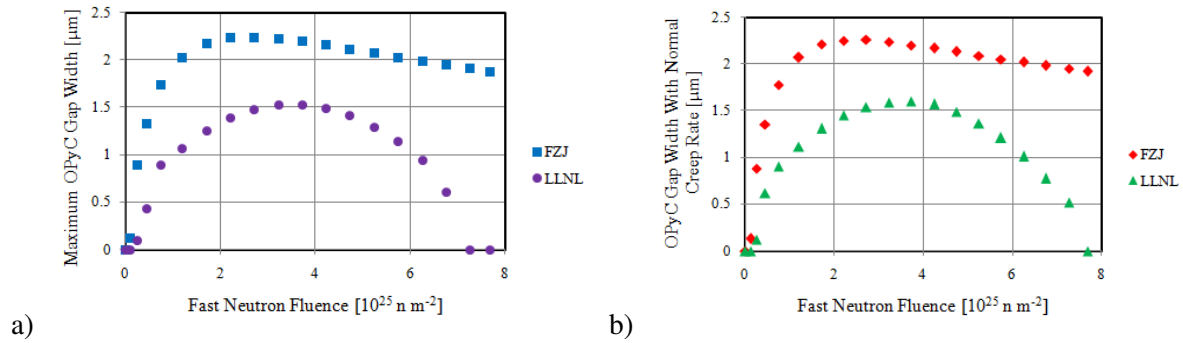


Figure 38. **a)** Plot of the OPyC/NITE-SiC gap widths when accelerated (2.9x CEGA) low temperature creep is used. **b)** Plot of the OPyC/NITE-SiC gap widths when normal (2x CEGA) low temperature creep is used. Only minor differences in the gap widths were predicted.

4.3 Alternate Irradiation Induced Dimensional Change Correlation for Pyrolytic Carbon

The FZJ and LLNL dimensional change correlations are independent of density, temperature, and Bacon Anisotropy Factor (BAF). Based on the above NPR and HFIR irradiation results, it seems probable that these variables have a notable impact on the PyC behavior and thereby TRISO fuel performance. As a result, it is desirable to account for these variables considering that the LWR environment and TRISO manufacturing processes span a wide range of conditions and material properties respectively.

The low density buffer has been observed to shrink isotropically, and was assumed to saturate for densities less than 1000 kg m^{-3} [9]. Initially, the high density PyC shrinks but was assumed to experience large volumetric swelling at high fluence [30]. It was also assumed that the transition between low and high density behavior was continuous. An additional assumption was made that the temperature and BAF effects would accentuate the anisotropic behavior, but density would function as the dominate volume change mechanism. This conclusion is based on observations from HOPG irradiations by Bokros at

various temperatures, BAFs, and densities [21]. The methods used to develop this correlation are similar to those used by Wang [32], which started with developing the isotropic correlation and then incorporated the anisotropy. Equation 12 provides the equations used for the IIDC correlation. The two primary terms can loosely be described as empirical estimates for dimensional change resulting from pore shrinkage and defect formation within the domains.

$$S_i = \frac{A_\rho}{B} \exp(B\Phi) + C_{Temp} (D_{i,BAF} E_\rho \Phi^2 + F_{i,BAF} G_\rho \Phi) \quad (\text{Eq. 12a})$$

$$A_\rho = 1.0728(1 - \exp(-1.04\rho_0^{1.4})) - 1.007 \quad (\text{Eq. 12b})$$

$$\rho > 1.73 \frac{\text{g}}{\text{cm}^3}; \quad B = -1.75 \quad (\text{Eq. 12c})$$

$$\rho \leq 1.73 \frac{\text{g}}{\text{cm}^3}; \quad B = 1.3515\rho - 4.0846$$

$$C_{Temp} = \frac{1.2}{1 + \exp(-0.011T_K + 8.5)} + 0.3 \quad (\text{Eq. 12d})$$

$$D_{BAF}^{Tan} = -0.075468BAF_0 + 1.0668 \quad (\text{Eq. 12e})$$

$$D_{BAF}^{Rad} = -4.0829BAF_0^2 + 17.202BAF_0 - 12.119 \quad (\text{Eq. 12f})$$

$$E_\rho = 7.846 \times 10^{-4} \rho_0^3 - 3.6289 \times 10^{-3} \rho_0^2 + 6.1409 \times 10^{-2} \rho - 3.2966 \times 10^{-3} \quad (\text{Eq. 12g})$$

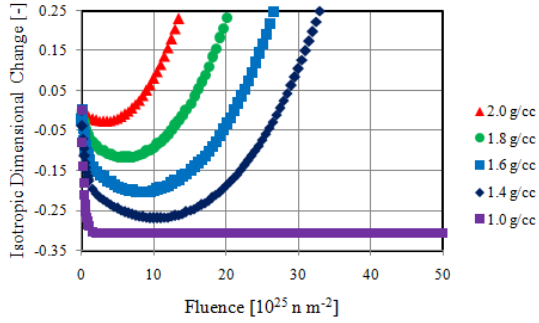
$$F_{BAF}^{Tan} = -1.7699BAF_0^2 - 7.8622BAF_0 - 5.0317 \quad (\text{Eq. 12h})$$

$$F_{BAF}^{Rad} = -0.16672BAF_0^2 - 1.0464BAF_0 + 2.2162 \quad (\text{Eq. 12i})$$

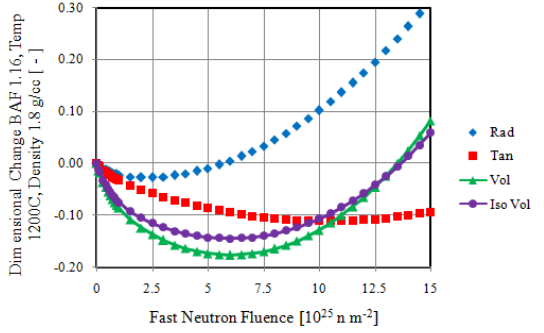
$$G_\rho = 0.01739\rho_0^4 - 0.11251\rho_0^3 + 0.028769\rho_0^2 - 0.34101\rho_0 + 0.14844 \quad (\text{Eq. 12j})$$

Equation 12. These are the equations used for the hybrid correlation. The fluence, Φ , has units of $1 \times 10^{-25} \text{ n m}^{-2}$, temperature, T , is in Kelvin, and initial density, ρ_0 , is in g cm^{-3} . The subscript, i , denotes tangential and radial directions. The designed BAF range is 1.0 to 1.5.

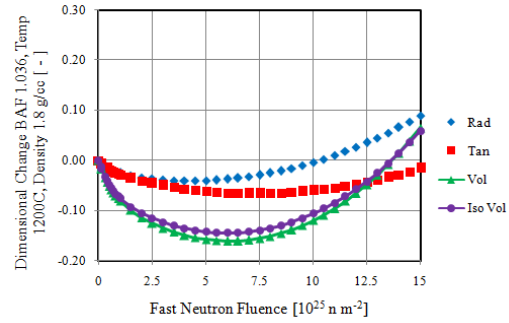
Figure 39 and Figure 40 plot and compare the effects of density, temperature, and anisotropy. The effect of density is to transition from shrinkage and saturation to an immediate and rapid swelling at nearly theoretical levels. Density is assumed to produce an isotropic behavior since it changes the pore concentration. However, the BAF is presumed to accelerate radial swelling and tangential shrinkage in a fairly but not completely constant volume behavior. The modeled effect of temperature is to amplify the second term of the equation that contains the anisotropy and high density behaviors. As a result, the correlation predicts temperature and anisotropy independent pyrolytic carbon at low densities, but highly dependent on these variables at theoretical density.



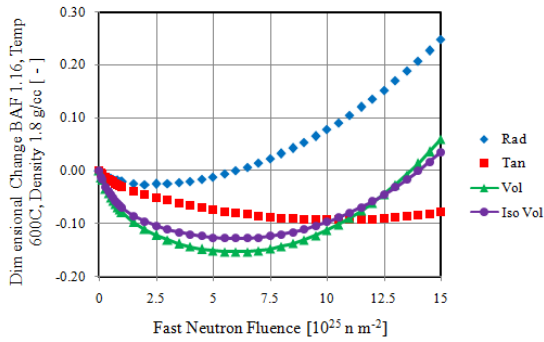
a)



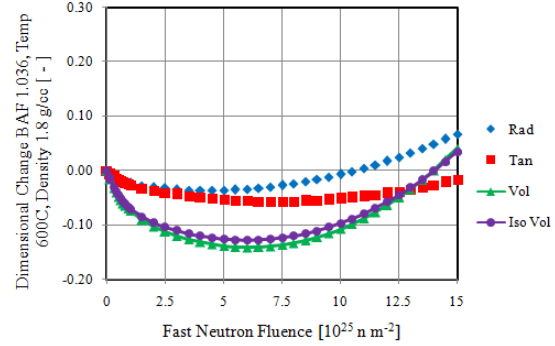
b)



c)



d)



e)

Figure 39. These are plots showing the dimensional change dependence on initial density, temperature, and anisotropy. **a)** Volumetric change at 800 °C and initially isotropic. **b)** Plot showing the tangential, radial behaviors and comparing the anisotropic and isotropic volume change at 1200 °C and BAF 1.16. **c)** Plot of the dimensional change at 1200 °C and BAF of 1.036. **d)** Plot of the dimensional change at 600 °C and BAF of 1.16. **e)** Plot of the dimensional change at 600C and BAF of 1.036. The density of figures b through d is 1.8 g cm⁻³.

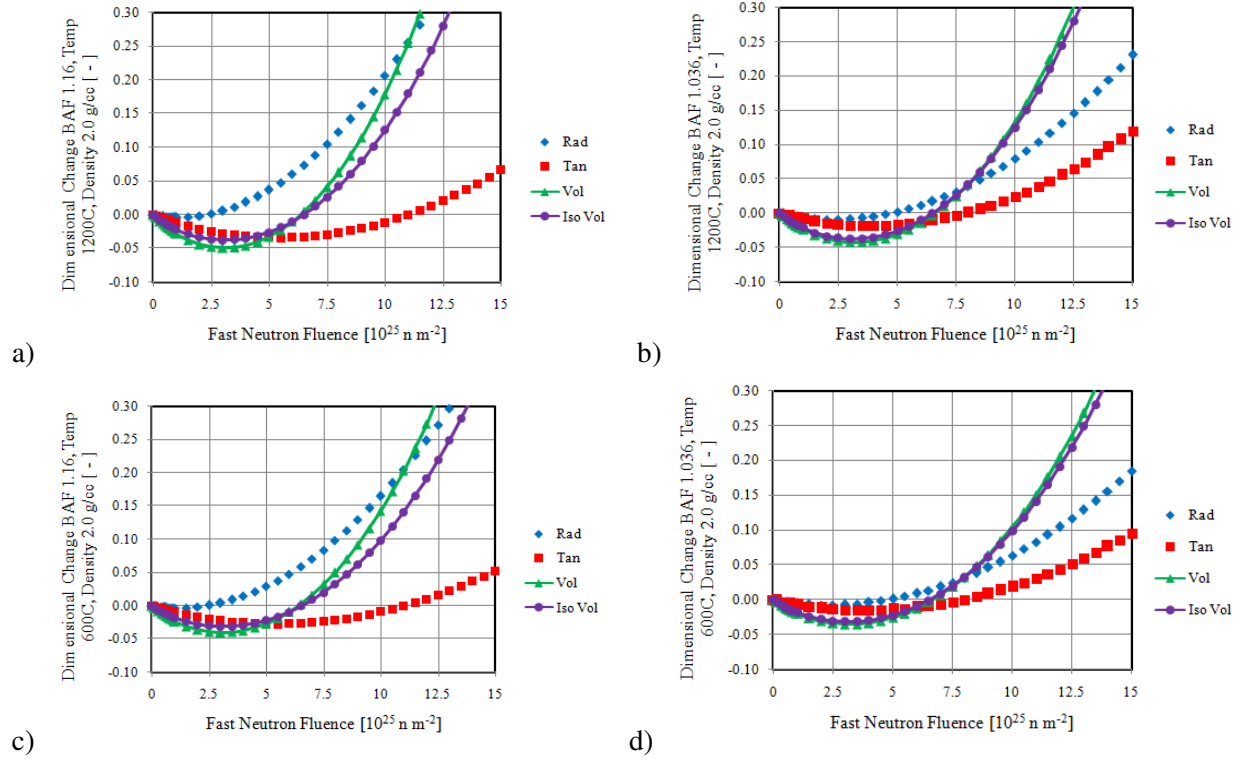


Figure 40. Plots showing the effect of anisotropy and temperature at 2.0 g cm^{-3} . **a and b)** Plots showing the modeled effect of anisotropy at $1200 \text{ }^{\circ}\text{C}$ and initial density of 2.0 g cm^{-3} . **c and d)** Plots showing the modeled effect of anisotropy at $600 \text{ }^{\circ}\text{C}$ and initial density of 2.0 g cm^{-3} .

A Poisson ratio in creep that is dependent on the minimum principal stress was also used [9]. Figure 41 plots the modeled Poisson ratio in creep. The NPR and HFIR simulations were again performed now with modified dimensional change correlation, accelerated low temperature creep, and a hydrostatic stress limit of 160 MPa. Table 14 and Figure 42 show the results of the simulations. The model predicts a greater sensitivity to temperature than what was observed in the NPR experiments, however, there is reasonable agreement with the NPR results. For the HFIR simulation, small patches of the OPyC were predicted to debond from the NITE-SiC shell, but the IPyC/SiC interface was predicted to remain intact. This was considered acceptable due to the small size of the predicted debonded patches and the resulting small gap widths. While there remains a large amount of uncertainty in the material properties for the pyrolytic carbon, these results give a greater degree of confidence in the ability to predict FCM fuel performance.

Table 14. Comparison of the predicted failure probabilities using the modified IIDC correlation with the experimental NPR results.

	Failed [%]	95% Interval [%]	Hybrid [%]	Hybrid Without Hydrostatic Stress Limit [%]
NPR-A4 IPyC	65	54 - 76	64.45	99.35
NPR-A5 IPyC	31	17 - 47	15.97	74.68
NPR-A8 IPyC	6	2 - 16	45.18	99.86
NPR-A9 IPyC	18	5 - 42	8.38	40.10

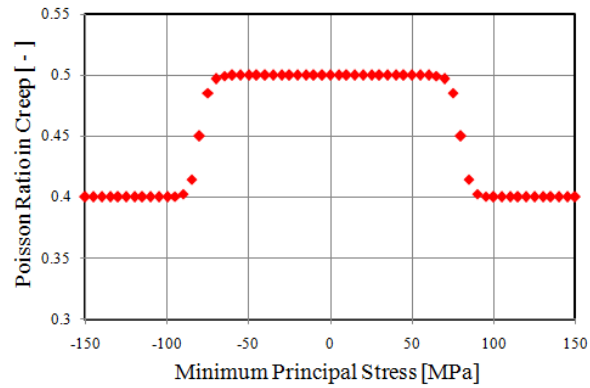


Figure 41. Plot of the Poisson ratio in creep for pyrolytic carbon as a function of minimum principal stress. The model can be configured to use the absolute value or only tensile stresses.

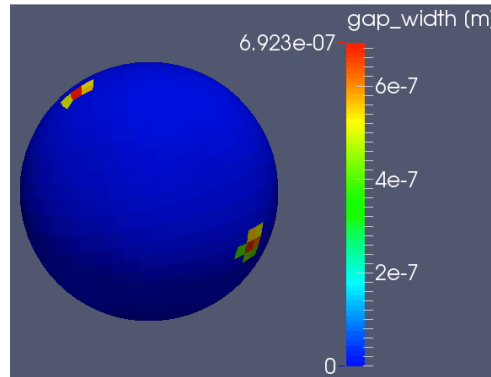


Figure 42. Maximum predicted OPyC interface debonding from the NITE-SiC shell at a neutron fluence of $4.25 \times 10^{25} \text{ n m}^{-2}$.

4.4 Recommendations for Additional Experiments to Define PyC Volume Change Behavior

The volumetric change of the PyC is the most important aspect of TRISO based FCM behavior under irradiation. The second factor of importance is its ability to generate stress in the surrounding materials, particularly silicon carbide. Existing experimental data is available for fluences up to about $4 \times 10^{25} \text{ n m}^{-2}$ and indicates that an initial shrinkage of a few percent volumetric can be expected [19,21]. However, data for high fluences is very limited [9]. Furthermore, there is limited data evaluating PyC behavior at various temperatures and initial densities. The expected fast neutron fluence for FCM applications reaches up to about $20\text{-}30 \times 10^{25} \text{ n m}^{-3}$. Thus, it is desirable to perform additional experiments to determine the PyC dimensional change behavior under irradiation at neutron high fluence.

It is recommended to use the High Flux Isotope Reactor (HFIR) to achieve the required high neutron fluences. Irradiation temperatures between 350 and 1100 °C would be useful. However, the recommended target temperatures are between 500C and 900 °C. There is also the possibility of a transition in defect type and mobility at about 600-700 °C. As a result, it is possible that the PyC in the interior and exterior

of a FCM pellet will experience different behavior at high fluence. The target initial density for the PyC should be about 2.0 g cm^{-3} , but a range from about $1.85\text{-}2.05 \text{ g cm}^{-3}$ may be useful. A very high density ($>2.1 \text{ g cm}^{-3}$) is much more likely to produce volume expansion and significant stresses at high neutron fluence due to the theoretical density of PyC being 2.26 g cm^{-3} .

It is important to capture the volume change under irradiation when the PyC sample is unconstrained and then compare that to a fully constrained sample. A partially restrained PyC sample would most likely be effective. However, there is a small possibility of irradiation creep confounding the volume change results. The PyC for the unconstrained sample could be deposited onto a graphite substrate, and then the substrate would be ground away. Alternatively, irradiating the deposited PyC and graphite substrate together may provide information on both materials. However, if the irradiation behavior is sufficiently dissimilar between the materials a fracture in the sample may occur. Reducing the number of directions the PyC can deform may decrease the uncertainty of the volume change measurement. A partially restrained sample could be produced by depositing the PyC onto a NITE-SiC disk, outer surface of a sphere, or the interior of a cylindrical shell.

The fully constrained PyC sample must employ a geometry that prevents expansion in all directions. A spherical shell of PyC with SiC materials on the interior and exterior surfaces would be analogous to an OPyC layer embedded in a SiC matrix. However, a cylindrical geometry may be easier to create. Figure 43 shows a representation of possible geometries for the fully constrained samples. It is also recommended to include samples where graphite has been substituted for the pyrolytic carbon. In the event that the irradiation temperature is insufficient to cause a volumetric turnaround in the PyC, there will be significant uncertainty in the maximum temperature at which the FCM fuel can be operated. However, graphite is known to experience a volumetric turnaround at 900°C , which is a temperature achievable in HFIR. Information on the amount of stress graphite can generate in surrounding materials due to irradiation swelling will be relatable to the pyrolytic carbon.

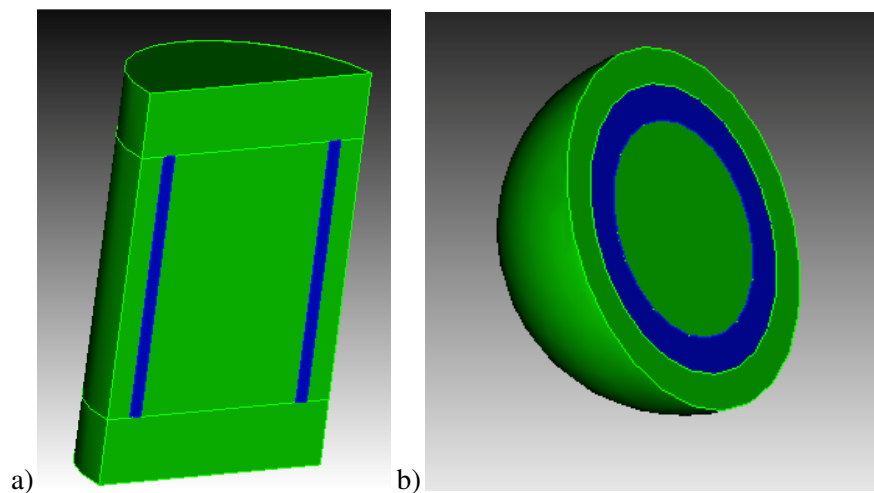


Figure 43. Two possible geometries for a fully constrained PyC sample. Green represents the SiC or constraining material, while blue indicates the PyC layer. **a)** A cylindrical geometry. **b)** A spherical geometry.

To estimate the stress generated by the PyC material it is recommended to produce multiple samples with varying thickness of the outer constraining material. If the PyC does expand volumetrically, a thinner surrounding SiC would experience higher stresses and thus higher probability of fracture. This would give an estimate for the sensitivity of PyC dimensional change to hydrostatic stress. Figure 44 plots some sample predictions for hoop stress in the outer SiC shell. It is expected that a range of shell thicknesses from about 0.08-0.23 mm would provide the range of failure probabilities necessary to estimate the PyC hydrostatic stress threshold for a PyC layer thickness of 0.25 mm. A plot of failure probability versus hoop stress is presented. The estimated element volume was $1 \times 10^{-12} \text{ m}^3$, which was representative of the mesh used in the simulations.

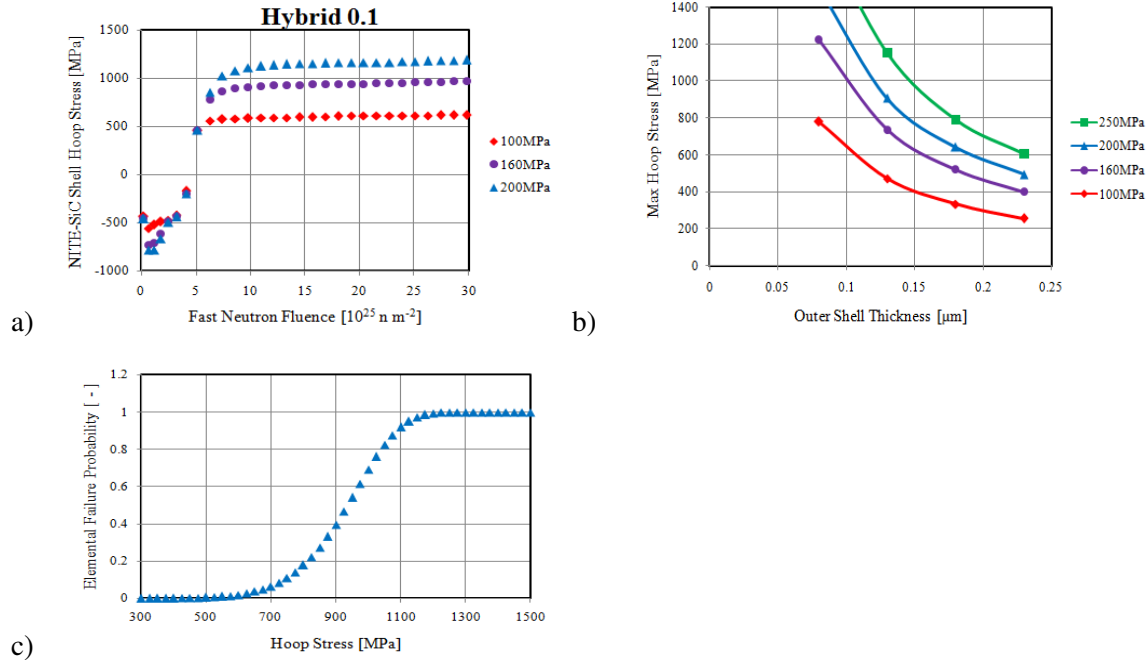


Figure 44. Plots of the expected hoop stress in the outer SiC shell surrounding a 0.25 mm thick PyC layer. **a)** In this simulation the outer SiC is 0.1 mm thick and the PyC stress threshold is varied from 200-100 MPa. Hybrid dimensional change correlation was used. **b)** The maximum hoop stress in the outer SiC shell, which occurs near the end of the simulation. **c)** A plot of the failure probability versus hoop stress. Due to the expansion of the PyC layer, the outer SiC shell is expected to be in tension tangentially and compression radially.

If the High Flux Isotope Reactor is selected for the irradiation facility, it is recommended to use the removable beryllium irradiation facility due to the smaller fast neutron flux gradient then in the periphery target region. It is expected that a 5 mm wide sample in the radial direction would accumulate about $2\text{-}2.5 \times 10^{25} \text{ n m}^{-2}$ by the end of the irradiation in the beryllium reflector as opposed to $5\text{-}10 \times 10^{25} \text{ n m}^{-2}$ in the periphery target region [65]. However, using the beryllium reflector would require 21 instead of 13 cycles to achieve the required fluence [65].

