TRISO Fuel Performance Modelling with BISON

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Abstract. Modeling of tristructural isotropic (TRISO)-coated particle fuel is being refined in the fuel performance code BISON. New developments include the implementation of an updated set of material properties, TRISO failure mechanisms, fission product diffusion parameters, and the design of a Monte Carlo scheme that allows BISON to calculate the probability of fuel failure within a population of TRISO particles and the subsequent fractional release of key fission products.

1. Introduction
BISON is an engineering-scale multidimensional finite-element based nuclear fuel performance code that has been under development at Idaho National Laboratory (INL) since 2008 [1]. The code can be applied to a variety of fuel forms including LWR pellets and fuel rods, TRISO-coated fuel particles, and metallic fuel in both rod and plate geometries. Modeling of these fuels is available in 1D-spherical, 2D-axisymmetric, or 3D geometries for both steady-state and transient fuel behavior and reactor operations.

BISON is built on the Multiphysics Object Oriented Simulation Environment (MOOSE [2]), a massively parallel, finite-element based framework that solves systems of coupled nonlinear partial differential equations using the Jacobian-free Newton-Krylov method [3]. This enables investigation of computationally large problems, as often encountered in nuclear fuel calculations. It also avoids the need for generating and inverting the Jacobian matrix, which is typically not analytically attainable and whose numerical approximation via finite-difference methods is not easily invertible.

In addition, MOOSE supports the use of complex two- and three-dimensional meshes and uses implicit time integration, which is important for the widely varied time scales in nuclear fuel simulation.

Although BISON has previously been used to demonstrate its capability to model TRISO fuel [4], a complete analysis requires a statistical treatment of a large population of particles to account for the particle-to-particle statistical variations in physical dimensions and fuel properties (layer thickness, density, etc.) that arise from the fuel fabrication process. It is well established that particles with properties that fall in the tail of their statistical distributions are more prone to failure and these cases must be captured to accurately compute the overall failure probability of the entire population of particles.

To this end, BISON has been updated with an enhanced TRISO model. The new model includes a comprehensive set of thermal and mechanical material properties, TRISO fuel failure mechanisms, and fission product diffusivities. BISON also includes an implementation of a Monte Carlo scheme that
allows the calculation of the probability of failure of a population of TRISO particles and of the subsequent release of fission products.

This paper provides a brief summary of TRISO fuel behavior that justifies the TRISO developments made in BISON. These developments are then detailed for the TRISO particle. Although BISON can also model the fuel element (compact or pebble), the focus here is on the demonstration of the failure probability capability, which is unaffected by the surrounding fuel form. Consequently, the developments associated to the fuel element are not discussed here.

The methodology to conduct failure probability and fission product release calculations is laid out and used on a benchmark case.

2. TRISO Fuel Behavior

2.1. TRISO Fuel Description

The TRISO-coated fuel particle is composed of a fissile fuel kernel surrounded by successive coating layers consisting of a porous carbon buffer layer, a dense inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and a dense outer pyrolytic carbon (OPyC) layer (Fig. 1). Historically, the kernel has been in an oxide or carbide form, but current developments in the USA favor the use of uranium oxycarbide (UCO - a mixture of UO\textsubscript{2}, UC, and UC\textsubscript{2}) which has shown superior performance [5]. The buffer accommodates the irradiation-induced swelling of the kernel, acts as a reservoir for fission gases to limit the internal pressure buildup in the TRISO particle, and protects the IPyC layer by absorbing fission product recoil. The IPyC protects the kernel from chlorine attack during chemical deposition of the SiC and, conversely, protects the SiC from the attack of fission products migrating from the kernel; it also serves as secondary structural layer to alleviate tensile pressure on the SiC and acts as a fission gas barrier. The SiC is both the primary structural layer and primary fission product barrier. It is protected by the OPyC layer during fuel handling; like the IPyC, the OPyC is a secondary structural layer and a fission gas barrier; it also provides a bonding surface to the overcoating matrix material. The TRISO particles are overcoated with resinated graphite powder before being pressed into the fuel element. The resinated graphite powder transforms into “so-called” matrix material upon pressing and subsequent heat treatments.

2.2. UCO TRISO Fuel Performance

In UO\textsubscript{2} TRISO fuel, excess oxygen generated by fission reacts with surrounding carbon from the buffer to form carbon monoxide [6]. CO is responsible for kernel migration [6], chemical degradation of the SiC layer [6], and increase of the internal pressure in the TRISO particle [6], which all increase the risk of fuel failure during irradiation. To mitigate these effects, UCO fuel has been developed by the Department of Energy Advanced Gas Reactor (AGR) Fuel Development and Qualification Program [7]. UCO TRISO fuel is planned to be used by current designers of small modular reactors such as Kairos Power.
In a TRISO particle, the primary function of the three outer coating layers (IPyC, SiC, and OPyC) is to contain the fission products produced in the kernel. The loss of structural integrity and leak-tightness to fission products of a coating layer constitutes a failure of this coating layer. Such failures can occur when TRISO-coated fuel particles undergo neutron irradiation. Under neutron flux, the accumulation of fission products in the kernel results in outward swelling. At the same time, the porous buffer shrinks as its porosity collapses. Both PyC layers also shrink early during irradiation but this reverts to swelling at longer irradiation times. As the buffer pulls away from the IPyC, a “buffer-IPyC” gap forms between the two layers. This gap fills with fission gases and provides the largest thermal resistance in the TRISO particle.

In the early phase of irradiation, the PyC layers are put into tension by shrinkage, which creates compressive forces on the more rigid SiC layer. However, if the tensile stress in the IPyC reaches its fracture strength, the layer can crack and concentrate a high localized tensile stress on the SiC layer. At longer irradiation times, the irradiation-induced creep of the PyC layers offsets their shrinkage, which relieves their tensile stress but also some of the compressive stress in the SiC. Concomitantly, fission gas pressure builds up in the free volume of the particle, reducing compressive stress in the SiC layer even more. As internal gas pressure increases, the tangential stress in the SiC layer can eventually become tensile. Failure of the SiC layer is then expected if the tensile stress reaches its fracture strength.

Historically, the following failure mechanisms of TRISO-coated fuel particles have been identified [6]:

- Pressure vessel failure of spherical or aspherical particles resulting in the failure of all three coating layers.
- Cracking of the IPyC layer leading to SiC failure.
- Partial debonding of the IPyC from the SiC leading to SiC failure.
- Kernel migration towards the SiC layer and its subsequent failure.
- Chemical attack of the SiC layer by fission products or CO leading to its failure.
- Thermal decomposition of the SiC layer at high temperatures.
- Buffer fracture leading to cracking of partially debonded IPyC.

As CO production is limited in UCO fuel, kernel migration and CO contribution to internal pressure and SiC corrosion are not considered in this UCO TRISO BISON model. Furthermore, thermal decomposition of the SiC is only expected at temperatures > 2100°C [8], far exceeding expected TRISO fuel operating or accident temperatures, and is also not modeled. Additionally, TRISO fuel manufactured to the German process requirements, including AGR fuel, has not exhibited IPyC-SiC debonding leading to SiC failure. Finally, there is currently no existing model for the cracking of a partially debonded IPyC layer because of lack of experimental data (e.g., buffer-IPyC bond strength).

2.3. Fission Product Transport
Several mechanisms might be involved in the transport of mobile fission products through the kernel and coating layers of TRISO particles. Such mechanisms could include lattice diffusion, grain boundary diffusion, pore diffusion, nano-cracking, or vapor transport [9]. Furthermore, effects like irradiation-induced trapping and adsorption, thermal decomposition of the coating layers, or chemical attack of the coating layers by other fission products, such as palladium or rare earth elements, could potentially impact these transport mechanisms.