4.5 Summary

A PyC dimensional change correlation has been developed to fit the available experimental data and reasonable agreement was obtained. The dimensional change of the PyC was considered a function of fast neutron fluence, density, temperature, and Bacon anisotropy factor. Considerations for hydrostatic stress are also included in the model, but data is extremely limited.

The correlation assumes an initial volumetric shrinkage followed by a graphite styled turnaround at high fluence. The available experiments do not provide sufficient information as to whether a volume expansion or constant volume extrapolation is more appropriate for high density PyC. As a result, it is recommended to perform additional experiments to determine the volume change behavior of PyC at high fluence.

CHAPTER 5: FCM SIMULATIONS IN AN HTGR ENVIRONMENT

5.1 FCM Model and Setup

Due to the highly anisotropic nature of the FCM geometry, it is necessary to model the FCM pellet. Each particle must be modeled discretely to obtain the proper stresses and temperatures. Since a considerable proportion of the heat will flow through multiple kernels and buffers before reaching the coolant, homogenous particles will not satisfactorily approximate the effects of interface debonding under these conditions. Also and as will be shown later, the thickness of the OPyC has an impact on the ability of the irradiation creep to relax the stress. As a result, a homogenous particle cannot accurately predict a TRISO particle for a wide range of parameters. Thus, it was important to develop the capability to simulate a large collection of discrete particles in a silicon carbide matrix.

The meshing limitations in the case of a TRISO particle used in the FCM pellet require the use of tetrahedral elements in the kernel and the subdivision of the kernel into inner and outer regions to provide sufficient constraint once the buffer debonds from the IPyC. Figure 45 shows the mesh of a FCM TRISO particle. Table 15 lists the geometry for the TRISO particles used in the LWR and HTGR FCM simulations.

In these HTGR simulations, the mesh has 9 million degrees of freedom (DOF). The arrays allocated for variables and aux-variables were 16.1 and 237.2 million DOF respectively. These simulations were performed on the FALCON cluster at Idaho National Laboratory. The required resources were 256 processors, 3.8 TB of ram and about three days to complete a simulation.

Table 15. List of the TRISO particle geometry used in the LWR and HTGR FCM simulation. LWR is listed on the left and HTGR is listed on the right.

Material	Outer Radius [μm]	Thickness [μm]	Outer Radius [μm]	Thickness [μm]
OPyC	565	30	450	30
CVD-SiC	535	40	420	40
IPyC	495	30	380	30
Buffer	465	75	350	80
Kernel	390	390	270	120

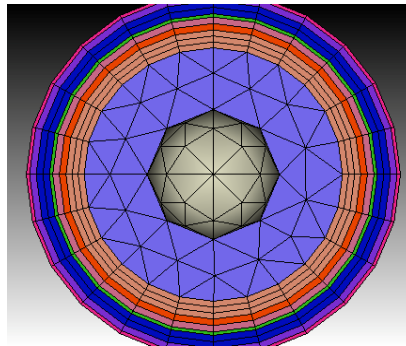


Figure 45. FCM TRISO particle mesh showing the various layers and debonding regions.

5.2 HTGR Simulations

The HTGR simulation features a FCM pellet with embedded TRISO particles in the center cylinder with three 120° sections of uniform NITE-SiC heat generating cylinders. Due to the lack of symmetry in the TRISO particle arrangement, it was necessary to have a central FCM pellet. The alternating 120° sections of homogenous fuel pellet and coolant channel is to complete the geometry for the single channel analysis.

Graphite is the material between the NITE-SiC cylinders. Three 120° coolant channels are also present. Due to meshing limitations, the simulated length of the fuel was only 5.08 mm. The heat generation was set to 10 kW m⁻¹ per fuel rod for a total of 101.6 W in total, and the duration was 671 full power days. The geometry used was listed in a paper by Travis and El-Genk [66] and is presented in Table 16. Figure 46 shows the HTGR mesh and schematic of the top down view of the general core layout. Due to the low linear power and resulting small temperature gradient across the pellet, the NITE-SiC swelling gradients do not cause much of a compressive perimeter. However, as will be later discussed the high power LWR cases expect significant compressive stresses at the perimeter of the pellet.

Table 16. List of the high temperature gas reactor and light water reactor geometry parameters as obtained from [66].

	HTGR	LWR
Coolant Temp [C]	700	290
Pellet Diameter [mm]	15.45	8.2
HTC [W m ⁻² K ⁻¹]	3000	38200
Linear Power [kW m ⁻¹]	10	35
Max Burnup [at%]	3.8	30
Packing Fraction [vol%]	40.4	41.5

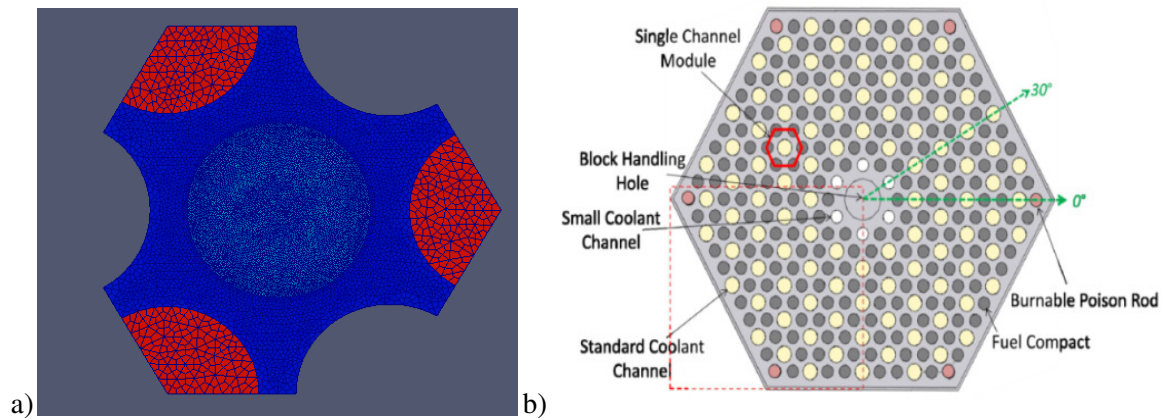


Figure 46. a) The mesh used in the HTGR simulation. b) A top down representation of the VHTR core [66].

The combination of moderate temperatures and burnup less than 1000 °C and 3.78 at% respectively are expected to produce low fission gas pressures, which are applied at the buffer/IPyC interface. This indicates that high thermal conductivity of the NITE-SiC and graphite allows the FCM fuel type to operate in this environment without high risk of fission gas overpressure. Figure 47 shows the results of the HTGR simulation at 10 kW m⁻¹ and a coolant temperature of 700 °C. Coolant channel diameter was set to 15.875 mm, the FCM pellet diameter was 15.45 mm, and the length of a single channel hex side was 18.8 mm. The verticle length of the single channel segment was 5.08 mm.

The total temperature difference from coolant interface to maximum fuel temperature was only about 140 °C. This temperature gradient is insufficient to generate the characteristic compressive perimeter in the NITE-SiC matrix. The matrix stress profiles are displayed in Figure 47e and f.

When using the LLNL correlation, a large increase in stress is predicted as the PyC beings to swell. Once the swelling is capped at 30% volumetric, the creep relaxes the stress. The maximum elemental stress is about 3100 MPa. While the stress at which 95% of the elements are below and the average hoop stress are only about 1400 and 550 MPa respectively. This indicates that the model predicts a small number elements with very high stresses that are predominately located between particles in close proximity.

The FZJ correlation assumes constant volume PyC behavior and partial interface contact for fluences of about 10x10²⁵ n m⁻² and higher. This produces the scatter observed in the maximum hoop stress trend. It is interesting to note that in some places the 95% and average hoop stresses are nearly identical. This indicates that many of the elements are in a narrow range of stresses.

The maximum temperature is predicted to rapidly increase as the buffer/IPyC gaps form and thermal conductivities degrade. However, at about 13x10²⁵ n m⁻² the LLNL correlation predicts re-contact at the IPyC/buffer interface while the FZJ simulation predicts that the gaps will remain open. This gap closure leads to a lower temperature in the LLNL simulation which results in a lower maximum fission gas pressure.

The graphite planes were assumed to be oriented in the horizontal direction to allow for better heat transfer. Additionally, the graphite was assumed to have free volume on the top and bottom surfaces. The resulting stresses in the graphite binder were less than 35 MPa and not considered to cause a significant probability of fracture.

5.3 High Temperature Gas Reactor Parameter Variations

In these simulations, the FCM pellets are surrounded by a binder that is modeled as graphite unless otherwise noted. The FCM pellet and coolant channel diameters are 15.47 and 15.875 mm respectively. The length of a single channel hex side was 18.8 mm [66]. The base coolant temperature used in these simulations was 700 °C with a heat transfer coefficient of 3000 W m⁻² K⁻¹ [66].

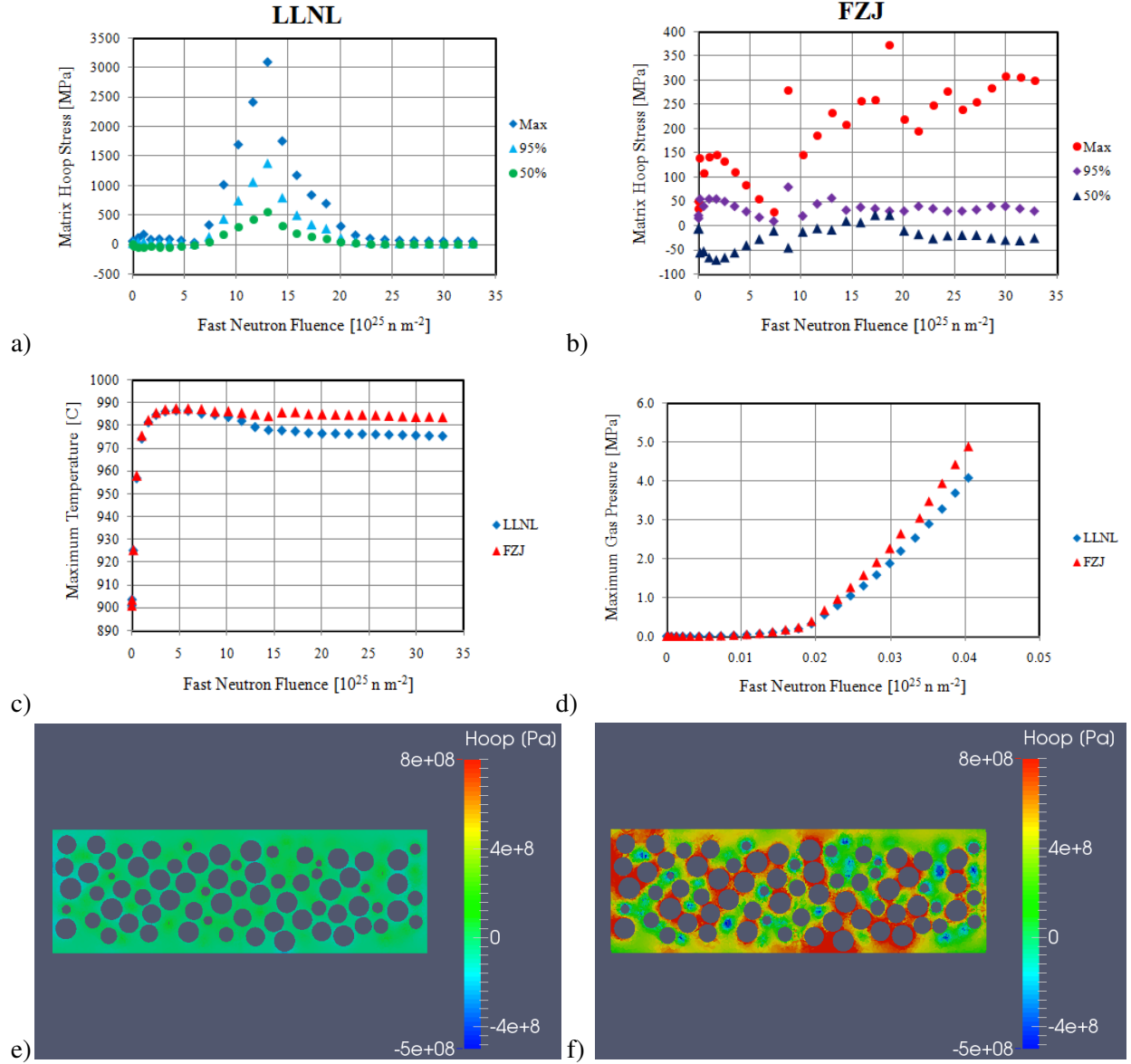


Figure 47. **a)** A plot comparing the maximum elemental hoop stress reported within the matrix of the central FCM pellet versus fluence for the FZJ and LLNL dimensional change correlations. **b)** A plot of the matrix hoop stress using the FZJ correlation. **c)** A plot of the maximum temperature within the matrix of the central FCM pellet. **d)** A plot of the fission gas pressure. **e)** A vertical slice through the center of the FCM pellet showing hoop stress profile at $2.56 \times 10^{25} \text{ n m}^{-2}$. **f)** A vertical slice through the center of the FCM pellet showing hoop stress profile at $13 \times 10^{25} \text{ n m}^{-2}$.

5.3.1 Irradiation Induced Dimensional Change

In this simulations the predicted hoop stresses from the FZJ, LLNL, and hybrid correlation are compared. The LLNL correlation is predicted to produce the characteristic large stress spike due to PyC swelling and creep relaxation. The FZJ correlation produces stresses less than 500 MPa with considerable scatter due to partial OPyC/matrix interface contact. While the hybrid correlation predicts a stress limited swelling that results in a slowly increasing hoop stress of about 1000 MPa. It should be noted that the 95% hoop stress is approximately half of the maximum hoop stress, and the average hoop stress is about a quarter of the maximum hoop stress. This indicates that very large maximum elemental hoop stresses will be encountered before long range cracks are expected in the matrix. Figure 48 plots the results.

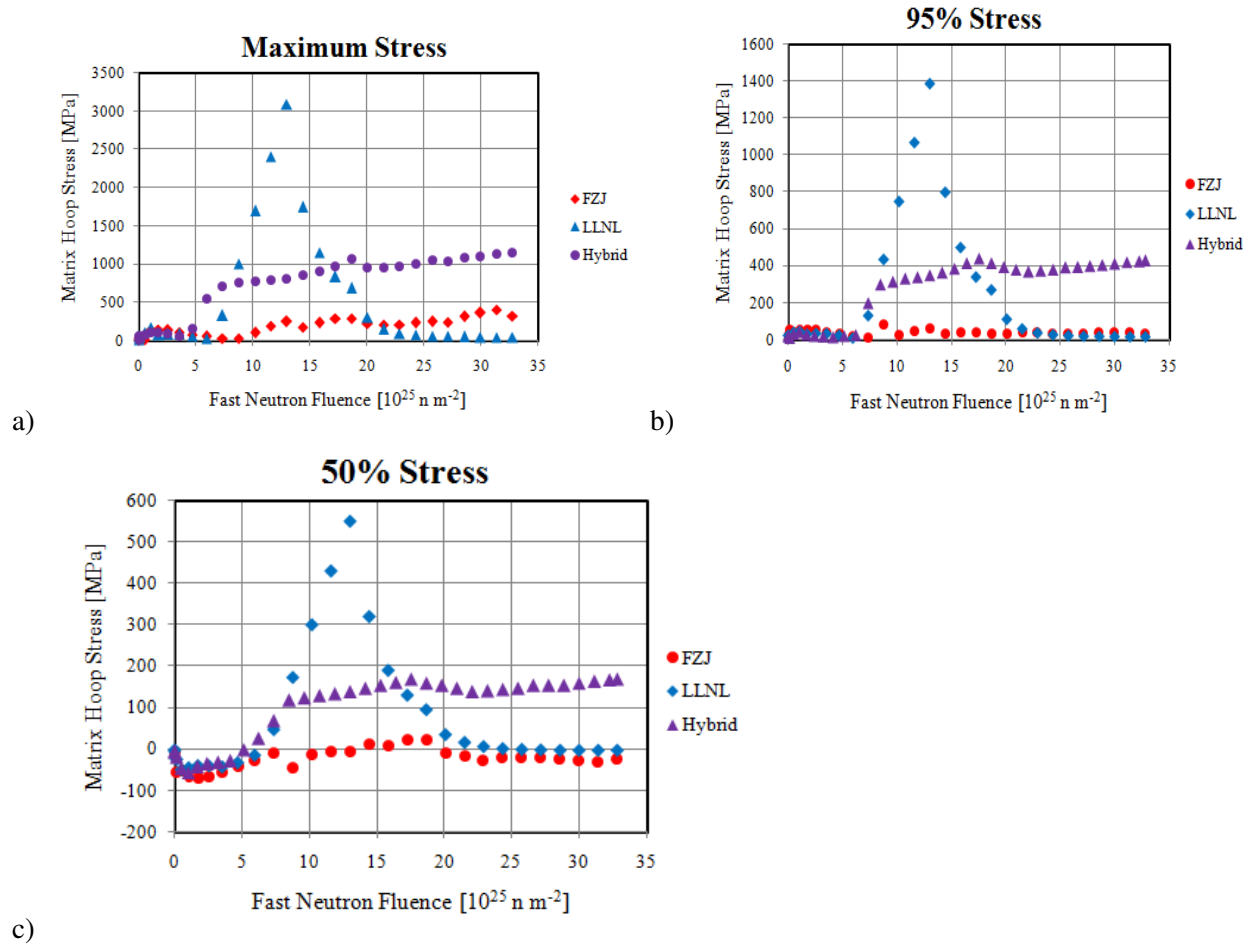


Figure 48. a) The maximum hoop stress induced in the FCM matrix when used in a high temperature low power environment. LLNL correlation predicts volume expansion, FZJ constant volume, and hybrid includes a stress-limited behavior. b) The stress level at which 95% of the matrix elements are at lower stresses. c) The matrix hoop stress level at which 50% of the matrix elements are at lower stresses.

5.3.2 Coolant Temperature

The effect of coolant temperature was considered. A range of coolant temperatures from 300 to 1100 °C were simulated at a linear power of 10 kW m^{-1} . There are three regimes for the SiC swelling: entirely saturated, mixed which is saturated at the perimeter but continuous near the centerline, and entirely

continuous. The following results illustrate the potential effects of all three regimes as shown in Figure 49. For coolant temperatures below about 700 °C and a linear power of 10 kW m⁻¹ the resulting matrix centerline temperature is below the 1000 °C threshold for continuous swelling.

As a result, for coolant temperatures less than 700 °C the stress profile is dominated by the OPyC volumetric behavior. However, at a coolant temperature of 900 °C, the mixed saturated/continuous swelling is predicted. This results in large stresses that linearly increase with fluence. At a coolant temperature of 1100 °C, an entirely continuous swelling condition is predicted and the excessive +5 GPa stresses are not expected. At this high of a coolant temperature, there is very little differential SiC swelling predicted by the model, which assumes temperature independent cavity formation. As a result, it is theoretically possible to operate FCM at very high temperatures according to the model. However as temperature increases, additional buffer volume will be required to accommodate the fission gas and kernel swelling.

In these simulations, the maximum and 95% hoop stresses have the same trends. However, the 50% stress for the 900 °C simulation does not have the characteristic linear increase at high fluence. This is due to the increasing number of elements contained in the compressive interior caused by the high temperature SiC swelling. Since at high fluence about half of the matrix elements are in the compressive region, this produces a compressive average hoop stress despite the large tensile stresses near the perimeter.

The pellet temperature is stable for temperatures below 1000 °C. However, at higher temperatures, the continuous SiC swelling degrades the conductivity of the NITE-SiC matrix and results in higher temperatures. The minimum matrix temperature plot also shows the matrix thermal conductivity is predicted to degrade more at low temperature than at high temperature.

5.3.3 Linear Power

The linear power was varied from 5 to 20 kW m⁻¹ with a coolant temperature of 700 °C. Figure 50 plots the results. The linear power predictions are similar to the coolant temperature simulations. At 10 kW m⁻¹ or less, the resulting matrix centerline temperature is below the 1000 °C continuous swelling threshold. At 15 kW m⁻¹ the very center of the matrix is slightly above the threshold and produces the slow linear increase. However, at 20 kW m⁻¹ the centerline is far above the continuous swelling threshold and extreme maximum stresses are predicted. As before, the maximum and 95% stresses have similar trends. However, the average stresses at 20 kW m⁻¹ become compressive due to the large number of elements contained in the continuously swelling matrix region.

It should also be noted that a linear power of 20 kW m⁻¹ is very high for a HTGR, but this power level was selected to show the potential effects of long term operation at very high powers. Additionally, the maximum gas pressures at end of simulation using the hybrid correlation ranged between 3.9 to 49.3 MPa for the 5 kW m⁻¹ and the 20 kW m⁻¹ respectively. This indicates that the additional fuel volume could be added to the particles, and that it is possible to operate at high powers for long durations without over pressurizing the particles.

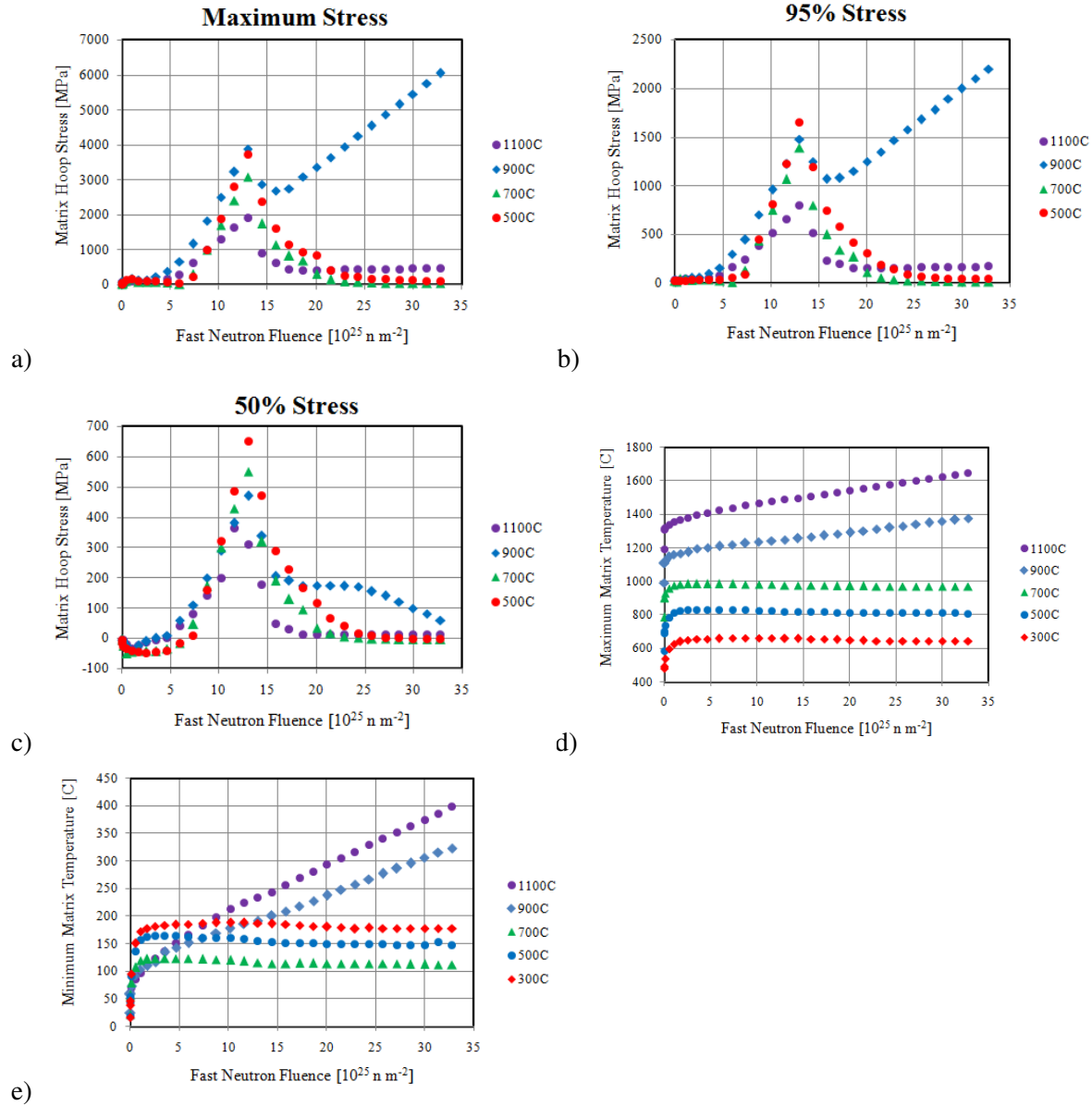
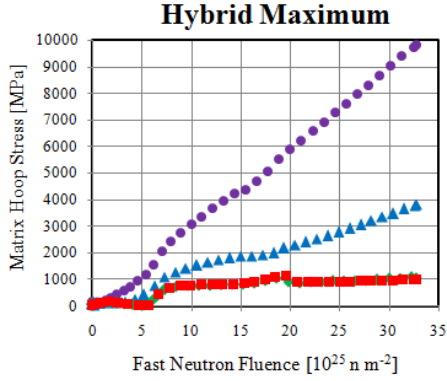
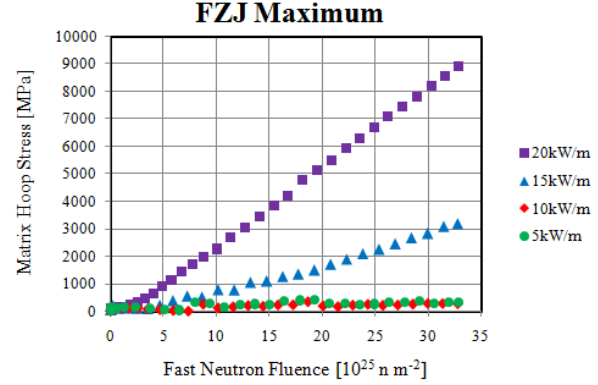


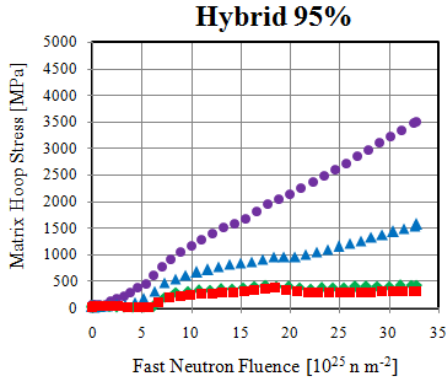
Figure 49. Effects of the coolant temperature on the matrix hoop stress. **a)** Maximum matrix hoop stress. **b)** Stress at which 95% of the matrix elements are less than. **c)** 50% matrix hoop stress level. **d)** Maximum temperature. **e)** Minimum predicted matrix temperature.



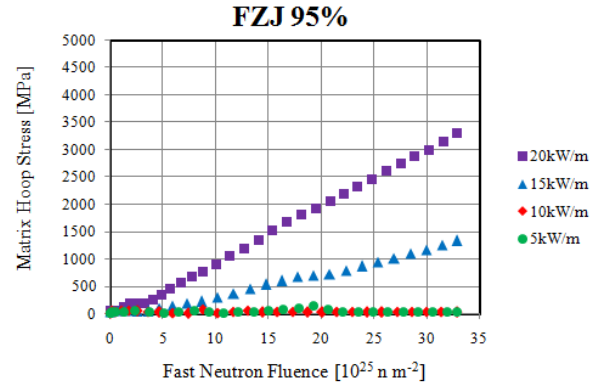
a)



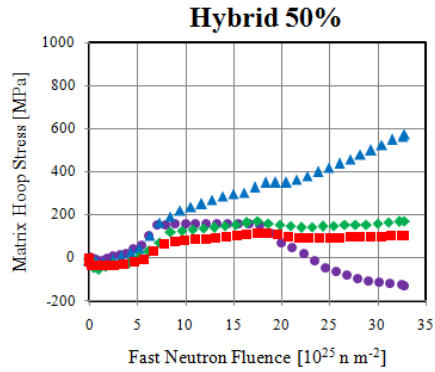
b)



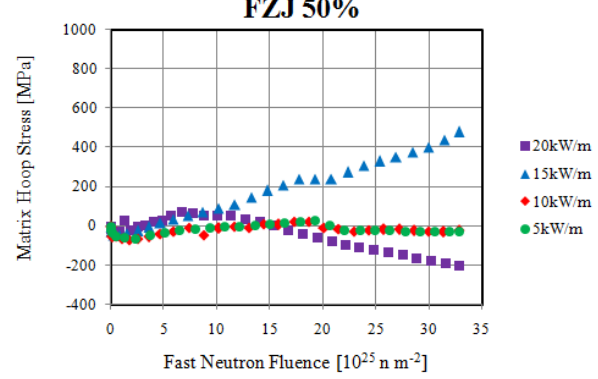
c)



d)



e)



f)

Figure 50. Effect of the linear power variation in a HGTR environment. **a, c, and e)** Maximum, 95%, and 50% matrix hoop stress levels using hybrid dimensional change correlation. **b, d, f)** Maximum, 95%, and 50% matrix hoop stress levels using FZJ dimensional change correlation.

5.3.4 Graphite and NITE-SiC Binder

The potential effects of a graphite or NITE-SiC binder were considered. The binder is the material between the FCM pellets. In traditional designs, graphite has been used, however NITE-SiC has the potential to provide additional resistance against radioactivity release and long range crack propagation from pyrolytic carbon swelling. The use of a NITE-SiC binder also avoids the potential problem of graphite ignition in the event of air ingress into the coolant system. Figure 51 plots the results. The free volume in the vertical direction allows the graphite to expand without causing large stresses in either the binder or FCM pellets, which indicates that the model predicts it to be a viable option.

A pair of simulations was performed using the FZJ constant volume dimensional change correlation. The FZJ correlation predicts larger gaps than the LLNL correlation. When combined with the lower thermal conductivity of the NITE-SiC, the resulting centerline temperature is sufficient to predict a small amount of amount of cavity generation in the matrix and some increasing stress. Figure 51 plots the results for the FZJ simulations.

The NITE-SiC binder does not prevent the large stresses in the matrix from occurring. However, the NITE-SiC binder experiences considerably lower stresses than those predicted in the matrix. As a result, extensive fracture is not expected to occur in the binder unless the FCM pellet has experienced complete failure. The NITE binder provides a very large diffusion distance to inhibit the release of fission products, but the NITE does have a lower thermal conductivity that will somewhat reduce the maximum operating linear power. The conclusion of these simulations is that both graphite and NITE-SiC are possible materials for the binder in HTGR applications.

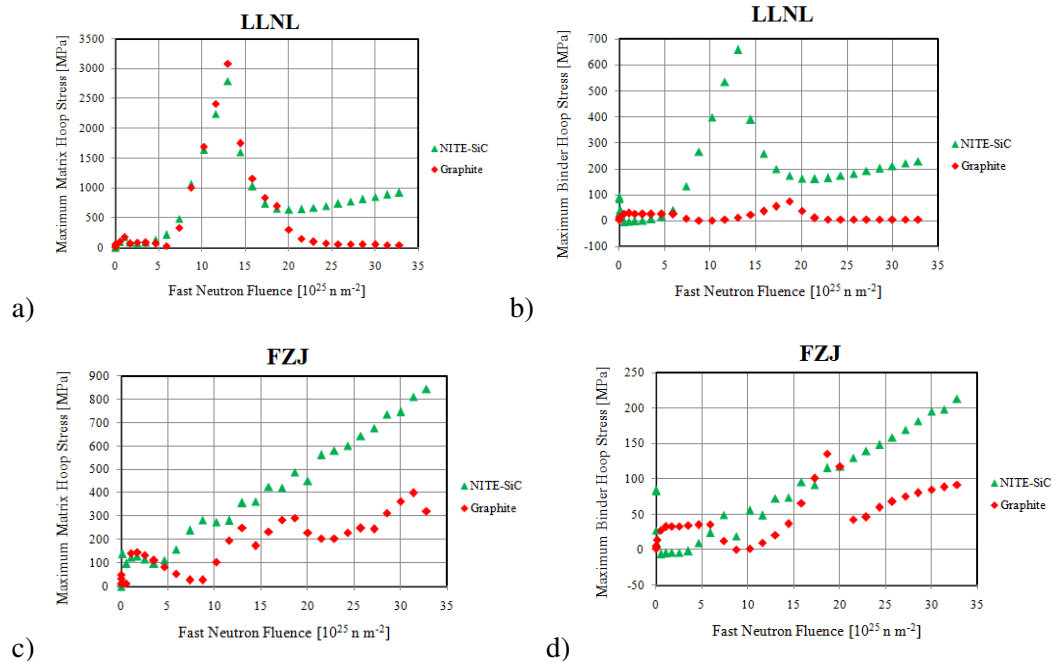


Figure 51. The maximum matrix hoops stress when using a NITE-SiC binder versus a graphite binder. **a and b)** Maximum matrix hoop stress and maximum binder hoop stress for LLNL dimensional change correlation. **c and d)** Maximum matrix hoop stress and maximum binder hoop stress for FZJ dimensional change correlation.

5.4 Summary

In summary, the techniques required to simulate a large collection of particles have been developed. The particles used in a FCM simulation employ a mixed hexahedral, tetrahedral, and pyramid elements. HTGR simulations are possible by simulating a central FCM pellet three 120° sections of coolant channel and homogenous NITE-SiC cylinders. It was found that the model predicts that the FCM fuel form should perform well in the HTGR environment, which is a low power and high temperature condition.

The results of the PyC IIDC variation showed that the volume change of the PyC is the parameter that could potentially generate large stresses in the matrix. It was also predicted that the hydrostatic stress could sufficiently reduce the stress in the event that the PyC experiences a large volume expansion.

The coolant temperature variation showed that the FCM should perform well for coolant temperatures less than about 700 °C and greater than 1100 °C. This is due to the mixed saturated and continuous swelling behaviors of the SiC matrix. It should also be noted that the model assumes temperature independent cavity formation for the SiC at high temperature.

Linear powers of less than about 10 kW m⁻¹ are expected to perform very well. However, higher linear powers of about 15 kW m⁻¹ are likely to produce high stresses from the SiC swelling. It is also expected that both a NITE-SiC and graphite would be suitable materials for the binder between FCM pellets.

CHAPTER 6: FCM SIMULATIONS IN AN LWR ENVIRONMENT

6.1 LWR Simulation Setup

This chapter focuses on simulating FCM pellets in a light water reactor environment. The same methods and models that were used for the HTGR simulations are likewise implemented in these simulations. Figure 52 shows the mesh used for the FCM pellet with the matrix removed for visibility. These simulations were likewise performed on the FALCON cluster at INL. The mesh used for the LWR simulations has 2.3 million degrees of freedom. The DOF allocated for the variables and aux-variables was 9.2 and 115.4 million respectively. In these simulations, 256 processors with 1.9 TB of ram were used and the resulting run time was about one day.

The modeled FCM pellet is 8.2 mm in diameter, 13.5 mm long, and contains 41.5 vol% TRISO particles. However, the dishes and chamfers commonly used in UO_2 pellets were not included in the FCM matrix. The dishes and chamfers can be neglected in this case because the NITE-SiC only swells about 2% under irradiation. The embedded TRISO particles are 1130 μm in diameter with 780 μm diameter kernels. Minimum particle separation was 35.2 μm , minimum radial pellet cover was 31.1 μm , and the minimum axial cover was 36.4 μm and 38.8 μm for the bottom and top surfaces respectively.

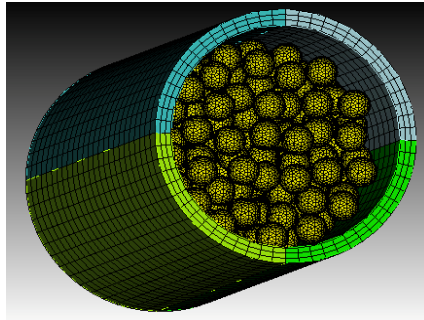


Figure 52. This is a representation of the mesh used for the FCM pellet in a LWR environment.

Table 17 lists the dimensions of the FCM pellet. The previous Table 15 lists the geometry of the embedded TRISO particles used in the simulation. A steady state simulation was run with a power level of 1.2 W per particle that corresponds to an average power of 662 W cm^{-3} averaged over the pellet, and a linear power of 350 W per cm. The coolant temperature was modeled to be 290 °C and 15.5 MPa.

The outer surfaces of the pellet were constrained using a penalty Dirichlet boundary condition. This allows for displacement at the perimeter but provides sufficient constraint so that the simulation is able to converge. The power history was an initial ramp up to full power over 2.78 hours, then remaining at a constant power for 671 days, and reaching an average burnup of about 290 MWd per kg of UN. Figure 53 shows the results of these simulations.

Table 17. The geometry for a RISO-III fuel pellet intended for use in LWRs. Dishes and chamfers were not used in the model. A smear power of 35 kW m⁻¹ or 1.2 W per TRISO particle with a 41.5 vol% packing fraction was used in this model.

Layer	[mm]
Outer clad radius	4.720
Inner clad radius	4.150
Outer fuel pellet radius	4.100
Fuel pellet length	13.50
Gap diametral	0.100

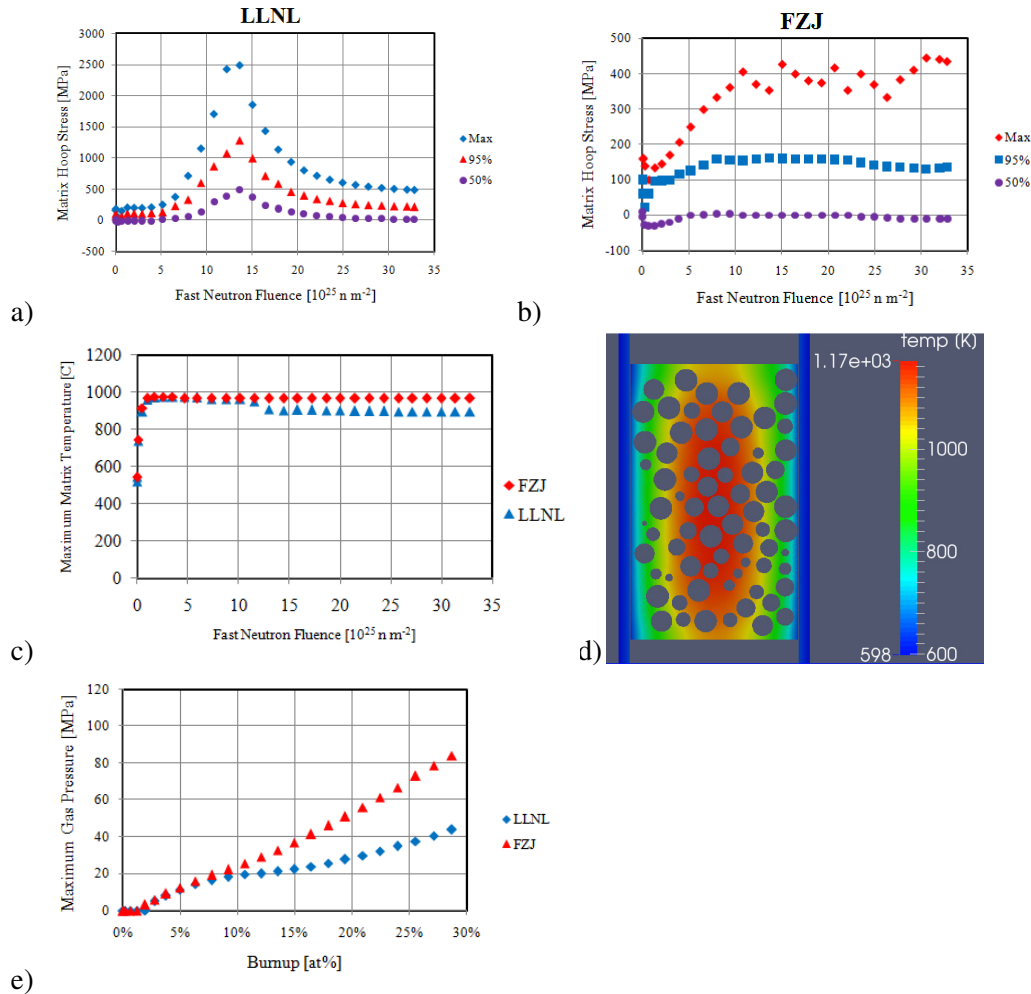


Figure 53. This figure illustrates the effects of constant volume growth versus large volumetric swelling in the PyC irradiation induced dimensional change. **a)** This is a plot comparing the maximum, 95%, and 50% matrix hoop stress levels using LLNL dimensional change correlations. **b)** This plot shows the maximum, 95%, and 50% matrix hoop stress levels using FZJ dimensional change correlation. **c)** This is a plot showing the maximum temperature in the matrix. **d)** This representation shows the temperature profile across the matrix and cladding at 33x10²⁵ n m⁻². The TRISO particles have been removed for visualization purposes. **e)** This figure compares the fission gas pressure for the LLNL and FZJ simulations.

Figure 53a plots the maximum, 95%, and 50% matrix hoop stress. This figure displays the results using the LLNL pyrolytic carbon dimensional change correlations. The global maximum matrix hoop stress will occur where particles are in close proximity to each other or other pellet surfaces and have very limited symmetry.

Figure 53b plots maximum, 95%, and 50% matrix hoop stresses using the German FZJ correlation. The primary difference is in the base assumptions of constant volume dimensional change for the FZJ and volumetric swelling in the LLNL correlations. Using the LLNL correlation results in the large stress increase at a fluence of about $13 \times 10^{25} \text{ n m}^{-2}$ due to a modeled PyC volume increase. The FZJ correlation results in partial interface contact, which produces scatter in the maximum matrix, hoop stresses. It is also important to note that for both the LLNL and FZJ simulations the maximum matrix hoop stresses are considerably larger than the 95% hoop stresses. This indicates that the maximum stresses are occurring in a few elements and that very large maximum stresses will be experienced before long range cracking occurs in the matrix.

Figure 53c compares the maximum temperature in the matrix between the LLNL and FZJ correlations. When using the LLNL dimensional change the buffer/IPyC gaps were predicted to close at a fluence of about $11\text{-}14 \times 10^{25} \text{ n m}^{-2}$. As a result, the maximum temperature decreased. Figure 53d shows a representation of the temperature profile across the matrix and cladding. A considerable amount of heat passes through additional particles on its way to the matrix surface. As a result, the thermal resistance caused by interface gaps has an impact on the temperature of the matrix and interior particles. This is an additional reason for homogenous particles being insufficient for use in FCM fuel performance modeling.

Figure 53e plots the global maximum fission gas pressure as a function of burnup. Initially the temperatures for the FZJ and LLNL pellets are almost identical at low burnup, and as a result so are the fission gas pressures. However, the different gas pressure trend occurs once the buffer/IPyC gaps close in the pellet using the LLNL dimensional change correlation and the temperature decreases.

Figure 54 shows vertical slices of the hoop stress through the pellet at 0.02 , 3.5 , 13.0 , and $33 \times 10^{25} \text{ n m}^{-2}$ respectively. Early in life, the matrix stresses are dominated by the differential thermal expansion of the NITE-SiC matrix. This produces a stress state that is tensile in the perimeter and compressive in the interior. At a fluence of about $1 \times 10^{25} \text{ n m}^{-2}$ the matrix stress is dominated by the matrix swelling gradient. This produces a stress state that is compressive at the perimeter and tensile in the interior. This is due to the fact that SiC swells more at low than high temperature. At $13.1 \times 10^{25} \text{ n m}^{-2}$ the LLNL IIDC correlation predicts very large volumetric swelling. This large volume expansion in combination with the geometry produces the profile seen in Figure 54c. After the IIDC has saturated, the 0.4 Poisson ratio in creep allows the OPyC to reduce its volume and relax the PyC swelling stresses. In Figure 54d, the stress state is now dominated by the saturated perimeter, kernel swelling, and gas pressure.

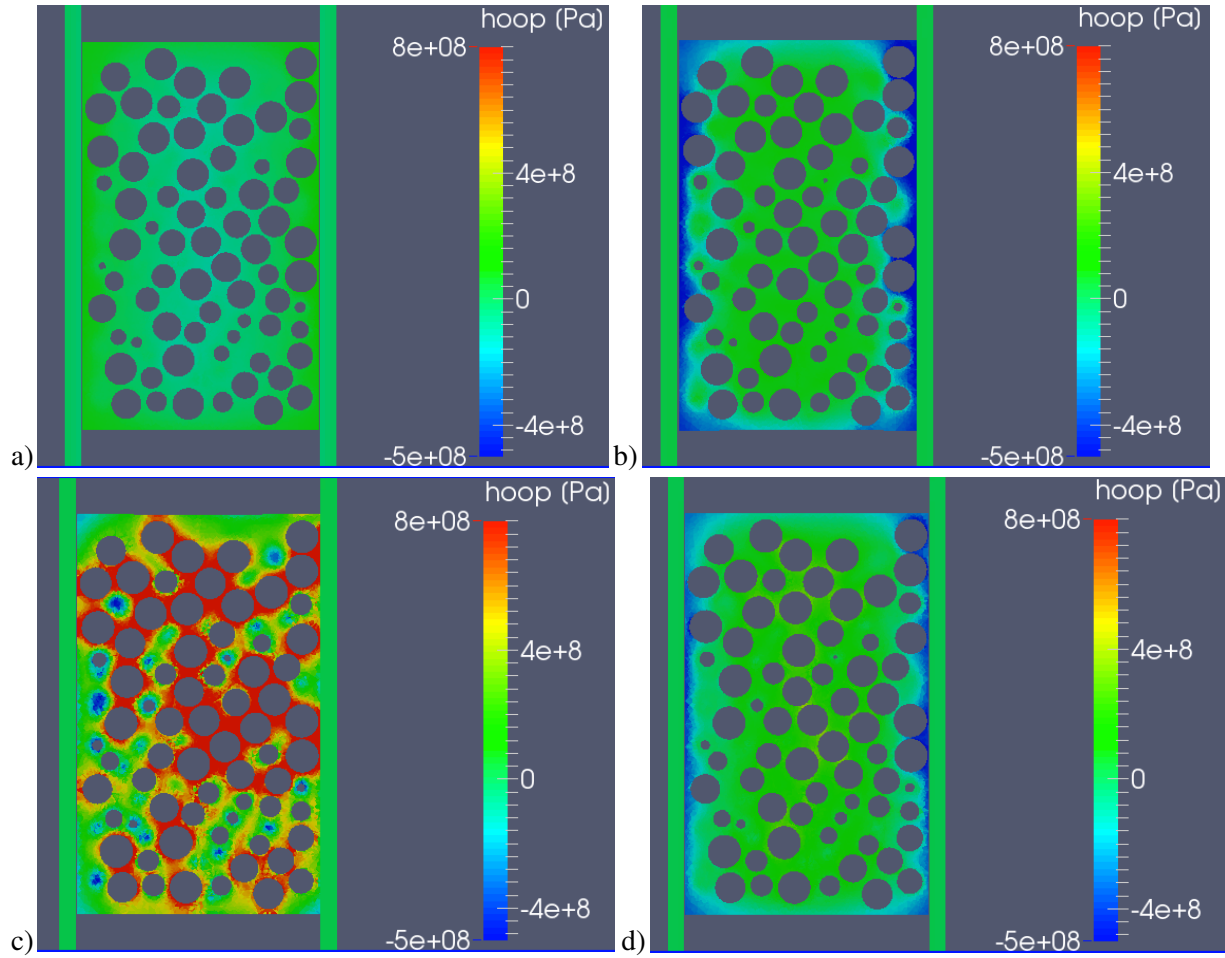


Figure 54. A vertical slice through the centerline of the pellet with the particles removed. The color scale shows the magnitude of the hoop stress. Tension is positive while compression is negative. **a)** The hoop stress profile at a fluence of $0.02 \times 10^{25} \text{ n m}^{-2}$. **b)** The hoop stress profile at a neutron fluence of $3.2 \times 10^{25} \text{ n m}^{-2}$. **c)** The hoop stress profile at a neutron fluence of $13.1 \times 10^{25} \text{ n m}^{-2}$. **d)** The hoop stress profile at a neutron fluence of $33 \times 10^{25} \text{ n m}^{-2}$.