To get by the lack of adequate models to conceptualize the fundamental knowledge of all possible transport mechanisms, Fick’s laws of diffusion are used with “effective” diffusivities to model fission product transport through a TRISO particles. “Effective” implies that the diffusivities describe the overall fission product transport using classical Fickian diffusion [6]. The application of these “effective” diffusion coefficients will result in the same fractional release of fission products from the TRISO particle as was observed in the integral release measurements from which they were derived.
3. UCO TRISO Fuel Modeling

3.1. Material Properties
TRISO fuel material properties include mechanical and thermal properties for the kernel and coating layers. BISON has the capability of modeling the fuel element in which TRISO particles are embedded, but the material properties of the matrix are not discussed here.

3.1.1. Kernel
Legacy TRISO fuel development programs have predominantly focused on UO\(_2\) fuel and, consequently, most kernel properties are based on UO\(_2\) experimental data.

Kernel swelling occurs throughout irradiation as solid and gaseous atoms released by fission accumulate in the kernel, resulting in a volume increase of the kernel. The volumetric change in kernel volume, or swelling S (-), is given by [10]:

\[ S = \frac{\Delta V}{V_0} = 0.8\% \times \Delta B_u \]  (1)

where \( V_0 \) (m\(^3\)) is the initial volume of the kernel, \( \Delta V \) (m\(^3\)) is the kernel volume increase, and \( \Delta B_u \) (%FIMA) is the burnup increment.

The Young’s modulus of the kernel, \( E \) (GPa), is given by [11]:

\[ E = 219 \times f(T) \times g(\rho) \]  (2)

\[ f(T) = 1 - 1.07 \times 10^{-4} \times T - 2.16 \times 10^{-7} \times T^2 + 3.10 \times 10^{-10} \times T^3 - 1.54 \times 10^{-13} \times T^4 \]  (3)

\[ g(\rho) = \frac{1.92 \times \rho - 0.92 \times \rho_{th}}{1.66 \times \rho - 0.66 \times \rho_{th}} \]  (4)

where \( T \) (°C) is the temperature of the kernel, \( \rho \) (g/cm\(^3\)) is the density of the kernel, and \( \rho_{th} \) (g/cm\(^3\)) is the theoretical density of UCO.

The Poisson’s ratio of the kernel, \( \mu \) (-), is derived from its Young’s modulus (see above) and its shear modulus [11]:

\[ \mu = 1.35 \times \frac{1.92 \times \rho - 0.92 \times \rho_{th}}{1.66 \times \rho - 0.66 \times \rho_{th}} - 1 \]  (5)

The thermal conductivity of the kernel, \( k \) (W/m-K), is given by [10]:

\[ k(T) = \begin{cases} 0.0132 \times e^{0.00188 \times T} + \frac{4.040}{1 + 0.23 \times 10^{-4}} & \text{if } T < 1650°C \\ 0.0132 \times e^{0.00188 \times T} + 1.9 & \text{if } T \geq 1650°C \end{cases} \]  (6)

where \( T \) (°C) is the temperature of the kernel.

The heat capacity of the kernel, \( c_p \) (J/mol-K), is given by [12]:

\[ c_p = 52.1743 + 87.951 \times \left( \frac{T}{1000} \right)^{-2} - 84.2411 \times \left( \frac{T}{1000} \right)^{-2} + 31.542 \times \left( \frac{T}{1000} \right)^{-3} - 2.6334 \times \left( \frac{T}{1000} \right)^{-4} - 0.71391 \times \left( \frac{T}{1000} \right)^{-2} \]  (7)

where \( T \) (K) is the temperature of the kernel.

3.1.2. Buffer
The Young’s modulus of the buffer, \( E \) (GPa), is given by [10]:

\[ E = 25.5 \times (0.384 + 0.324 \times \rho) \times (1 + 0.23 \times \phi) \times (1 + 1.5 \times 10^{-4} \times (T - 20)) \]  (8)

where \( \rho \) (g/cm\(^3\)) is the density of the buffer, \( \phi \) (×10\(^{25}\) n/m\(^2\), E > 0.18 MeV) is the fast neutron fluence, and \( T \) (°C) is the temperature of the buffer.