An additional simulation was performed to examine and compare the potential effect of hydrostatic stress on the PyC dimensional change and the resulting stresses in the matrix. The dimensional change was modeled with a linear dependence on hydrostatic stress. Additionally the effect of hydrostatic stress was modeled as being capable of accelerating or inhibiting the dimensional change depending on the direction of the hydrostatic stress and volumetric change. Figure 55 shows the effects of using a stress limited PyC IIDC. In the simulation, an elemental hydrostatic stress value of 50 MPa was considered a sufficient stress to prevent further volumetric increase in that element. The limiting of the IIDC prevented the characteristic peak in matrix hoop stress and maintained the compressive perimeter and tensile interior as shown in Figure 55c. Figure 55e and f show that the predicted matrix hoop stresses can be significantly reduced when a stress limiting term is used for the PyC IIDC. It also shows the 95% stress when using a stress limited behavior remains about half of the maximum stress. This produces a lower probability of nucleating and propagating cracks through the matrix.

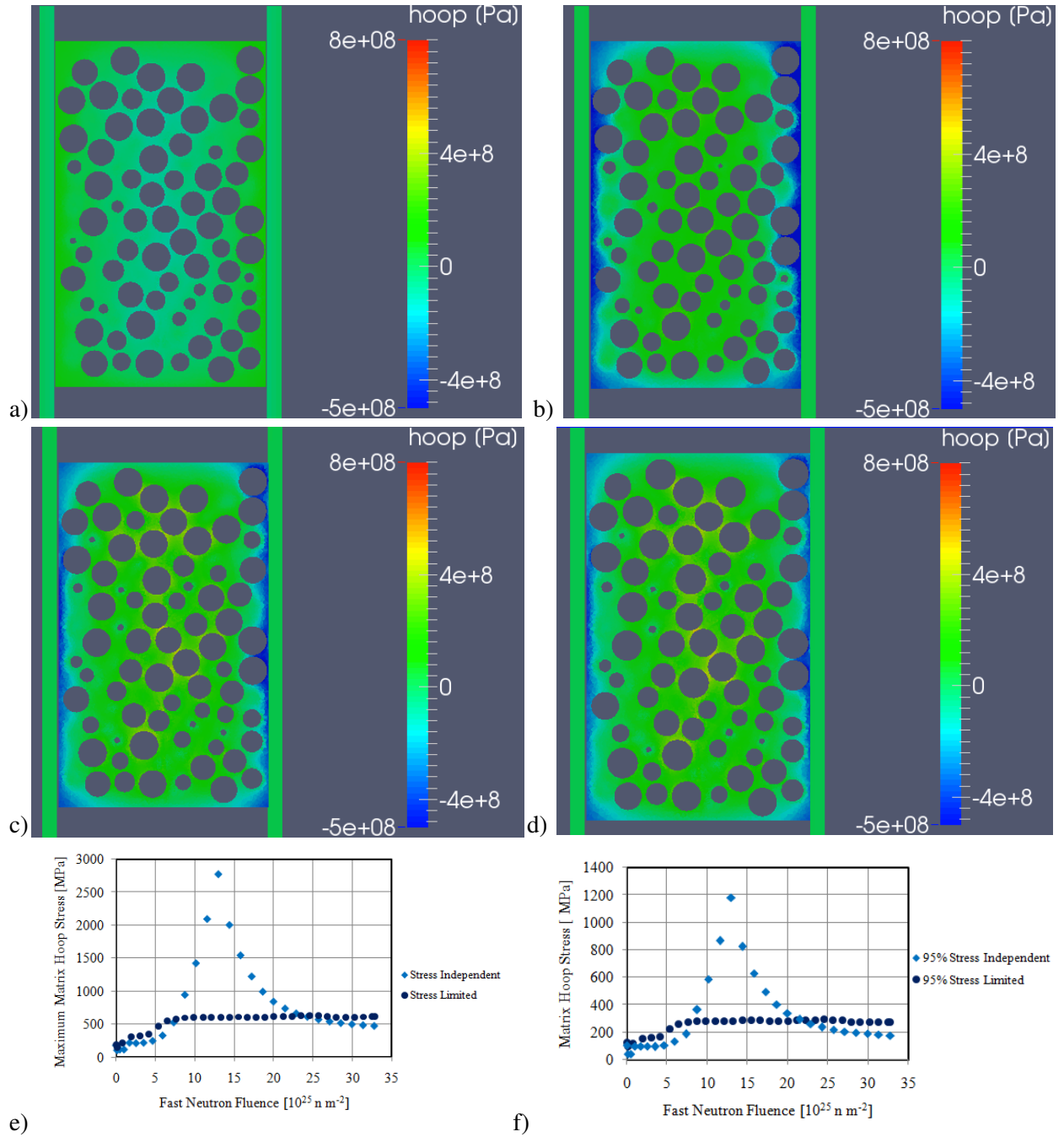


Figure 55. A vertical slice through the centerline of the pellet with the particles removed. The color scale shows the magnitude of the hoop stress. **a)** The hoop stress profile at a fluence of $0.02 \times 10^{25} \text{ n m}^{-2}$. **b)** The hoop stress profile at a neutron fluence of $3.2 \times 10^{25} \text{ n m}^{-2}$. **c)** The hoop stress profile at a neutron fluence of $13.1 \times 10^{25} \text{ n m}^{-2}$. **d)** The hoop stress profile at a neutron fluence of $33 \times 10^{25} \text{ n m}^{-2}$. **e)** Plot comparing the global maximum hoop stress in the matrix for stress independent and stress limited IIDC. **f)** A plot of the 95% hoop stress which refers to the level that 95% of the matrix elements are less than.

Due to each element being assigned a random value for the fracture threshold criterion, it was necessary to consider the uncertainty from using this method. It proved difficult to establish random seed that would provide a unique distribution for each simulation. As a result, four simulations were conducted that called the threshold distribution function different number of times. This was successful in generating four unique distributions to provide a comparison of the results. The FZJ dimensional change correlations were selected for these FCM simulations due to the predictions of partial debonding and re-contact. The remaining parameters are the same as the previous LWR FCM simulations, which include 8.2 mm diameter by 13.5 mm long pellet operating at 35 kW m^{-1} . Figure 56 shows the results. The different distributions do have an impact on the maximum matrix hoop stress. However, the trends are the same and the values are similar with the characteristic scatter for fluences above $10 \times 10^{25} \text{ n m}^{-2}$. This gives confidence to continue moving forward with the FCM model.

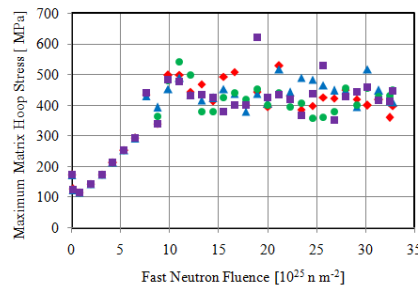


Figure 56. A comparison of the maximum matrix hoop stress using four different distributions for the debonding threshold values. The results show differences but the same general trends.

6.2 FCM Pellet Radial Power and Fast Neutron Flux Distribution

A radial power distribution was included to examine its impact on the thermo-mechanical response of the FCM pellets. Additionally, a reciprocal fast neutron flux profile was also included. A factor of two variation from min to max was used for these simulations following a simple R squared profile as shown in Figure 57.

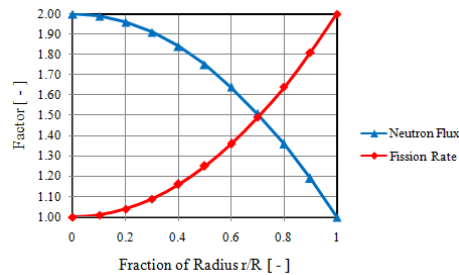


Figure 57. Radial power and fast neutron flux profiles across the FCM pellet. Spherical power profile within the kernels was not considered.

A FCM pellet simulation was performed to examine the effects. The average linear power remained 35 kW m^{-1} and the maximum fast neutron fluence of $43.7 \times 10^{25} \text{ n m}^{-2}$ was obtained at the end of the

simulation. The FZJ correlation was used for the PyC dimensional change with constant volume Poisson ratio in creep. The predicted centerline temperature was somewhat lower. However, the initial thermal stresses near the perimeter of the pellet were considerably higher despite the reduced thermal gradient across the pellet. This is most likely due to the higher thermal expansion coefficient for the PyC than the NITE-SiC near the perimeter of the pellet. The thermal expansion coefficients were 5.6 and $4.5 \times 10^{-6} \text{ K}^{-1}$ for the PyC and SiC respectively. The stresses at fluences above about $1 \times 10^{25} \text{ n m}^{-2}$ were very similar to those predicted by the uniform power distributions. The temperature and stress profiles were nearly identical at high fluences. This indicates that FCM should perform well with wide range of radial power profiles. Figure 58 shows the results.

6.3 LWR Parameter Variations

6.3.1 Irradiation Induced Dimensional Change

The irradiation induced dimensional change of the pyrolytic carbon has the potential to cause significant stresses in the matrix. This assumes that the PyC elastic properties do not deteriorate under volumetric expansion, and hydrostatic stress does not effectively limit the volumetric swelling in these applications. The Lawrence Livermore dimensional change correlation predicts an initial shrinkage followed by radial and tangential swelling. The German FZJ correlation predicts initial shrinkage followed by radial expansion and tangential shrinkage such that volume remains approximately constant. Modifications to these correlations include the swelling rate for LLNL and net volumetric expansion for the FZJ while maintaining radial expansion and tangential shrinkage [67,30]. Figure 59 plots the results.

Reducing the swelling rate in the LLNL correlation lowers the maximum stress but does not prevent high stresses from occurring. This result assumes a Poisson ratio in creep of 0.4. If volume is conserved in creep (Poisson ratio of 0.5) then the PyC volume swelling rate does not affect the maximum stress. This is due to a lack of other mechanisms in the model, which can reduce the volume increase other than elastic strain.

The effect of using the LLNL correlation with a stress limited term and sensitivity to stress of 160 MPa was considered. For this simulation, the 30% volume cap was disabled. Additionally, the LLNL swelling rate was varied from 1.0-0.1x as in the previous simulation. The results show that the saturation stress level remained approximately constant, but the fluence required to saturate increased.

The FZJ correlation predicts maximum stresses of about 500 MPa. While the FZJ with a reduced tangential shrinkage predicts very high stresses due to the volume increase. This illustrates the importance of the volume increase instead of the individual radial and tangential components. Due to the high creep rate, it is possible for PyC to experience large radial and tangential strains without generating large stresses provided the volume change is less than a few percent.

Another simulation was performed to compare the predicted matrix hoop stresses using the LLNL, FZJ, and hybrid correlations. The hybrid correlation predicts a saturation stress of about 1000 MPa, which falls between the predictions of the LLNL and FZJ correlations.

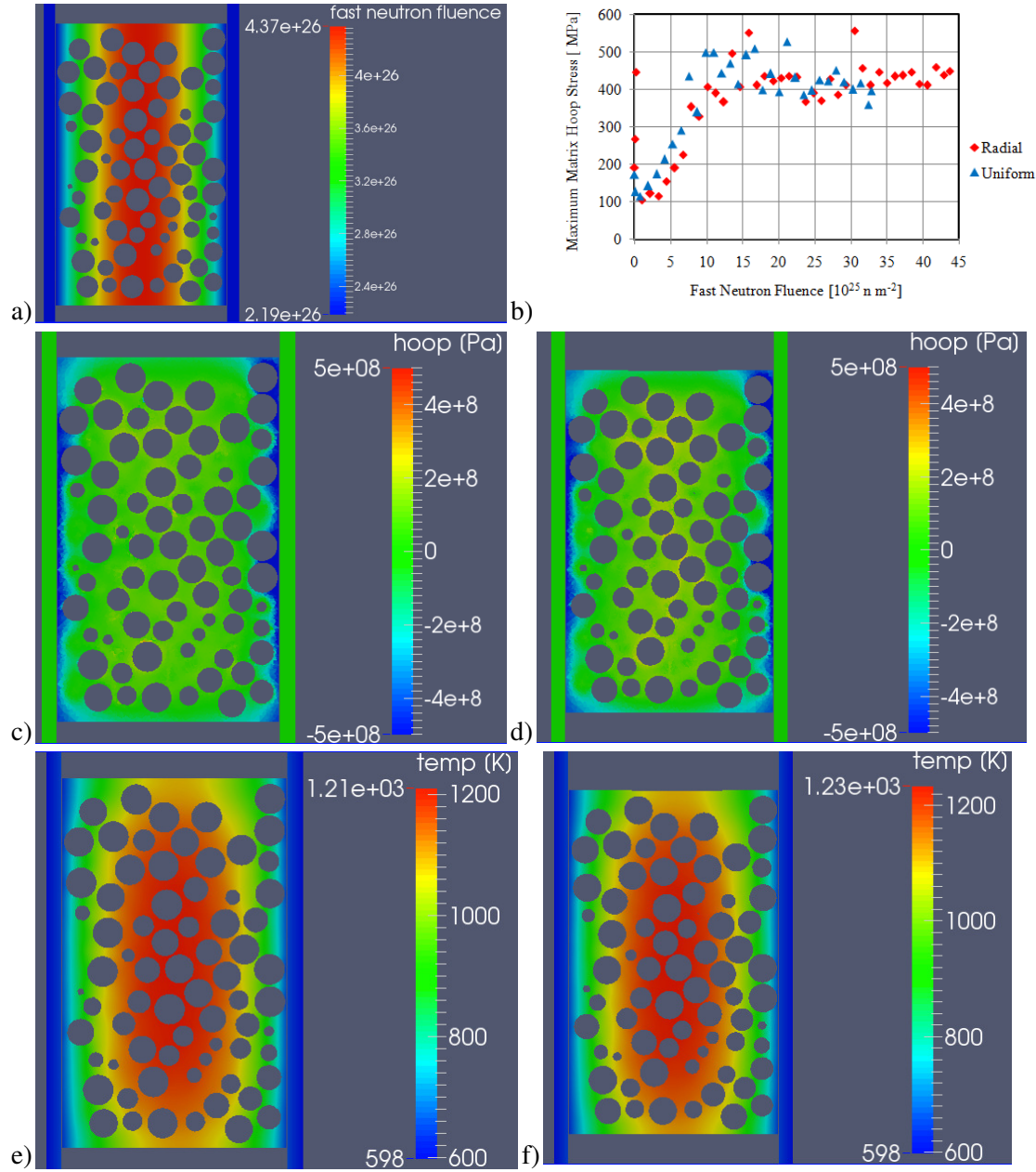


Figure 58. Comparison of the radial power and fast neutron flux profiles with uniform distributions. A factor of two variation was used. **a)** Fast neutron flux profile used in the radial distribution. **b)** Plot of the global maximum hoop stress in the matrix. **c)** Hoop stress profile for the radial distribution at end of simulation $43.7 \times 10^{25} \text{ n m}^{-2}$ **d)** Hoop stress profile for the uniform distribution at end of simulation $33 \times 10^{25} \text{ n m}^{-2}$ **e)** Temperature profile for the radial distribution at $43.7 \times 10^{25} \text{ n m}^{-2}$. **f)** Temperature profile for the uniform distribution at $33 \times 10^{25} \text{ n m}^{-2}$.

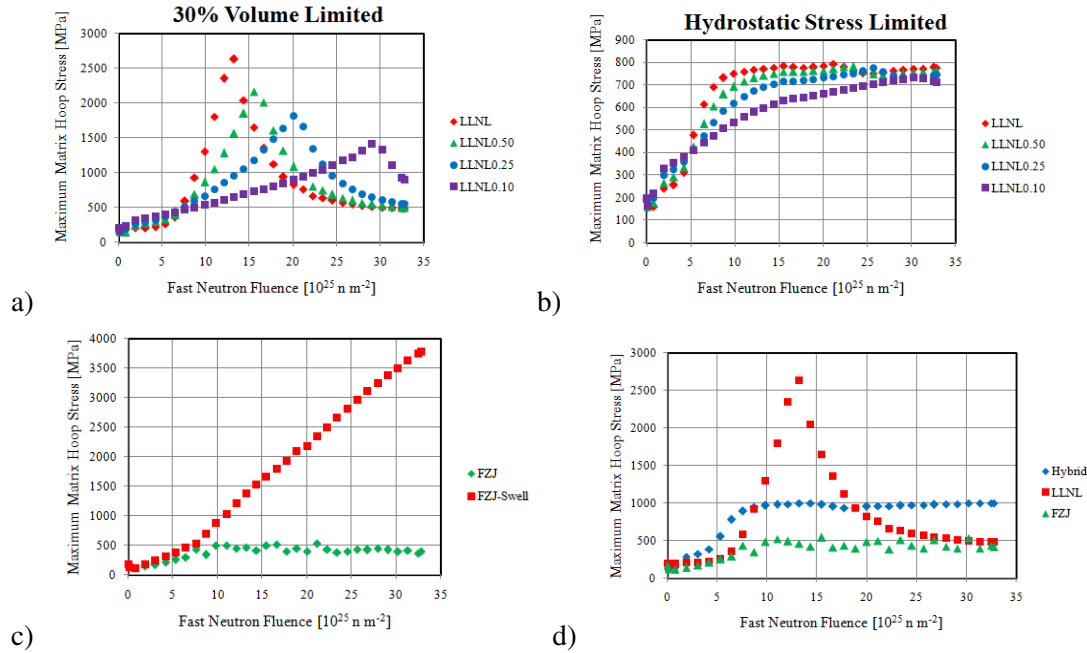


Figure 59. Plots of the predicted maximum hoop stress in the matrix for various dimensional change relationships. **a)** Plot of the maximum hoop stress using the LLNL correlation with reduced swelling rates of 0.5x, 0.25x, and 0.1x. **b)** Plot showing the minimal effect of swelling rate when hydrostatic stress is active. **c)** Plot of the maximum matrix hoop stress using the FZJ correlation and the FZJ with a reduced tangential shrinkage rate. **d)** Plot comparing the LLNL, FZJ, and hybrid correlations.

6.3.2 Pyrolytic Carbon Creep

A set of simulations was also performed to examine the potential effect of pyrolytic carbon creep. The creep rate and Poisson ratio in creep were the two parameters of interest, and Figure 60 plots the results. The CEGA correlation with a 2x multiplier was used as a base configuration [38,67].

The predictions are that a higher creep rate will produce a lower maximum stress and that the stresses will relax sooner. The Poisson ratio in creep can also have a substantial impact on the stresses in the matrix if the PyC is fully constrained. The OPyC has the NITE-SiC matrix on the outside and the CVD-SiC layer on the inside. The result is that the OPyC does not have any free volume to move into like the IPyC layer. The methods included in the model for a material to reduce its volume are creep and elastic deformation. If a Poisson ratio in creep of 0.5 is used then volume is conserved in creep and thus the volume expansion must be compressed elastically. This induces large stresses that remain even after swelling has been capped at 30% by volume. After the swelling has been capped, creep continues until the stress is uniform in all principal axes and then ceases. However, a Poisson ratio in creep of 0.4 allows the OPyC to reduce its volume and thereby the resulting stress. It is important to note that this behavior and the importance of the Poisson ratio in creep are only for the case of fully constrained PyC. It must be noted that in the case of a partially constrained PyC, such as the IPyC layer, the effect of the Poisson ratio in creep is expected to be almost unnoticeable due to the additional volume provided by the buffer and high pyrolytic carbon creep rate. As a result, an experiment aimed at determining an effective Poisson ratio in creep for PyC must consider a fully constrained geometry as a partially constrained sample would almost certainly produce inconclusive results.

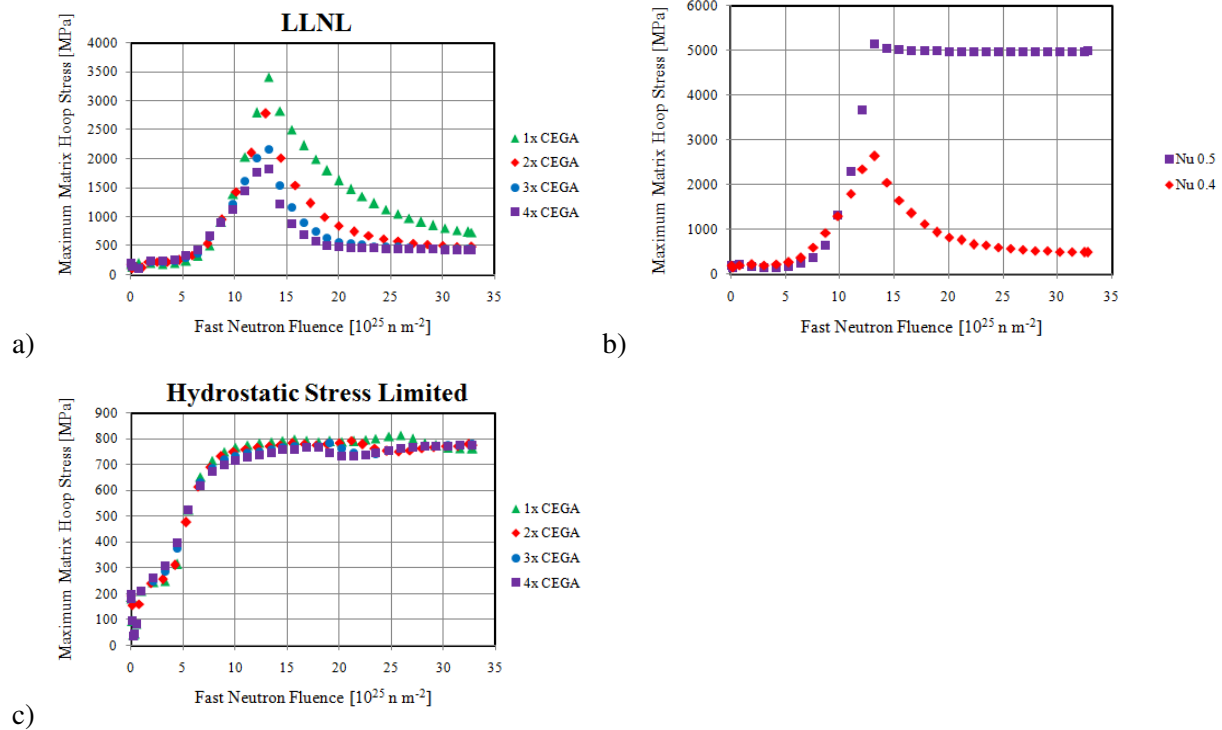


Figure 60. Plots comparing the effects from PyC creep rate and Poisson ratio in creep. **a)** Plot of the maximum matrix hoop stress using creep rates ranging from 1x to 4x the recommended CEGA correlation. The normal value used in other simulations 2x CEGA. **b)** Plot of effect of Poisson ratio in creep. **c)** Effect of creep rate when hydrostatic stress limited dimensional change is used.

The effect of creep rate when stress limited dimensional change is included was considered. A stress sensitivity of 160 MPa threshold with linear stress dependence was used. The results show that the creep rate has minimal influence over the hoop stress when stress limited dimensional change is included.

6.3.3 Hydrostatic Stress Limited Dimensional Change

The effect of hydrostatic stress was considered. In theory, the hydrostatic stress term provides an additional resistance to the formation of defects. In experiments, this component has proven much harder to evaluate. There is a paper by Bates et al. on the effects of hydrostatic stress in the zircaloy [48]. The recommended effect on the dimensional change is a linear reduction in the volume behavior with increasing compressive hydrostatic stress. However, the data points were sufficiently sparse that the following simulations are purely speculative. Figure 61 plots the results using a linear dependence.

As expected, a higher stress threshold allows larger stresses in the matrix. However, the general pattern of increase and plateau are consistently predicted. It is interesting to note that the 50 MPa threshold produces a similar trend compared to the FZJ constant volume dimensional change correlation. The 95% and 50% stresses are expected to have the same trends as the maximum stresses but with considerably lower values.