The Poisson’s ratio of the buffer, \( \mu \) (-), is given by [10]:

\[ \mu = 0.33 \]  (9)
The irradiation creep of the buffer, that leads to its gradual deformation in response to irradiation-induced damage, is directly proportional to fast neutron fluence. The proportionality factor, i.e., the irradiation-induced creep coefficient of the buffer, $K_\text{S} \left( \times 10^{-25} \text{ (MPa-n/m}^2\text{)} \right)$, is given by [10]:

$$K_\text{S} = 2 \times [1 + 2.38 \times (1.9 - \rho)] \times (2.193 \times 10^{-4} - 4.85 \times 10^{-7} \times T + 4.0147 \times 10^{-10} \times T^2)$$

(10)

where $\rho$ (g/cm$^3$) is the density of the buffer and $T$ (°C) is the temperature of the buffer.

The Poisson’s ratio in creep of the buffer, $\nu$ (-), is given by [10]:

$$\nu = 0.5$$

(11)

The irradiation-induced dimensional change (strain) of the buffer, $\varepsilon$ (-), is given by [10]:

$$\varepsilon = a_1 \times \phi + a_2 \times \phi^2 + a_3 \times \phi^3 + a_4 \times \phi^4$$

(12)

where the $a_i$ coefficients depend on density and temperature and $\phi \left( \times 10^{25} \text{ n/m}^2, E > 0.18 \text{ MeV} \right)$ is the fast neutron fluence. The $a_i$ coefficients are detailed in reference [10] and in the online BISON documentation.

The thermal conductivity of the buffer, $k$ (W/m-K), is given by [10]:

$$k = \frac{k_0 \times k_{th} \times (\rho_{th} - \rho_0)}{k_{th} \times (\rho_{th} - \rho_0) + k_0 \times (\rho - \rho_0)}$$

(13)

The thermal conductivity of the buffer depends on its initial and theoretical densities ($\rho_0$ and $\rho_{th}$ = 2.25 g/cm$^3$) and on the thermal conductivities at these two densities ($k_0$ = 0.5 W/m-K and $k_{th}$ = 4 W/m-K).

The specific heat capacity of the buffer, $c_p$ (J/kg-K), is given by [13]:

$$c_p = 720$$

(14)

The coefficient of thermal expansion of the buffer, $\alpha \left( \times 10^6/\text{°C} \right)$, is given by [10]:

$$\alpha = 5 \times \left(1 + 0.11 \times \frac{T - 400}{700}\right)$$

(15)

where $T$ (°C) is the temperature of the buffer.

3.1.3. PyC

The Young’s moduli (GPa) of the PyC in the tangential ($E_t$) and radial ($E_r$) directions are given by [10]:

$$E_t = 25.5 \times (0.384 + 0.324 \times \rho) \times (1 + 0.23 \times \phi) \times \left(1 + 1.5 \times 10^{-4} \times (T - 20) \times (0.481 + 0.519 \times \text{BAF}_0)\right)$$

(16)

$$E_r = 25.5 \times (0.384 + 0.324 \times \rho) \times (1 + 0.23 \times \phi) \times \left(1 + 1.5 \times 10^{-4} \times (T - 20) \times (1.463 - 0.463 \times \text{BAF}_0)\right)$$

(17)

where $\rho$ (g/cm$^3$) is the density of the PyC, $\phi \left( \times 10^{25} \text{ n/m}^2, E > 0.18 \text{ MeV} \right)$ is the fast neutron fluence, $T$ (°C) is the temperature of the PyC, and BAF$_0$ (-) is the initial anisotropy of the PyC measured by its Bacon Anisotropy Factor.

The Poisson’s ratio of the PyC, $\mu$ (-), is given by [10]:

$$\mu = 0.33$$

(18)

The irradiation-induced creep coefficient of the PyC, $K_s \left( \times 10^{-25} \text{ (MPa-n/m}^2\text{)} \right)$, is given by [10]:

$$K_s = 2 \times [1 + 2.38 \times (1.9 - \rho)] \times (2.193 \times 10^{-4} - 4.85 \times 10^{-7} \times T + 4.0147 \times 10^{-10} \times T^2)$$

(19)

where $\rho$ (g/cm$^3$) is the density of the PyC and $T$ (°C) is the temperature of the PyC.