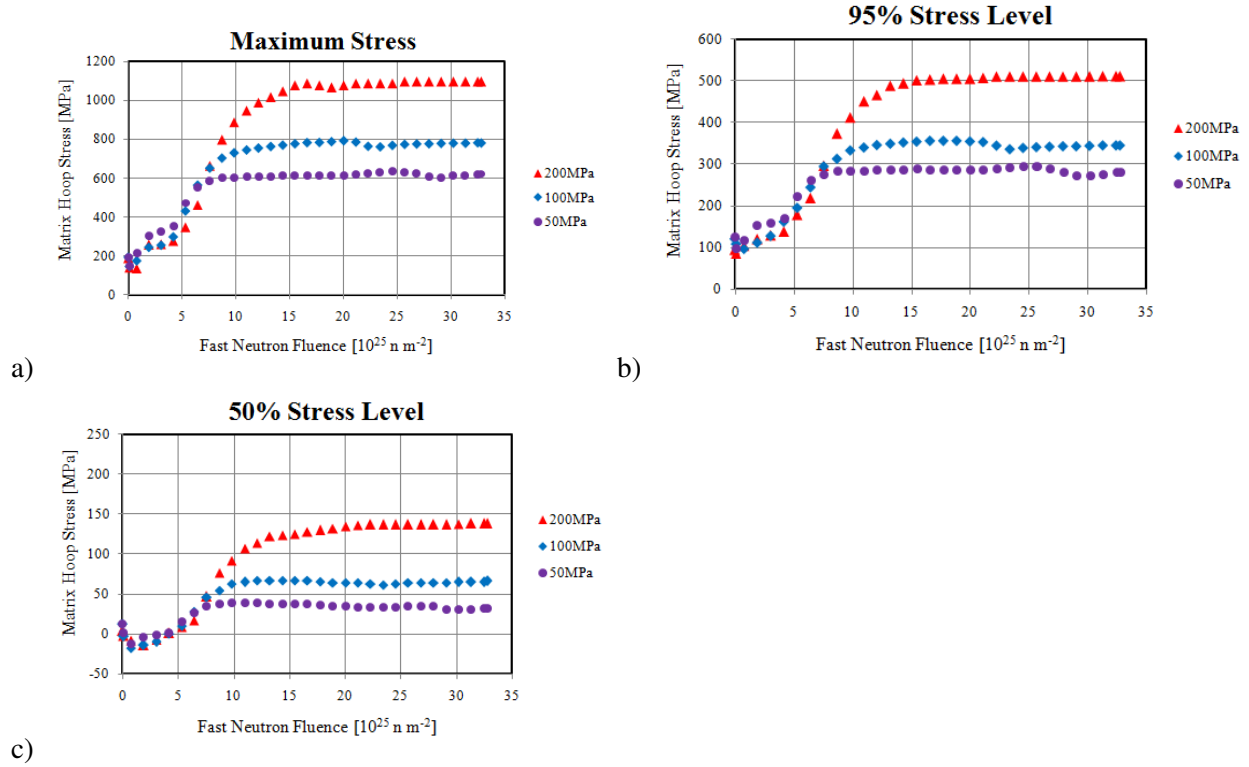


Figure 61. The effects from hydrostatic stress limited dimensional change on maximum matrix hoop stress as a function of neutron fluence. The threshold which was considered sufficient to prevent any additional volume increase was varied from 50 to 200 MPa. **a)** Maximum elemental matrix hoop stress. **b)** 95% matrix hoop stress level. **c)** 50% matrix hoop stress level.

6.3.4 Linear Power

The effect of linear power is important since it has significant performance implications. In addition to the PyC volume change, the SiC swelling in the matrix can have a significant effect due to the temperature gradient. Below 1000 °C, the SiC swelling is modeled as saturating at about $1 \times 10^{25} \text{ n m}^{-2}$ which is desirable for reactor operations. However, there is a predicted change to cavity generation that is expected to occur between 1000 and 1250 °C. The cavity generation is modeled as temperature independent. In the model, the transition from saturated to continuous swelling begins at 1000 °C and is completed at 1250 °C. The result is three regimes. When the centerline temperature is less than 1000 °C the SiC is operating entirely with saturated swelling. This produces a very stable swelling behavior, and since SiC swells more at low temperature than at 1000 °C the perimeter has compressive stresses while the interior is tensile. The second regime is when the centerline temperature is above 1000 °C but the perimeter is below 1000 °C. This produces mixed saturated and continuous swelling regions in the matrix and eventually leads to high tensile stresses once the interior has swelled more than the perimeter. The third case is operating completely above 1250 °C. Assuming the cavity generation is temperature independent, this would allow for high temperature operations without inducing very large stresses from differential swelling at high fluences.

Figure 62 plots the results of varying the linear power from 15 to 55 kW m^{-1} . For linear powers less than about 40 kW m^{-1} , the continuous swelling of the SiC is not expected to occur. The predicted gas pressures

were less than 40 MPa despite the very high burnup of 30 at%. As a result, gas pressure is not expected to be the primary limiting criterion for FCM in light water reactor applications. At 45 kW m⁻¹ there is a prediction of some high temperature SiC swelling that produces a slow linear increase in matrix hoop stress. However, at 55 kW m⁻¹ the region of continuous SiC swelling is larger and the matrix hoop stress increases more quickly. In this simulation at 55 kW m⁻¹ the continuously swelling region of the matrix did not include more than half of the elements in the matrix. Thus, the 50% stress trend follows the maximum and 95% stress behaviors. The maximum temperature increase at a reasonably consistent 100 °C for every 5 kW m⁻¹ increase in linear power.

It should also be noted that long term operation at 35 kW m⁻¹ is an extreme condition. However, it is necessary to simulate extreme conditions for further understanding of the potential behavior and failure methods of TRISO based FCM. This strongly suggests the FCM fuel form is robust and durable design.

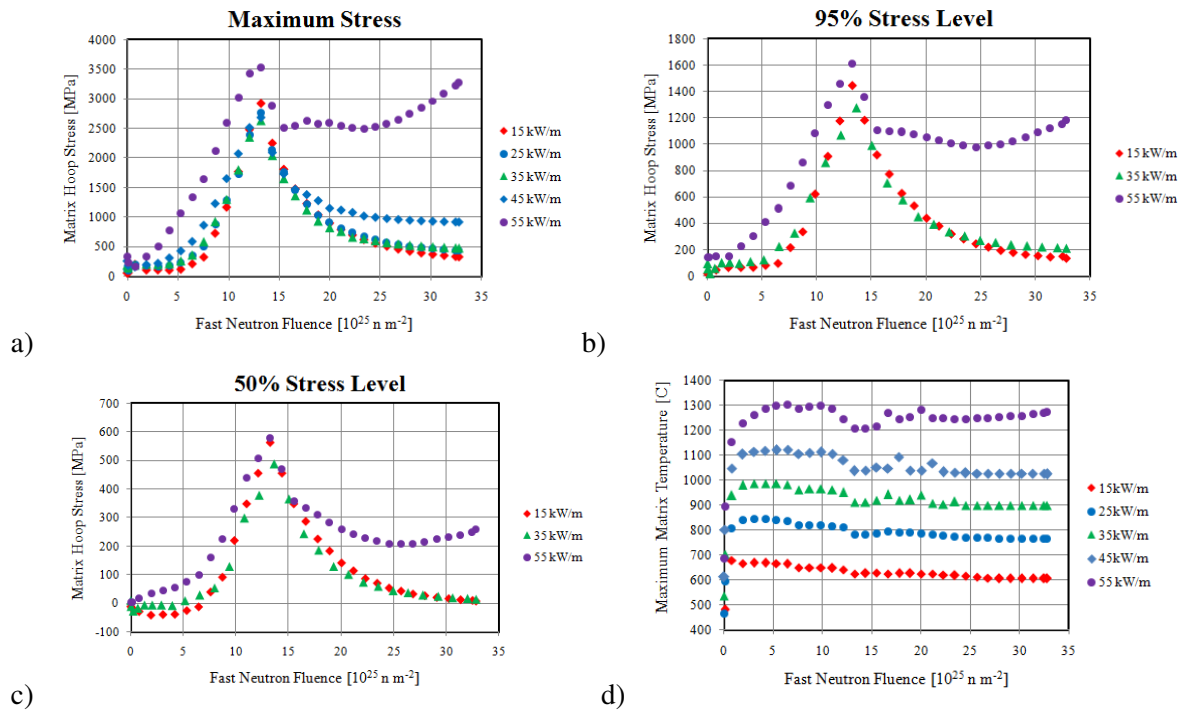


Figure 62. Plots of the effects from linear power varied from 15 to 55 kW m⁻¹. **a)** Maximum matrix hoop stress. **b)** 95% matrix hoop stress level. **c)** 50% matrix hoop stress level. **d)** The maximum temperature.

The effect of stress limited dimensional change was also considered when using the FZJ and Hybrid correlations. The linear power was varied from 55 to 15 kW m⁻¹. Figure 63 plots the FZJ results. When using the FZJ correlation for PyC dimensional change, the results for linear powers from 15 to 35 kW m⁻¹ were reasonably low stresses and temperatures as expected. Centerline temperature and gas pressure increased somewhat with linear power, but hoop stress was mostly unaffected. However, at 45 and 55 kW m⁻¹ the kernel swelling was sufficient to cause re-contact at the Buffer/IPyC interface for a large majority of the particles. This leads to a reduction in temperature that reduced the continuous swelling of the matrix. Also, the boundary between saturated and continuous swelling in the matrix moved closer to the centerline. This produced a reduction in rate of stress increase for the 55 kW m⁻¹ case and a net reduction in matrix hoop stress for the 45 kW m⁻¹ simulation.

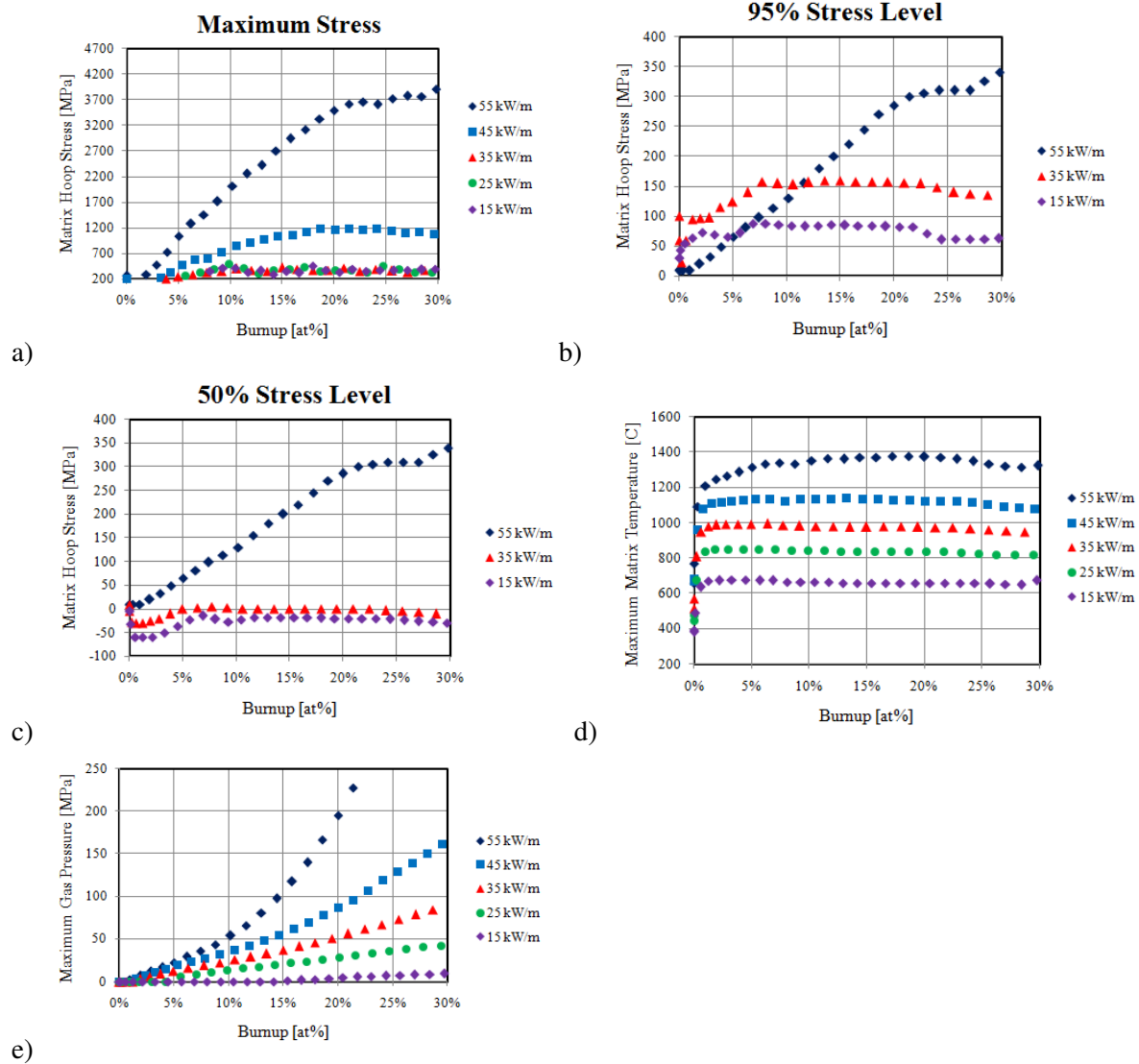


Figure 63. The effect of linear power using the constant volume FZJ dimensional change correlation. **a)** Global maximum matrix hoop stress. **b)** Stress level at which 95% of the matrix elements are less than. **c)** Stress level at which 50% of the matrix elements are less than. **d)** Maximum temperature in the matrix. **e)** Maximum gas pressure for a particle near the centerline of the pellet.

The same linear power variation was performed using the Hybrid correlation and Figure 64 plots the results. The Hybrid correlation predicts a volume expansion that is limited by hydrostatic stress. The result that the gaps are predicted to close and this reduces the temperatures and gas pressures compared to the FZJ simulations. The volume expansion does generate a maximum matrix hoop stress of about 1 GPa. However, it is expected to require about 1.5 GPa to generate long range cracking the in matrix. The predicted gas pressures are reasonably low for linear powers less than 35 kW m^{-1} , but increase rapidly with temperature.

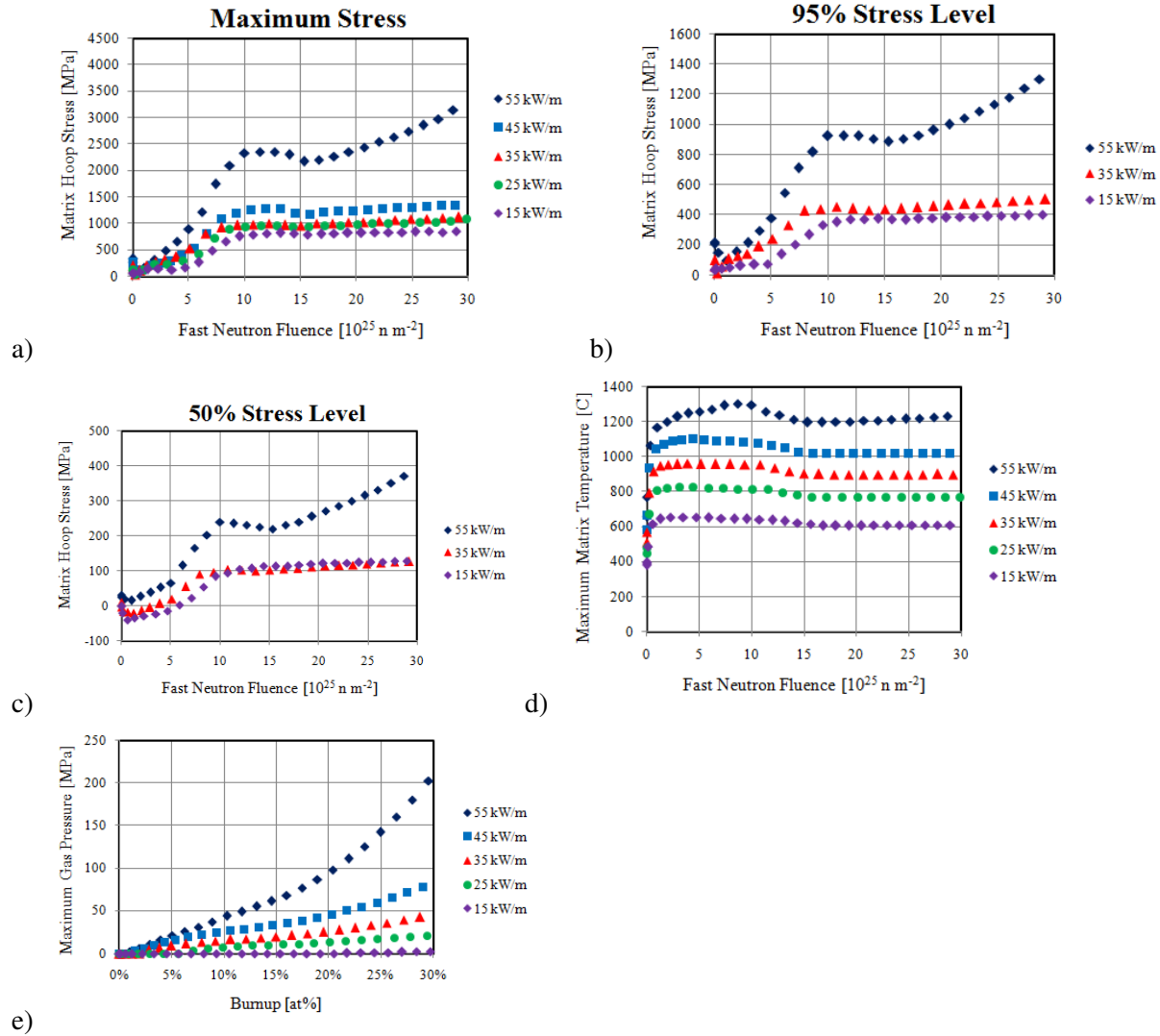


Figure 64. The effect of using the hybrid dimensional change correlation that assumes volume expansion with a stress limited behavior. **a)** Maximum elemental hoop stress in the matrix. **b)** 95% matrix hoop stress level. **c)** 50% matrix hoop stress level. **d)** Maximum temperature in the matrix **e)** Maximum gas pressure in a particle near the centerline.

6.3.5 TRISO Particle Geometry

The effects of the TRISO geometry were considered, and the minimum particle spacing and OPyC layer thickness were varied. The particle diameter was 1130 μm , and the results are shown in Figure 65. The minimum particle spacing was varied from 20 to 50 μm , which produced TRISO packing fractions from 41.75 to 33.5 vol%. The model predicted a minor change in maximum matrix hoop stress when the particle spacing was varied. Previous simulations comparing the effects of particle spacing predicted about a factor of three reduction in stress for a factor of eight increase in spacing. A reduction of only 12% in stress from PyC swelling suggests an emphasis on the particle packing fraction rather than the minimum particle spacing. Since TRISO particles have the disadvantage of a low uranium content, this parameter is not a practical means to control the matrix stresses.

The OPyC layer thickness was then varied from 10 to 50 μm and was predicted to have a large effect on the matrix stresses. A factor of five reduction in OPyC thickness is predicted to be able to reduce the matrix hoop stress from PyC swelling by about a factor of 3.7. This ability to reduce the stress is due to a thinner OPyC causing less displacement for the NITE-SiC matrix to constrain. The results also show that the ability of the creep to relax the stress is proportional to the layer thickness. The creep rate is proportional to the difference in principal stresses, and as the layer thickness decreases, the differences become smaller. The results are shown in Figure 65.

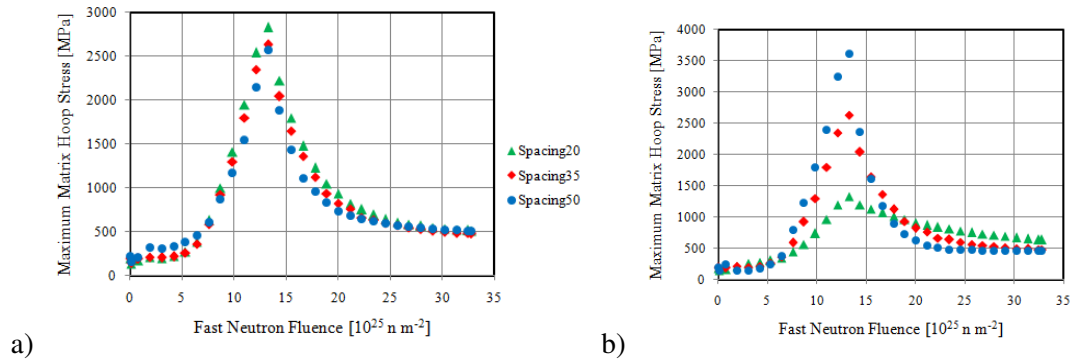


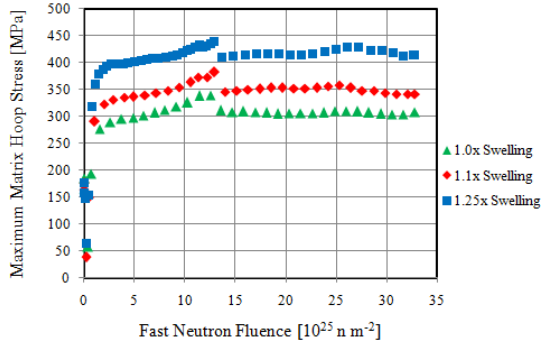
Figure 65. Effect of the TRISO particle spacing and OPyC layer thickness. **a)** Maximum matrix hoop stress versus increasing minimum particle spacing. **b)** Matrix hoop stress with a range of OPyC layer thicknesses.

6.3.6 BISO (Bilayer ISotropic) Particles

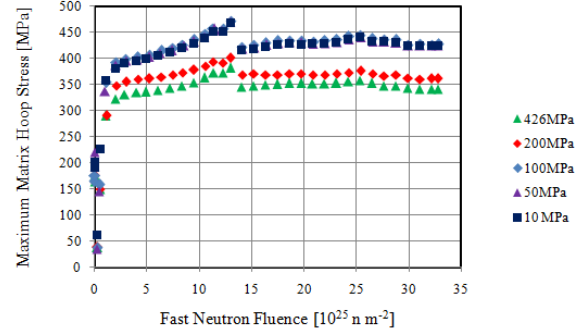
The BISO particle is similar to a TRISO particle, but without the OPyC layer. Thus, the CVD-SiC layer is in direct contact with the matrix. In this design the CVD-SiC layer is the outermost shell of the particle, which is composed of the SiC, IPyC, Buffer and Kernel regions. The removal of the OPyC layer was considered due to the potentially large stresses that may occur because of the possible volume increase in a fully constrained geometry. The OPyC normally provides a means to deflect cracks in the matrix around the particle and a weaker material to cushion the particle.

Figure 66a plots the results from varying the NITE-SiC swelling. It was presumed that the NITE-SiC would swell more than the CVD-SiC due to the additives in the NITE-SiC. The swelling range was 1.0-1.25x where the NITE-SiC has the same swelling as the CVD-SiC to 25% more volume increase. In this figure the bond between the CVD and NITE SiC was considered monolithic. The results indicate that the stress does increase with the NITE-SiC swelling. However, the stresses remain insufficient to generate long range cracking in the matrix. The discontinuity at a fluence of about $13 \times 10^{25} \text{ n m}^{-2}$ is due to the IPyC swelling cap.

Figure 66b plots the results various bond strengths assuming the NITE-SiC swells by 10% more than the CVD-SiC. The bond strength was varied from a monolithic 426 MPa to a very low 10 MPa. The characteristic volume was set to 1.57 mm^3 and the scale parameter to 8.0. The results show the stress does increase when the bond strength is reduced from 426 to 100 MPa. However, when the stresses are further reduced below 100 MPa the resulting stresses are approximately constant. This indicates that BISO particles should perform well regardless of the CVD to NITE-SiC interface bond strength.



a)



b)

Figure 66. Plots for the effects of BISO particles on the matrix. **a)** Maximum matrix hoop stress for NITE-SiC having the same swelling (1x) as CVD-SiC, 1.1x, and 1.25x the CVD swelling. **b)** The maximum matrix hoops stress for various interface bond strengths between the CVD and NITE-SiC.

6.4 Summary

The transition from 2D to 3D was completed. Methods to mesh and simulate a large random arrangement of discrete TRISO particles were developed. This provides the ability to determine stresses, temperatures, and gas pressures for FCM fuel in both LWR and HTGR environments. Due to meshing limitations, tetrahedral and pyramid elements were used for the fuel kernels. As a result, the model can predict temperatures but not stresses within the UN kernels. This is not expected to be significant limitation for the current applications.

The effect of IIDC was considered and as before, the volume change is the important parameter. Stress limited dimensional change was also included and found to significantly reduce the predicted stresses in the matrix.

A range of linear powers was examined, and the model predicts the FCM fuel would perform well for linear powers less than about 40 kW m^{-1} . This limitation is due to the mixed SiC swelling. Thus, it is possible for the FCM fuel to operate at higher linear powers for short durations.

The model indicates that the use of BISO particles in a NITE-SiC matrix should also perform well. However, it is expected that the BISO particles will be more susceptible to manufacturing defects than a TRISO particle.

CHAPTER 7: CRACKING AND FISSION PRODUCT TRANSPORT

7.1 Cracking Model

This chapter focuses on the development and implementation of fracture and fission product transport through the FCM matrix. The cracking model is based on the interface debonding and recontact model discussed in Chapter 3.

When the failure criterion is met using Weibull statistics, the element's modulus and thermal conductivity are reduced to approximate a cracked element. During the crack propagation, the time step size is reduced and the elements with the highest failure probabilities crack first. The selection process is done by using a Weibull modulus of about 20 to provide a wide spread in the resulting values which creates a reliable selection process even at high stresses.

The transport model is based on thermal diffusion. In cracked elements, the diffusion coefficient is increased to account for the crack pathway. As a result, the model is able to approximate fission product transport as a function of stress and temperature.

7.1.1 Plate Crack Propagation

To test the cracking model on a simple geometry, a plate one element thick was simulated. The plate contained five circular heat generating regions with pressure boundary conditions to create large stresses. Figure 67a shows the mesh. The intact element modulus was 300 GPa while the cracked element modulus was 1 GPa. The total heat generation was small but still sufficient to show the temperature discontinuities caused by the cracked elements. The heat was rejected through the left surface. Figure 67b and c show the results.

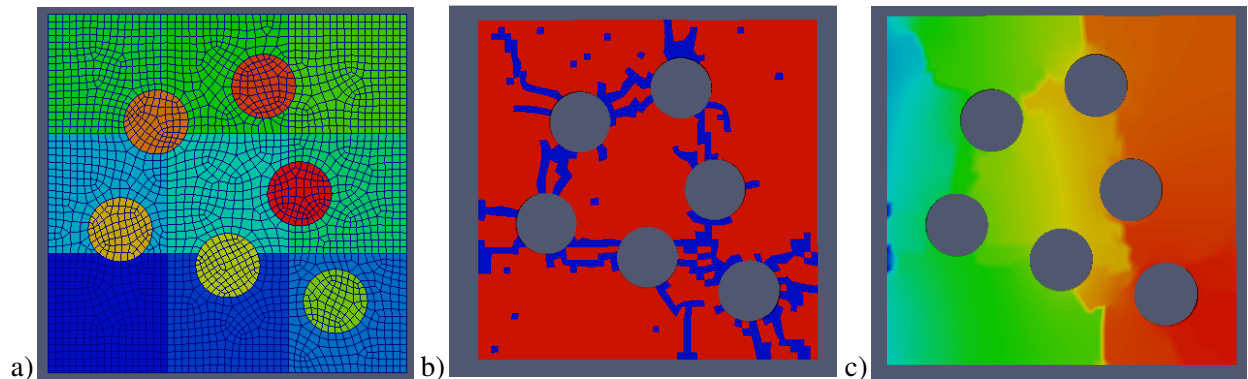


Figure 67. The results of a test simulation of the cracking model. This geometry was selected due to its simplicity. **a)** The mesh used in the simulation with the five circular regions to provide the stress necessary to cause significant cracking in the surrounding SiC plate. **b)** Resulting crack patterns predicted by the BISON model from pressure boundary conditions applied in the circular regions. **c)** Temperature profile and discontinuities from cracks. Heat was rejected through the left surface.

7.1.2 Uranium Dioxide Pellet Thermal Expansion Crack Development

The next simulation involves a UO_2 pellet to further evaluate the cracking model. The cylinder is 8.2 mm in diameter and 13.5 mm long. Linear power was set to 25 kW m^{-1} and the power is uniformly distributed throughout the pellet. The characteristic fracture stress was set to 200 MPa with a characteristic volume 1.57 mm^3 and scale parameter of 7.25. The mesh type was the “thex” form. This was selected due its use in the FCM matrix. The element density was $230 \text{ elements mm}^{-3}$. The intact modulus was 200 GPa with a cracked element modulus of 10 GPa. Figure 68 shows the results. The radial cracking pattern with a depth of about 40% appears to be a reasonable prediction. The axial cracks near the midplane of the cylinder are due to the axial thermal expansion of the interior, which is restrained by the perimeter. This prediction gives a reasonable amount of confidence in the usefulness of the cracking model for FCM fuel performance.

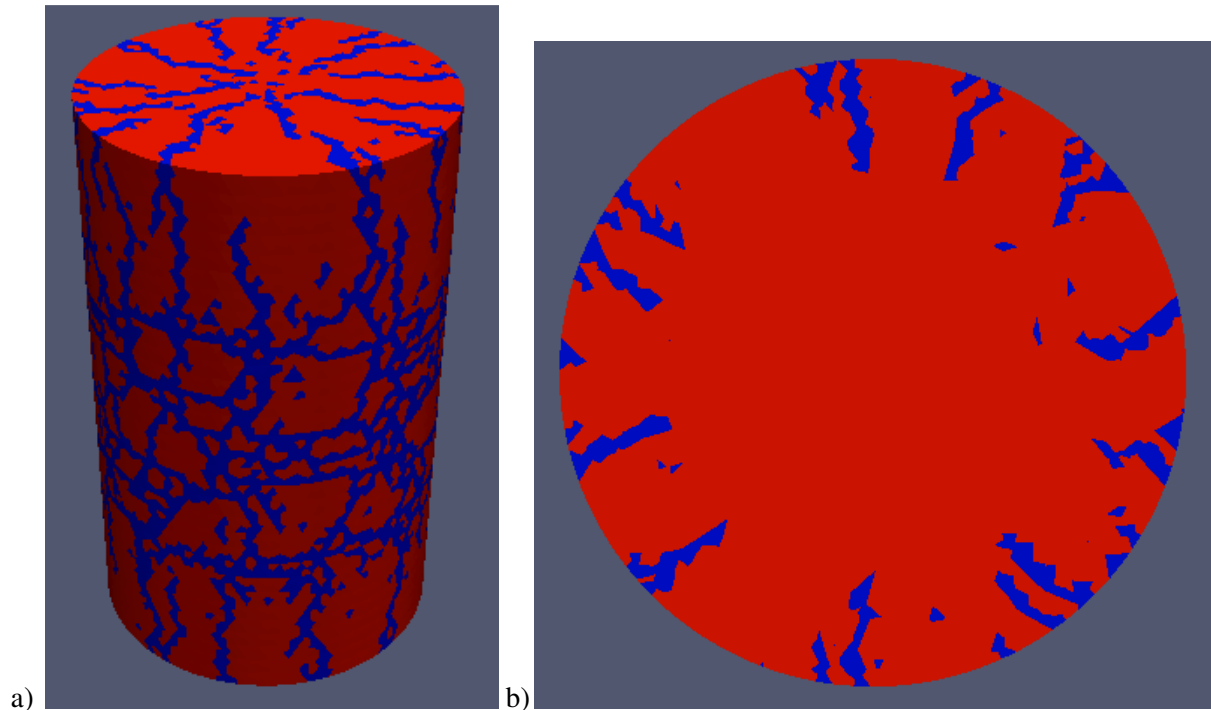


Figure 68. The cracking patterns for a UO_2 pellet predicted at 25 kW m^{-1} . **a)** Overview of the predicted surface cracks in the UO_2 pellet. **b)** Cross section view of the UO_2 pellet 3.5 mm below the midplane that shows the radial crack profile.

7.1.3 FCM Pellet Crack Propagation Principal Stress Fracture Criterion

The purpose of this simulation was to investigate how a FCM pellet might crack if it were overstressed from pyrolytic carbon swelling and the PyC maintained its elastic properties while swelling. However due to the uncertainty in dense pyrolytic carbon behavior under irradiation at high fluences, the implications of this simulation are purely speculative. The same LWR geometry as before was used, which is an 8.2 mm diameter 13.5 mm long pellet containing 41.5 vol% TRISO particles. The pellet was operated with a total power of 472.5 W, which is about 35 kW m^{-1} .

The characteristic stress was set to 426 MPa and the scale parameter to 8.0 with a characteristic volume of 1.57 mm^3 [3]. The model assumes constant failure parameters. However, the characteristic stress may

increase substantially with fluence. Figure 69 shows the predicted pellet surface crack profile while Figure 70 shows the interior cracking patterns. The elements that were assigned a small failure probability at fracture began to crack at about $8 \times 10^{25} \text{ n m}^{-2}$. However, the cracks did not propagate until the matrix stress was much higher. Bulk cracking was predicted to begin at about $9.9 \times 10^{25} \text{ n m}^{-2}$ and to follow a mostly chaotic pattern with some circumferential cracking. However, with a crack thermal conductivity on the order of $10^{-4} \text{ W m}^{-1} \text{ K}^{-1}$, the centerline temperature was increased by about 100°C . The simulation was stopped at about 20% volumetric swelling of the PyC or $11.65 \times 10^{25} \text{ n m}^{-2}$ due to substantial crack development. Figure 71 shows the temperature profile across the pellet.

Cracking of the TRISO particle layers was included in the simulation. The failure criterion is based on the value of the tensile normal stresses and since these are all compressive, the model did not predict much cracking within the particles. The expected large shear stresses of about 1-2 GPa make the model prediction of minimal TRISO layer failure somewhat concerning. However, ceramics typically fail from normal tensile stresses instead of shear stress. As a result, it is likely that the characteristic shear failure stress is considerably higher than the tensile normal stress. However, the large magnitude of the shear stresses may potentially cause problems for this assumption. When a simulation using the signed Von mises failure criterion with a 426 MPa characteristic stress was performed the CVD-SiC shells fractured extensively, but the matrix was not predicted to experience additional fracture.

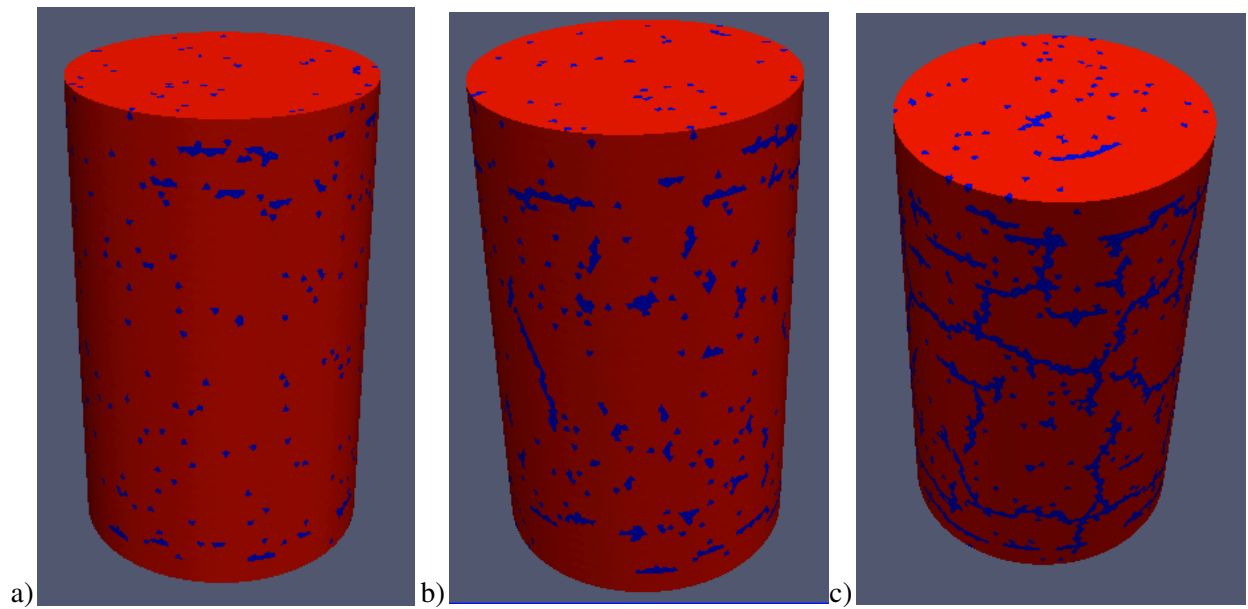


Figure 69. Plots of the predicted cracking at the FCM pellet surface. Representations are at PyC volumetric swellings of 12.61, 16.48, and 20.76% for a, b, and c respectively.

A simulation was performed to compare the cracking patterns if the FZJ IIDC correlation is used instead of the LLNL correlation. The Poisson ratio in creep was set to a constant volume 0.5, but all other parameters were unchanged from the previous LLNL cracking simulation. The results did not predict any large or propagating cracks. This indicates that the PyC volumetric change is much more important to the NITE matrix failure than the separate effects of radial or tangential dimensional change. Figure 72 shows the predicted cracking patterns when using the FZJ dimensional change correlation.

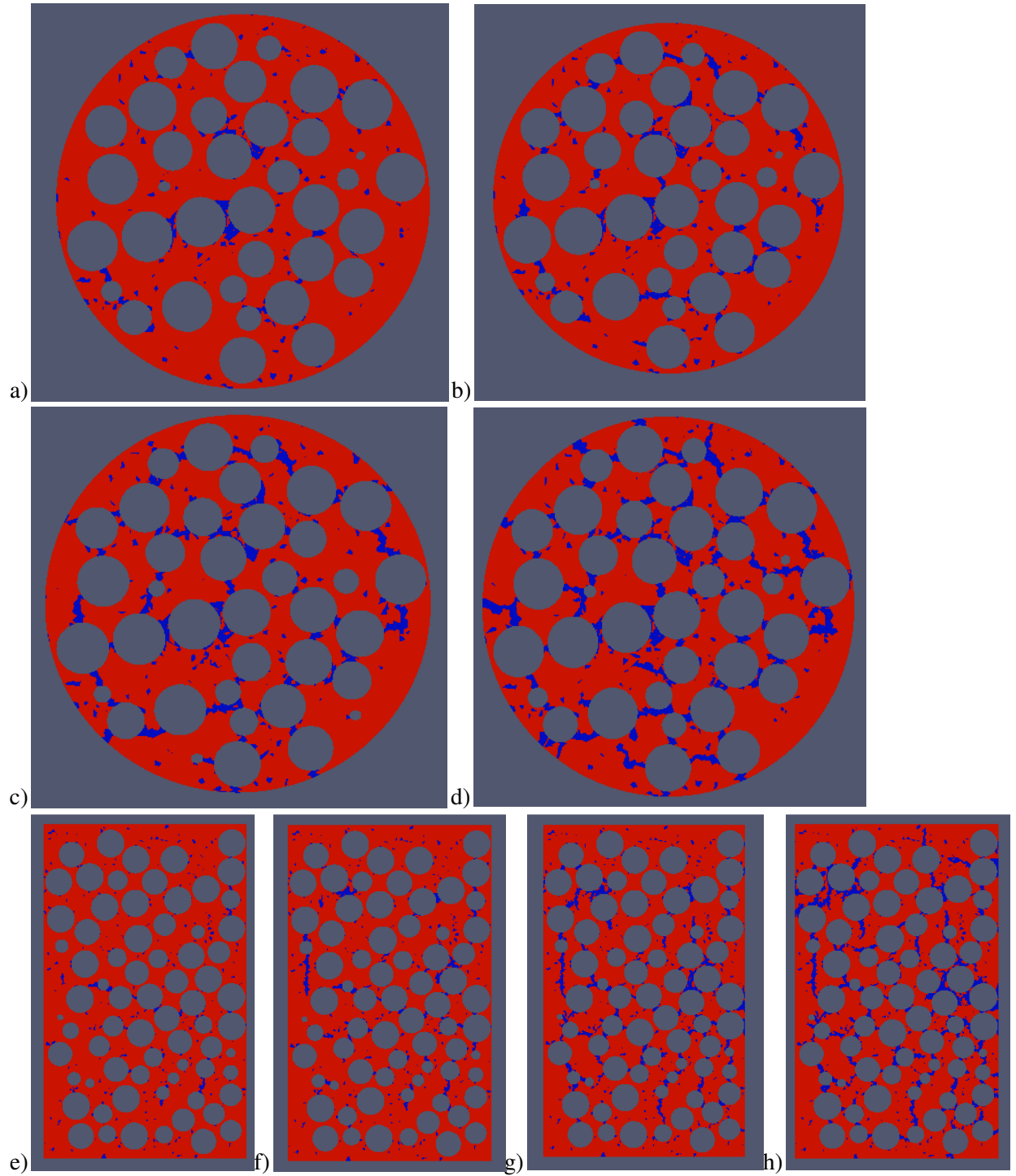


Figure 70. This shows the predicted development of the cracks within a FCM pellet with a characteristic stress of 426 MPa. **a-d)** Rθ cross section view of the predicted cracking patterns at midplane for PyC volumetric swellings of 9.15, 12.61, 16.48, and 20.76%. **e-h)** RZ cross section view of the predicted cracking patterns at midplane for PyC volumetric swellings of 9.15, 12.61, 16.48, and 20.76%.

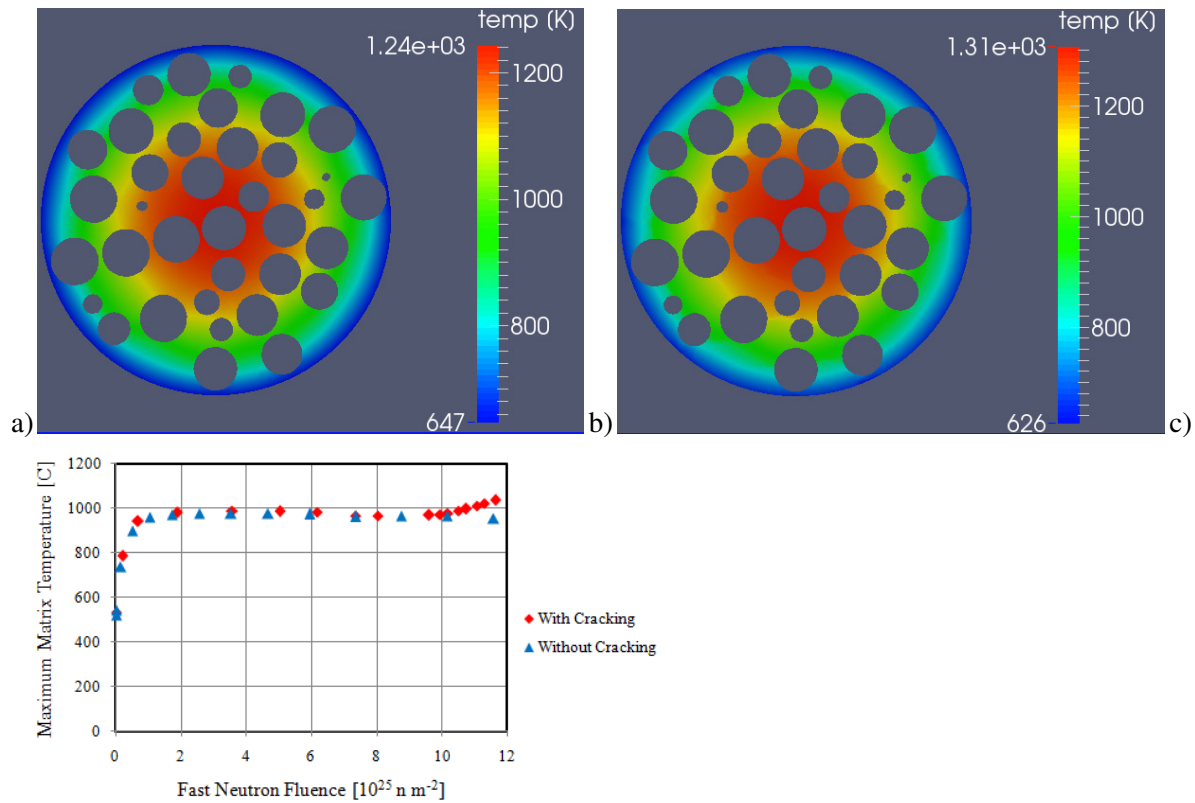


Figure 71. a and b) Temperature profiles at 9.15 and 20.76% volumetric swelling. c) Maximum temperature in the pellet or particles versus fluence.

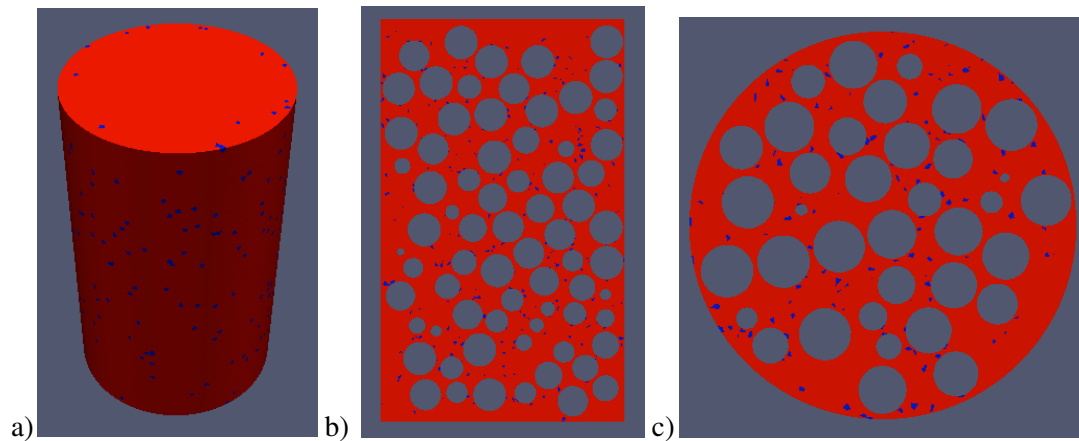


Figure 72. Representations of the predicted cracking patterns using the FZJ pyrolytic carbon dimensional change correlation which assumes a constant volume behavior. a) Overview of the predicted cracking patterns on the surface of the NITE matrix at $33 \times 10^{25} \text{ n m}^{-2}$. b) Vertical slice through the matrix that shows the predicted cracking patterns within the NITE matrix at $33 \times 10^{25} \text{ n m}^{-2}$. c) Horizontal slice through the matrix that shows the predicted cracking patterns within the NITE matrix at $33 \times 10^{25} \text{ n m}^{-2}$.

7.2 Silver and Cesium Transport

7.2.1 Transport Setup

The release of silver and cesium is primarily dependent on the temperature and cracks or faults in the SiC materials. The temperature dependent diffusional transport was modeled with the Arrhenius diffusion equation. Elements that are considered cracked are given a factor of a thousand larger diffusion coefficient. This assumes that temperature is important to release even along a crack.

Silver has two stable and several short lived isotopes. As a result, the assumption that the silver is generated in the kernel and then transported out without loss or gain is not always sufficient. Hence, radioactive decay, neutron activation and diffusion were coupled together. Below is the resulting equation. In case of short parent half lives or large activation cross sections, the grandparent source term is used to allow for convergence of the solution. Equation 13 shows the pde used for calculating silver and cesium transport.

$$\frac{dN}{d\tau} = \sum_{i=1}^3 \phi \sigma_i N_i + \sum_{i=1}^3 \lambda_i N_i - \phi \sigma N - \lambda N - D \nabla^2 N - \nabla \left(D Q \frac{N}{T^2} \nabla T \right) + f''' \quad (\text{Eq. 13})$$

Equation 13. N is the concentration and f''' is the fission source term. The equation was configured to account for up to three parent isotopes. The Soret effect that accelerates transport along temperature gradients was not used in any of these simulations due to a lack of coefficient data.

The Soret effect was added due to the noticeable temperature gradient across the matrix. However, due to lack of coefficient data this effect remained disabled. As for the activation and decay terms, Silver-109 has three primary parents. Hence, the kernel was configured to handle zero to three possible parent isotopes. Decay and activation chains for silver and cesium were modeled. The isotopic data used in the simulation was obtained from the Korean Atomic Energy Research Institute (KAERI) and Japanese Atomic Energy Agency (JAEA) [68,69]. The neutron activation cross sections were set to a value that is one half of the thermal cross sections. This was to obtain a rough estimate of the one group neutron cross sections.

7.2.2 Comparisons to Analytical Calculations

A set of simulations to compare the BISON results with analytical calculations for silver diffusion rates in silicon carbide were performed. A constant concentration source with one dimensional diffusion was setup. Equation 14 shows the relationship between concentration, time and distance for the simulations.

$$\frac{c}{c_0} = \text{ERFC} \left(\frac{x}{2\sqrt{Dt}} \right) \quad (\text{Eq. 14})$$

Equation 14. This equation describes the analytical solution for the time dependent concentration with a source configuration.

The maximum diffusion distance was 2 mm. The selected temperatures were 1800, 2000, and 2400 °C, and a total time of 14 days was used for the short duration. The long duration set of simulations used a final time of 1600 days and temperatures of 1200, 1400, and 1600 °C to compare the predicted diffusion over a reasonable fuel lifetime. Figure 73 compares analytical and BISON results of the silver the diffusion. The accuracy of the transport model increases with concentration. Also due to the high activation energy, long range silver diffusion is not expected through intact silicon carbide for temperatures below 1000 °C during the operating time of the fuel.

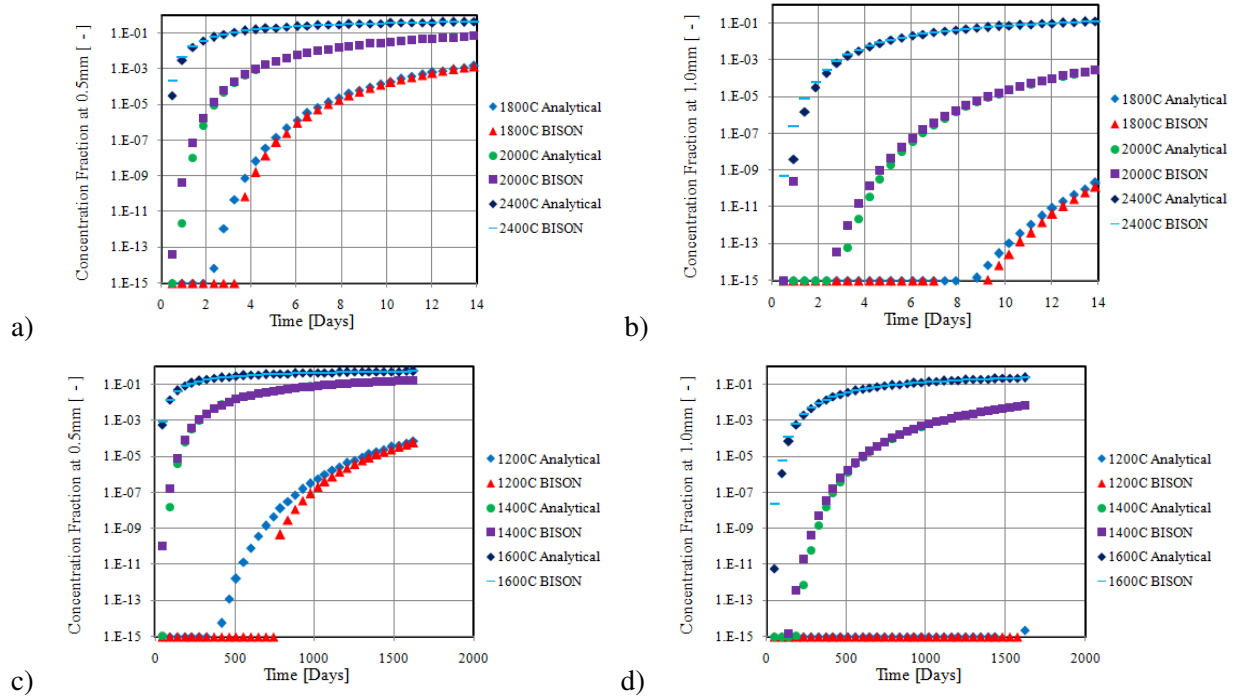


Figure 73. The plots above compare the BISON and analytical solutions to a time dependent 1D silver diffusion. The accuracy of the BISON model improves with increasing concentration. **a)** Short term and high temperature comparison plot of the silver concentration 0.5 mm from the source. **b)** Short term and high temperature comparison plot of the silver concentration 1.0 mm from the source. **c)** Long term and lower temperature comparison at 0.5 mm. **d)** Long term and lower temperature comparison at 1.0 mm.

The next set of simulations shows the effect of adding a small crack to the 1D diffusion at low temperatures but over a long duration. The SiC plate is 40 μm across with cracks 0.1, 1.0, and 5.0 μm wide. The temperatures were 600 and 800 °C and the duration was 1620 days. Figure 74 shows the results. The model predicts a significant dependence on the width of the crack even at elevated temperatures. The model predicts minimal release even with cracks in the SiC and over short distances for temperatures less than 600 °C. The implications are that the FCM fuel type should be effective at retaining fission products during normal operating conditions. During adverse conditions, the long diffusion distances provided by the NITE-matrix should provide additional time for resolving the situation.

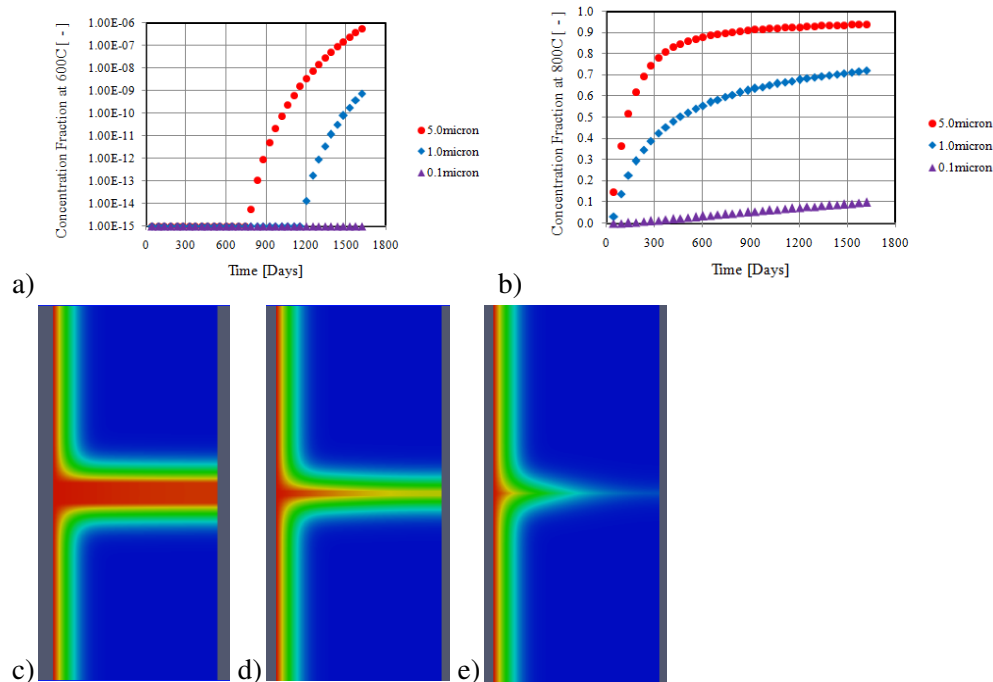


Figure 74. Plots of figures of the one dimensional silver diffusion through a cracked plate of silicon carbide. The crack diffusion coefficient was 1000x the intact coefficient. **a)** Plot comparing the concentration at the crack end for crack widths of 5, 1, and 0.1 μm . Temperature was 600 $^{\circ}\text{C}$. **b)** Plot comparing the concentration at the crack end for crack widths of 5, 1, and 0.1 μm . Temperature was 800 $^{\circ}\text{C}$. **c)** Silver concentration at 1620 days and 800 $^{\circ}\text{C}$ for the 5 μm wide crack. **d)** Silver concentration at 1620 days and 800 $^{\circ}\text{C}$ for the 1 μm wide crack. **e)** Silver concentration at 1620 days and 800 $^{\circ}\text{C}$ for the 0.1 μm wide crack.

7.2.3 FCM Simulation with Cracking and Transport

A simulation was performed that combined the cracking and transport models. A light water reactor FCM pellet with linear power of 35 kW m^{-1} was selected with tensile principal stress failure criterion. The LLNL IIDC correlation was used but an 18% volume expansion cap was used instead of the recommended 30% cap. The result was the prediction of extensive cracking in the matrix but continued numerical convergence of the BISON model was still possible. Both the silver and cesium chains were simulated and the diffusion coefficients were assumed to be 1000x higher in a crack than in intact material. Both open and closed cracks were considered to have accelerated diffusion coefficients. Due to the low temperatures near the pellet perimeter and long diffusion distances, no appreciable release from the matrix was predicted. However, transport near the center of the pellet was predicted and the acceleration from cracks can be seen. It is interesting to note that the model predicts the silver transport as being mostly crack driven whereas thermal diffusion had a much greater influence on the predicted cesium transport. Figure 75 shows the predicted cracking patterns in the matrix. Figure 76 shows the silver and cesium transport in the matrix at 671 full power days and about 440 days after cracking was completed. This point in time corresponds to a fluence of $33 \times 10^{25} \text{ n m}^{-2}$. The silver profile is largely crack driven whereas the cesium profile is a mix of bulk and crack transport. This indicates that the silver release will be more dependent on the quality of the matrix while the cesium release more related to the temperature.

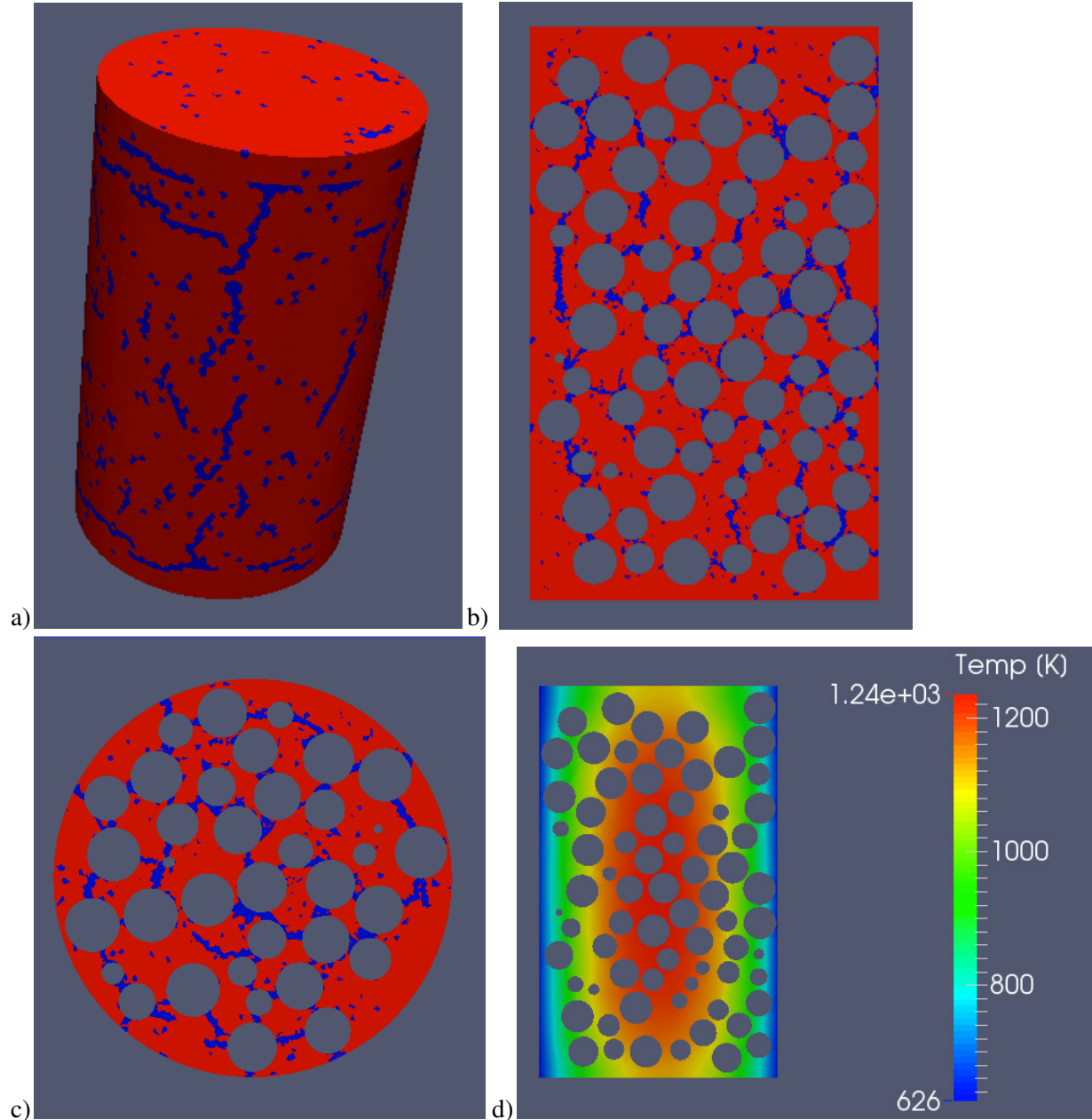


Figure 75. Representations of the predicted cracking patterns and temperature profiles in the matrix at $33 \times 10^{25} \text{ n m}^{-3}$ and 671 full power days. **a)** External cracking pattern. **b)** Vertical slice through the centerline of the pellet. **c)** Horizontal slice through the midplane of the pellet. **d)** RZ slice showing the temperature profile in the matrix.

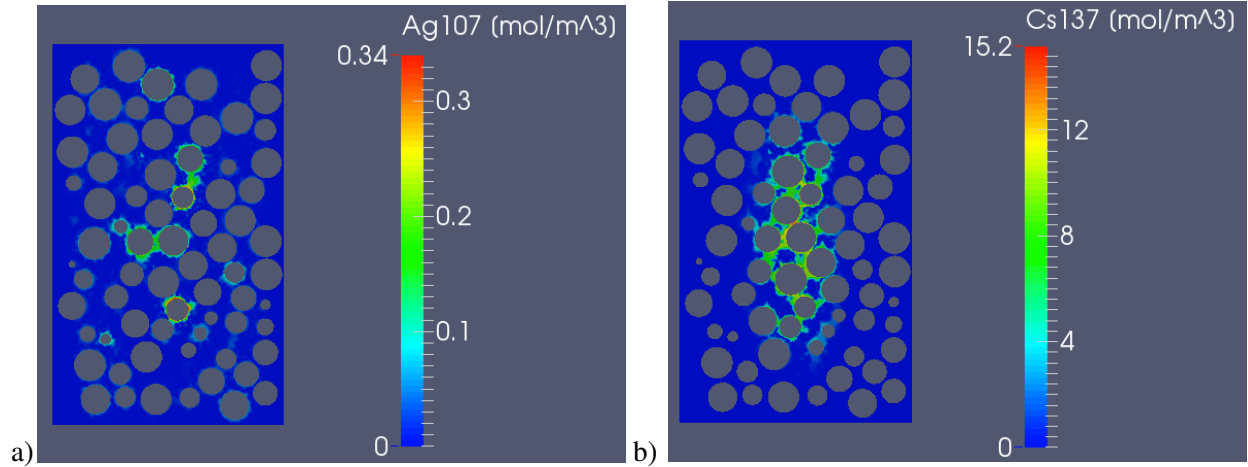


Figure 76. Representations of the silver and cesium transport in the matrix at fifty hours after temperature ramp to 2100 K. **a)** Silver transport in the matrix. **b)** Cesium transport in the matrix.

This simulation was then restarted at the 671 full power day mark. The power was set to $1.5 \times 10^{-4} \text{ kW m}^{-1}$ and the coolant temperature was increased to 1500 K. This condition was held for 12.5 days. This process was repeated for coolant temperatures of 1800 and 2100 K. Due to convergence issues, it was necessary to remove thermal expansion from the restarted simulations. However, an extensive cracking network was still present in the simulations. The model predicted small release fractions ($\sim 10^{-2}\%$ of inventory) at 1500 K. However, as temperature increased substantial release fractions were predicted after several days. While the 2100 K simulation did predict large release fractions, it should be noted that the 1% threshold for cesium release was not reached until about 50 hours. Figure 77 shows the results. The cesium release fractions are about an order of magnitude higher than the silver release due to the selected pre-exponential factor for thermal diffusion. Figure 78 compares the radial profile of the silver and cesium after 12 days of high temperatures.

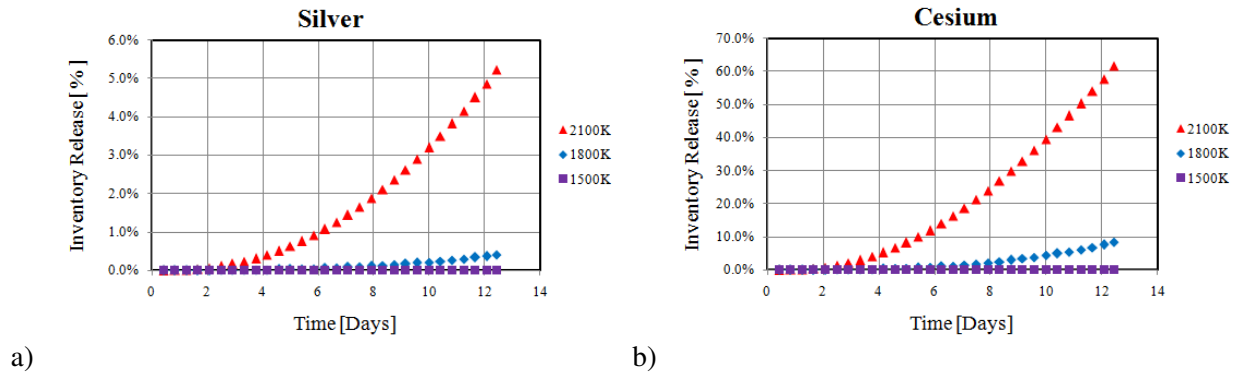


Figure 77. The silver and cesium release from the NITE-SiC matrix. The power generation was removed and the coolant temperature was increased for about 12 days. **a)** Total silver release fraction. **b)** Total cesium release fraction.

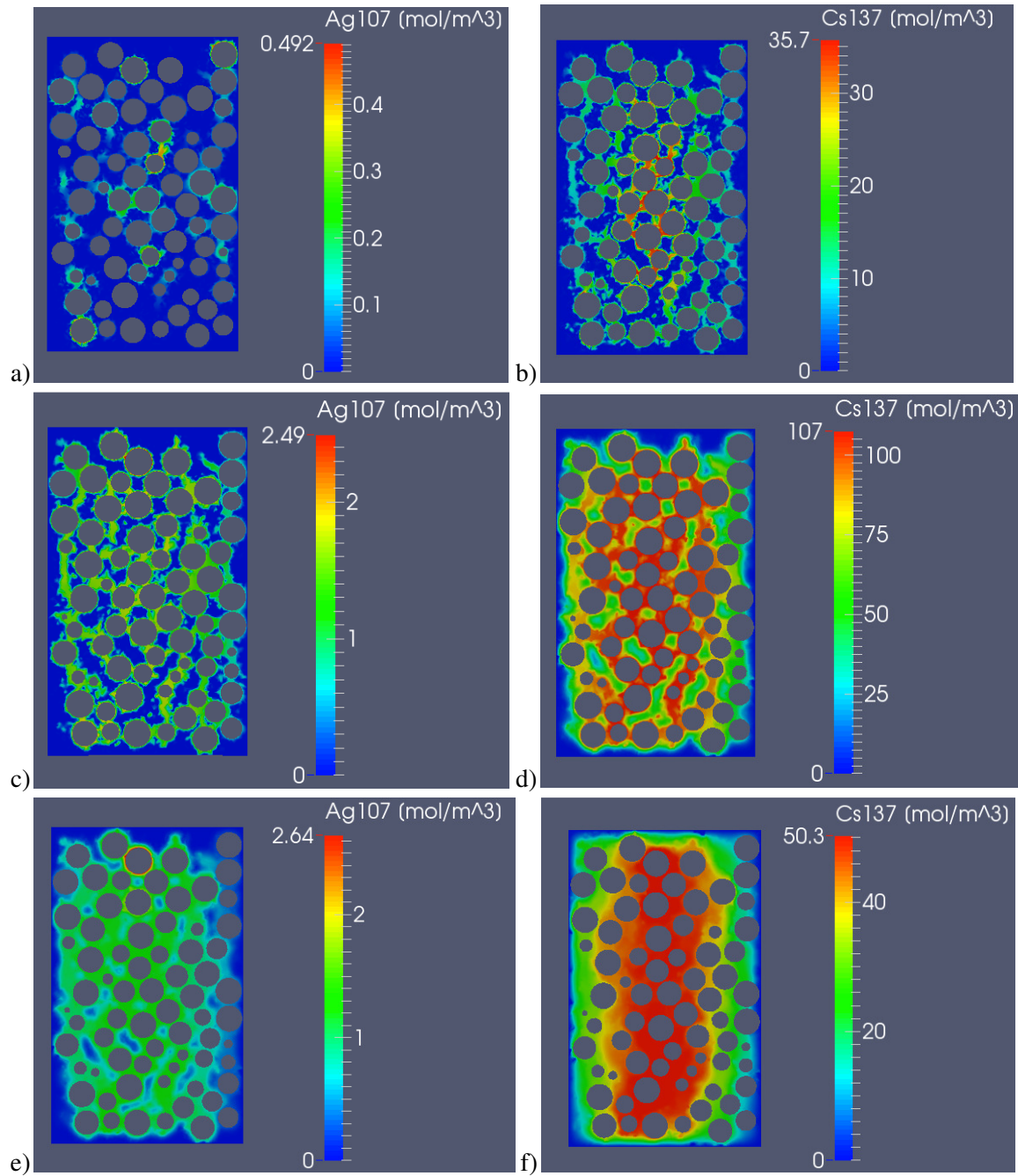


Figure 78. Representations of the silver and cesium transport through the matrix after 12 days at elevated temperatures. **a, c and e)** Silver transport at 1500, 1800, and 2100 K respectively. **b, d, and f)** Cesium transport at 1500, 1800, and 2100 K respectively.

7.3 Summary

A fracture model was developed to predict cracking patterns in the matrix and TRISO particles. The fracture model uses a reduced timestep size during crack propagation to decouple the process from other effects. Additionally, only the elements with the highest failure probabilities were allowed to fracture during each time step. This allows the crack to propagate in a believable fashion rather than resembling a stress concentration. However, this model is computationally intensive and shear stresses are not included in the element failure probability.

The cracking model assumes that the silicon carbide characteristic stress is independent of fast neutron fluence. In the event that this value increases substantially, it is expected that the matrix cracks would be significantly reduced in number and length. This would also improve the fission product retention for temperatures less than about 1800 K.

A preliminary model for silver and cesium transport was developed. The transport model is based on thermal diffusion. The crack pathways are included as a diffusion coefficient multiplier. In these simulations, a factor of 1000x was used since there is very little information for the effects of cracks on the movement of silver and cesium. It should also be noted that for convergence, the effective diffusion coefficient is limited to a range from about 1×10^{-8} to $1 \times 10^{-27} \text{ m}^2 \text{ s}^{-1}$. This produces some limitations on the diffusion sensitivity to crack pathways and maximum temperature.

The high temperature FCM transport simulations predict that about 50 hours at a temperature of 2100 K would be required to release 1% of the cesium inventory and in excess of two weeks at 1500 K. These simulations included a significant crack network in the FCM matrix.

CHAPTER 8: CONCLUSIONS AND FUTURE WORK

8.1 Conclusions

A comparison between BISON and PARFUME using the IAEA Case 11 benchmark was performed, and good agreement in stress and gas pressure was obtained. The stress components were examined individually, and the resulting trends appeared to be reasonable based on the selected correlations. The mesh size was varied, and the results were found to converge as the mesh size decreased. This provided confidence in the setup of the BISON model.

Interface debonding was added using a reduction in modulus and thermal conductivity. This approach avoids the convergence issues and interface overlap experienced when using an unmeshed gap. Also, this method allows for recontact of a pressurized interface.

A PyC dimensional change correlation has been developed to fit the available experimental data and reasonable agreement was obtained. The dimensional change of the PyC was considered a function of fast neutron fluence, density, temperature, Bacon anisotropy factor, and hydrostatic stress. The correlation assumes an initial volumetric shrinkage followed by a graphite styled turnaround at high fluence.

The techniques required for simulating a large collection of discrete particles for use in a LWR or HTGR environment have been developed. The particles used in a FCM simulation employ a mix of hexahedral, tetrahedral, and wedge elements. This configuration allows each particle to behave independently with its own interface debonding and fission gas release.

A fracture model was developed to predict cracking patterns in the matrix and TRISO particles. The fracture model uses a reduced timestep size during crack propagation to decouple the process from other effects. The elements with the highest failure probabilities were allowed to fracture during each time step.

A model for silver and cesium transport was developed. The transport model is based on thermal diffusion. The crack pathways are included as a diffusion coefficient multiplier. Simulations predicted that the FCM fuel form should provide a substantial improvement in fission product retention even with an extensive crack network in the matrix.

The primary source of uncertainty in the performance of FCM fuel is the volumetric change of the pyrolytic carbon. An increase in volume above ~15% potentially has the ability to cause excessive failure in the NITE-SiC matrix assuming all other parameters remain constant. In the event that PyC experiences a large volumetric increase under neutron irradiation, the next important factor is the amount of pressure that PyC can exert on surrounding materials if fully constrained. Factors such as stress limited dimensional change and elastic properties may affect the ability of the PyC to generate stress in other materials. In addition, the fully constrained geometry of the OPyC is important due to its high irradiation creep rate. If the PyC has free volume to expand into then only minor stresses are expected in the surrounding materials.

In the event that PyC has undesirable dimensional change properties and can fracture the matrix, there are available means to mitigate the volume expansion effects. The thickness of the OPyC is expected to have a significant effect on the amount of stress generated in the matrix. This is due to the smaller displacement that must be enforced on the OPyC by the matrix. Also, it may be possible to remove the OPyC entirely. However, this will leave the particle more vulnerable to cracks in the matrix, and to cracks that could extend from the matrix to defective particles. Alternatively, reducing the as deposited density of the OPyC is expected to increase the amount of the neutron fluence required to reach the volume turn around point. This would increase the neutron fluence limit, but also decrease the thermal conductivity and the maximum sustainable linear power due to SiC cavity formation.

In the case where stress limited dimensional change can prevent large stresses from occurring in the matrix due to PyC volume increase, then the sensitivity of the dimensional change to hydrostatic stress is expected to be the dominant factor. Normally important parameters such as creep rate, PyC volume increase rate, and Poisson ratio in creep are likely to become unnoticeable.

The remaining probable behavior for the PyC dimensional change is significant radial expansion and tangential shrinkage at approximately constant volume. Provided the volume change remains less than several percent, this behavior is not expected to generate significant stresses in the matrix or limit the fuel performance. Under this condition, fission gas pressure and SiC swelling will be the remaining factors that could cause significant stresses in the matrix.

Fission gas pressure can be an issue in both the LWR and HTGR environments. The amount of fission gas released is related to the temperature and burnup of the kernel. While limiting the burnup is undesirable, reducing the temperature can be done through the linear power. Alternatively, increasing the thermal conductivity of the buffer by using a graphite foam such as POCO graphite may be effective [70,71]. Furthermore, increasing the size of the buffer to accommodate the fission gas will reduce the pressure, but this also reduces the amount of fuel that can be embedded in the matrix.

SiC swelling behavior under irradiation exhibits saturation, mixed, and continuous swelling regimes. The effect of saturation swelling is to place the perimeter of the pellet in compression due to greater swelling at low temperatures compared to 1000 °C. This is the optimal environment for operation due to the irradiation stability and prevention of crack propagation through the perimeter of the pellet. The continuous swelling regime is expected to occur for temperatures above 1250 °C. In the model, the continuous swelling rate is considered temperature independent. If this assumption is essentially true, then FCM can operate at very high temperatures without generating large stresses from SiC swelling. In the remaining case where the perimeter of the pellet is saturated but the interior is continuously swelling, then large stresses can occur once the interior has swelled more than the perimeter. If the estimated continuous swelling rate of 0.129% per 1×10^{25} n m⁻² fast neutron fluence is accurate then the fuel can operate in this regime for an extended period, but not for the entire lifetime of the fuel.

8.2 Future Work

Experiments to provide additional information on PyC dimensional change behavior at high neutron fluences should be performed. It is also important to estimate the ability of the PyC to induce stress in the surrounding materials. To achieve these goals, it will be necessary to examine the behavior of both stress free and fully constrained PyC samples. The stress free samples would provide the volume change behavior, while the failure fractions in the constraining materials allow estimates of mitigating effects.

The modeled PyC creep assumed that the swelling and creep phenomena are unrelated. In most models, the PyC volume behavior is assumed to be a constant. Thus, coupling the swelling and creep effects is unimportant. However, coupling these effects should be investigated given that a large PyC volume expansion may occur at high fluence and could generate significant stresses in the matrix. Additionally, swelling and creep are known to be coupled effects in ceramics [50].

There is considerable uncertainty in the behavior of the PyC modulus. German sources predict a constant behavior, while British Nuclear Fuel Laboratory (BNFL) modeled a saturation trend, and the CEGA corporation suggested a linear increase [67]. However, the ability of irradiation creep to reduce stress is proportional to the modulus since the creep strain rate is modeled as being independent of the modulus. As a result, very similar stresses would be predicted even if the PyC modulus changes by a factor of two or three. Thus, there is a significant uncertainty involving the coupling of the PyC creep rate and modulus.

Additional sources of uncertainty in the model are the fission gas release, nitrogen production, swelling, and thermal conductivity degradation of uranium nitride. The model assumes that UN has the same fission gas release and swelling behavior during irradiation and burnup as UO_2 . The model also assumes that the nitrogen production from UN will be the same as the CO produced from UO_2 , which is probably a conservative assumption about the resulting gas pressure. If FCM fuel is used for commercial power generation, the TRISO particle geometry will be optimized for maximum fuel content. Under these conditions, particle over pressure due to fission gas and nitrogen release will become a limiting factor. Thus, it is desirable to understand this behavior as accurately as possible.

During partial interface contact, the model predicts a large amount of scatter in the maximum matrix hoop stress. It seems likely that these predicted stresses would not be experienced in experiments and are an artifact of the explicit formulation used in the debonding model. It would be desirable to improve the accuracy of the debonding model during partial contact.

At this time, the model assumes isotropic elastic properties in all materials. For the PyC and graphite materials, this limitation is not desirable particularly for the graphite. In the case of the PyC, the material is nearly isotropic and the effects are not expected to be excessive. However, it would be very useful to compare the effects of isotropic and anisotropic elastic properties. In an HTGR environment, the graphite is used as the binder between FCM pellets and coolant channels. The model assumes that the graphene planes are aligned horizontally, and that there is free volume in the vertical direction. Thus, the model avoids the issue of anisotropic graphite properties since there is minimal heat transfer in the vertical direction and the predicted stresses are insignificant. However, replacing the PyC layers with graphite is not a current capability of the model.

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APPENDIX

Appendix of Related Features

Ductile Failure

Ductile failure consists of plastic deformation leading to fracture. Unlike the brittle fracture this is not a sudden effect. The general method was to use a plastic damage model that depends on the stress triaxiality and temperature. As the material gains more plastic damage, the yield strength decreases. Once the plastic damage reaches one, the element is considered cracked and the time step is reduced until propagation is completed. The yield strength was enforced by removing excess strain from the elastic strain tensor. This concept of plastic damage and reducing the yield strength was recommended by Wei Hua Tai and Nikaido et al [72,73]. This allows for the formation of a neck and the typical ductile failure patterns. The following simulations use data from INL for SS 316L [74]. Figure 79 shows the specifications and mesh use for the simulations. Table 18 and Figure 80 display the results of work performed by Blandford et al [74]. Figure 81 shows the equations used to calculate plastic failure. Figure 82 shows the resulting necking and failure patterns.

Table 18. This list the experimental data from Blandford et al. for SS 316L.

Temp[F]	Yield Strength[ksi]	UTS[ksi]	UE[-]	Neck Strain[-]	Area Reduction [%]
70	41.6	92.8	61.6	0.48	88
300	33.6	70.4	36.6	0.31	82
600	21.2	68.1	31.3	0.27	81

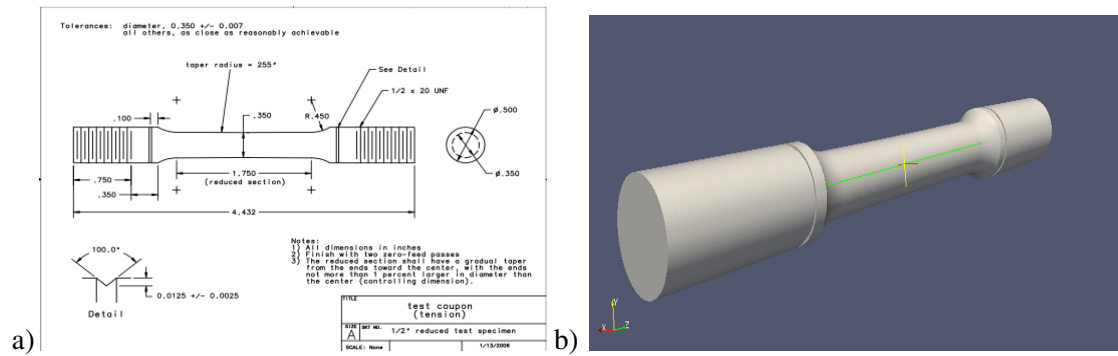


Figure 79. a) Tensile specifications from INL. Blandford et al. b) Mesh of the INL specimen.

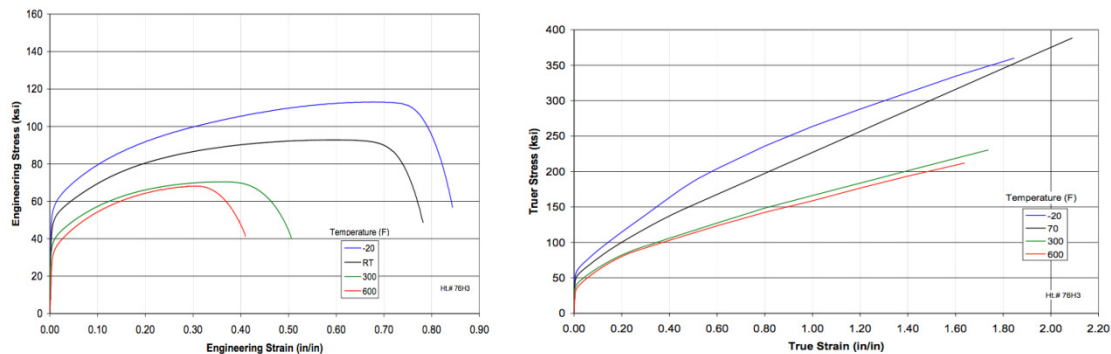


Figure 80. Figures from Blandford et al. showing the plots of the engineering and true stress for SS 316L [74].

$$PD = \sum \frac{\Delta |\bar{\epsilon}_p|}{\epsilon_f}$$

$$\epsilon_f = A * EXP \left(- \frac{B \sigma_m}{\sigma_v} \right)$$

$$\bar{\epsilon}_p = \frac{\sigma_v - \sigma_y}{E_e + E_p} \frac{\sigma}{\sigma_v}$$

Figure 81. Plastic damage equation. The plastic damage is equal to the plastic strain divided by the failure strain. The failure strain is a function of the mean and vonMises stresses. The “A” and “B” variables are functions of temperature and curve fits to data from Blandford et al [74].

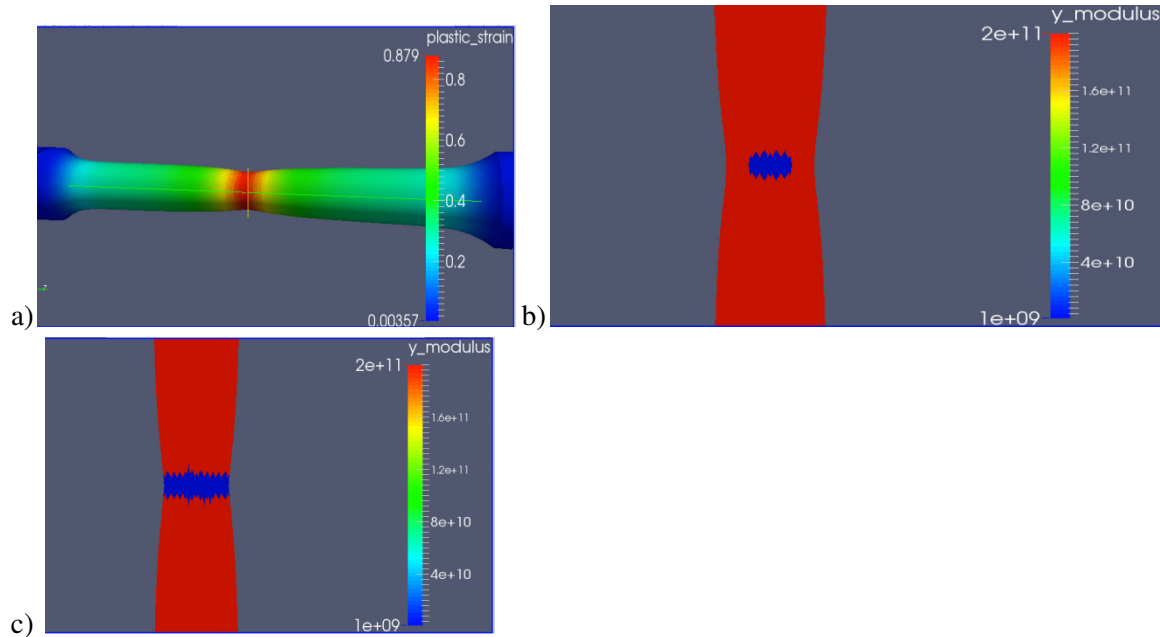


Figure 82. a) Plot of the plastic strain and resulting necking effect. **b and c)** Crack initiation and propagation patterns.

Thermal Fatigue

Thermal fatigue was added as a failure mode for the NITE-SiC to investigate the potential for load following applications. The model assumes an intact material with initial flaws distributed throughout the material. The flaws are assumed to be spherical in shape with the “flaw size” being the average diameter. The model assumes that there is at least one flaw on average per element, and that the flaw diameters have a normal distribution. This assumption of one flaw per element can be an issue if the material has a low concentration of large flaws. It may be necessary to curve fit the modeled initial flaw size to experimental observations.

Flaw growth is modeled to occur when the material is repeatedly placed in tension but not in compression. Hence, the signed von Mises or max principal stresses are used. Signed von Mises has the same magnitude as the von Mises or effective stress but takes the sign of the greatest principal stress. This formulation has the advantage in a bi or triaxial stress condition because it accounts for all principal and shear stresses. However, in the case of a compressive max principal followed closely by a tensile principal stress, the model would not predict any crack growth. The max principal uses the largest tensile principal stress for crack growth. However, it does not account for the other principal or shear stresses which may be tensile. The assumption is that largest principal stress will dominate crack growth rate. The crack growth per cycle, da/dn , is calculated using Equation 15 which is a modified Paris law [75].

$$\frac{da}{dn} = C \Delta K^p K_{\max}^n \quad (\text{Eq. 15})$$

Equation 15. Where C, p, and n are material constants. K is the stress intensity as shown in Equation 16.

$$K = \sigma \sqrt{2\pi a} \text{EXP}[C'(a - a_0)] \quad (\text{Eq. 16})$$

Equation 16. Where σ is the signed von Mises or max principal stress, a is the current crack size, a_0 is the initial flaw diameter, and C' is a constant currently set to 0.08 per mm to help account for increasing stress in the mesh element as the crack grows.

Using data and recommendations from Chen et al [75] for ABC (Al, B, and C additives) SiC, the material constant C was modeled as temperature dependent. The constant “p” was modeled as temperature and load ratio dependent, while “n” was set to a constant 75.3 as shown in Table 19. The load ratio (R) is the ratio of the min over the max stress intensity. Figure 83b plots the resulting crack growth rates da/dn versus max stress intensity $K_{\max}$ for 25-1300 °C. Figure 83c plots crack growth rate for load ratio.

Table 19. List of the material constants used to calculate the crack growth per cycle [75].

	C	N	P
25C	5.9e-73	75.3	8.6
1300C	3.3e-61		13.2
25C R=0.5			12.73
1300C R=0.5			20.26

Mesh element size stability was done by scaling the crack growth rate by Equation 17. Since the mesh is an imaginary construct, it is important that any changes to it do not affect the fatigue rate. This equation takes into account that larger elements will contain more flaws than smaller elements, and each flaw is independently growing their own cracks that eventually coalesce.

$$Scale = \left(\frac{V_e^{1/3} - a_0}{\left(\frac{\frac{4}{3}\pi \left(\frac{a_0}{2} \right)^3}{\frac{\rho_{th} - \rho}{\rho_{th}}} \right)^{1/3} - a_o} \right)^{\frac{2}{n+p}} \quad (Eq. 17)$$

Equation 17. V_e is the mesh element volume, a_0 is the initial flaw diameter, ρ is the current density, and ρ_{th} is the theoretical density.

A simulated bar measuring 5x5x50 mm was modeled with a pressure applied on the end of the bar and cycled at a load ratio (R) of 0.1, initial flaw size of 25 μm and temperature of 25 °C. Heat from the fatigue process is not considered. Figure 83a shows the results for the same bar with different sized meshes. It should be noted that the initial flaw size of 25 μm was taken from data for B₄C and NITE-SiC may be quite different. Figure 83b and c plot the crack growth rate versus stress intensity for various temperatures and load ratios. Figure 84 shows the failure profile for the bar using signed von Mises and max principal criterion.

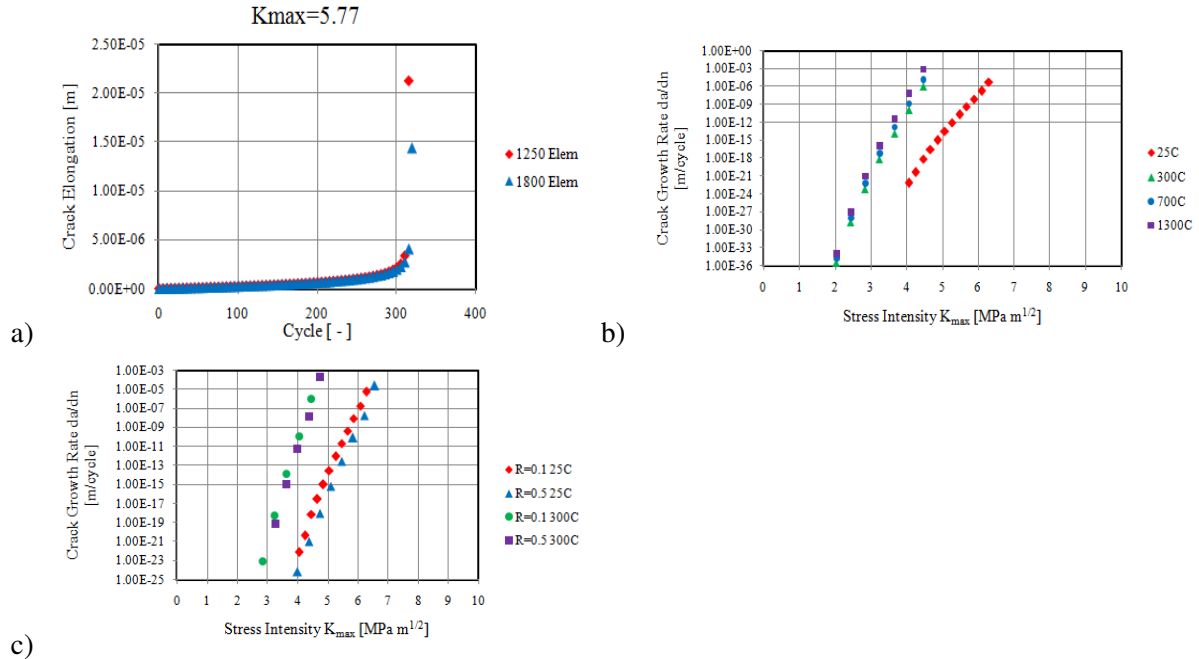


Figure 83. a) This plots the crack length for the 5x5x50 mm bar with 1250 and 1800 mesh elements. b) This plots the crack growth rate for various temperatures. c) This plots the crack growth rate for load ratio 0.1 and 0.5 at 25 and 300 °C.

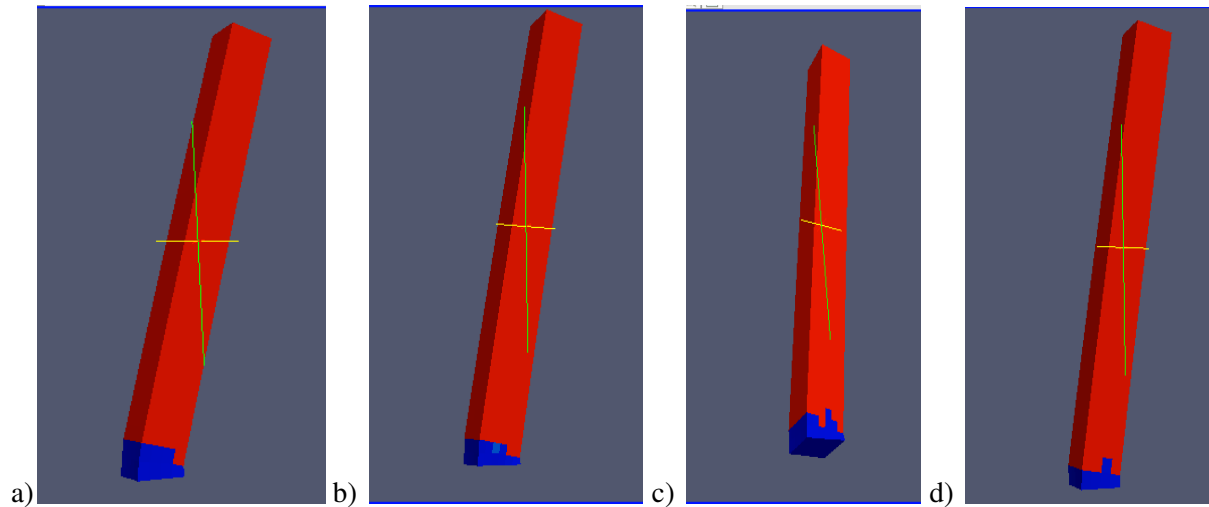


Figure 84. **a)** Signed von Mises failure criterion with 1250 elements. **b)** Signed von Mises with 1800 elements. **c)** Max principal stress failure criterion with 1250 elements. **d)** Max principal stress with 1800 elements. The 1800 element mesh using max principal had some difficulty cracking the last row of elements. As a result, using signed von Mises is recommended.

Zircaloy and Steam Reaction

The zirconium and steam reaction produces considerable quantities of heat at high temperatures which can influence the fuel failure and creep rupture of the cladding. Traditionally the reaction rate is written with units of mass squared per area squared. BISON uses energy per unit volume, thus some reformulation is required. Equation 18 gives the relationship for the heat production that is used in the BISON model. Table 20 lists the material properties for stainless steel 316 and Zircaloy-4. It should be noted that Zircaloy has three different regimes and associated values due to changing crystal structure shown in Figure 85 [76,77].

Table 20. List of the material parameters used in the clad-steam reaction kernel [78,76,77].

Material	Rate Constant [mg cm ⁻² s ⁻¹]	Activation Energy [kJ mol ⁻¹]	Heat of Reaction [J g ⁻¹]
SS-316	3e7	209.0e3	500-1000
Zircaloy-4 T<890C	5.52e4	121.3e3	6300
Zircaloy-4 890C<T<1577C	3.58e5	140.2e4	6300
Zircaloy-4 T>1577C	1.04e11	329.7e3	6300

$$q''' = 2 \frac{W}{\Delta r} \frac{\sqrt{t} - \sqrt{t_{old}}}{\Delta t} Q$$

$$W = \sqrt{A \exp\left(\frac{-E}{kT_K}\right)}$$
(Eq. 18)

Equation 18. q''' is the energy density and t is the time in seconds. Δr is the thickness of the meshed zirconium reaction layer. This is thickness of the meshed layer that generates this heat not the actual estimated depth of the reaction although it is recommended that these values be similar. Q is the heat of reaction, and W is the reaction rate.

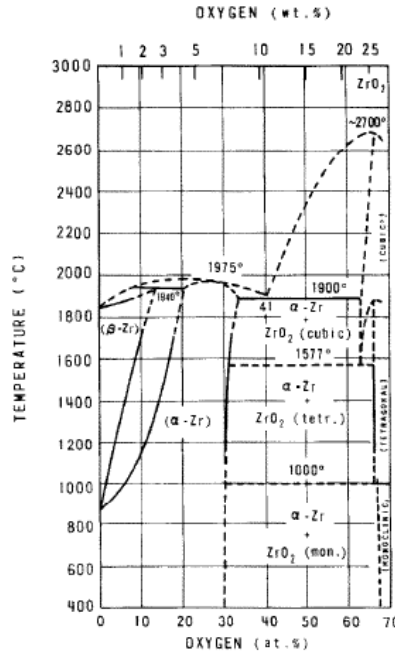


Figure 85. Diagram of the zirconium and oxygen phase diagram adapted from Urbanic and Heidrick [76].

Low temperature beta zirconium oxide is monoclinic, alpha zirconium oxide is tetragonal, and at high temperatures a cubic structure is formed.

VITA

Daniel Schappel was born in Orlando, Florida to the parents of David and Ruth Schappel. He earned a Pre-engineering Associates of Arts degree from Seminole Community College. Later, he attended University of Florida and completed a Bachelors of Science degree in Nuclear Engineering. Following this, he was accepted into the University of Tennessee PhD program in Nuclear Engineering.