The Poisson’s ratio in creep of the PyC, $\nu$ (-), is given by [10]:

$$\nu = 0.5$$

(20)
The irradiation-induced dimensional change (strain) of the PyC, $\varepsilon$ (-), is given by [10]:

$$\varepsilon = a_1 \times \phi + a_2 \times \phi^2 + a_3 \times \phi^3 + a_4 \times \phi^4$$

(21)

where the $a_i$ coefficients depend on BAF, density, temperature, and the direction (radial or tangential) of the strain and $\phi \times 10^{25}$ n/m$^2$, $E > 0.18$ MeV) is the fast neutron fluence. The $a_i$ coefficients are detailed in Ref. [10] and in the online BISON documentation.

The thermal conductivity of the PyC, $k$ (W/m·K), is given by [10]:

$$k = 4.0$$

(22)

The specific heat capacity of the PyC, $c_p$ (J/kg·K), is given by [13]:

$$c_p = 720$$

(23)

The coefficients of thermal expansion of the PyC ($\times 10^{-6}$/°C) in the radial ($\alpha_r$) and tangential ($\alpha_t$) directions are given by [10]:

$$\alpha_r = \left(30 - 37.5 \times \frac{2}{(2 + BAF)}\right) \times f(T)$$

(24)

$$\alpha_t = \left(1 + 36 \times \frac{1}{(2 + BAF)^2}\right) \times f(T)$$

(25)

$$f(T) = 1 + 0.11 \times \frac{T - 400}{700}$$

(26)

where BAF (-) is the Bacon Anisotropy Factor of the PyC and T (°C) is the temperature of the PyC.

Pyrocarbon is a brittle material and, as such, its probability of failure is calculated using Weibull statistics. The Weibull characteristic strength, $\sigma_0$ (MPa·m$^{1/6}$), and modulus, $m$ (-), of the PyC are given by [10]:

$$\sigma_0 = 16.8 \times \sqrt{f(\phi) \times g(T)}$$

(27)

$$f(\phi) = 1 + 0.23 \times \phi$$

(28)

$$g(T) = 1 + 1.5 \times 10^{-4} \times (T - 20)$$

(29)

$$m = 9.5$$

(30)

where $\phi \times 10^{25}$ n/m$^2$, $E > 0.18$ MeV) is the fast neutron fluence and T (°C) is the temperature of the PyC.

3.1.4. Buffer-IPyC Gap

Heat produced in the kernel is transferred to the outer coating layers through the buffer-IPyC gap via a gap conductance model using the width of the gap and the conductivity of the gas mixture (Kr and Xe) in the gap. Radiation (limited temperature difference between the buffer and IPyC) and convection (small gap width) are not included in the model.

The thermal conductivity of the Kr-Xe gas mixture, $k_{gas}$ (W/m·K), is given by [14]:

$$k_{gas} = \frac{f_{Kr} \times k_{Kr}}{f_{Kr} + f_{Xe} \times \Psi_{KrXe}} + \frac{f_{Xe} \times k_{Xe}}{f_{Xe} + f_{Kr} \times \Psi_{XeKr}}$$

(31)

where $f_{Kr}$ (-) and $f_{Xe}$ (-) are the molar fractions of Kr and Xe, respectively, and $k_{Kr}$ (W/m·K) and $k_{Xe}$ (W/m·K) are their thermal conductivities. The thermal conductivities depend on the average temperature of the gap, T (K), and are given by:

$$k_{Kr} = 8.247 \times 10^{-5} \times T^{0.8363}$$

(32)

$$k_{Xe} = 4.351 \times 10^{-5} \times T^{0.8616}$$

(33)

and the “$\Psi$” functions are given by:

$$\Psi_{KrXe} = \left(1 + 2.41 \times \frac{(M_{Kr} - M_{Xe}) \times (M_{Kr} - 0.142 \times M_{Xe})}{(M_{Kr} + M_{Xe})^2}\right) \times \Phi_{KrXe}$$

(34)
\[ \Psi_{\text{XeKr}} = \left( 1 + 2.41 \times \frac{(M_{\text{Xe}}-M_{\text{Kr}})\times(M_{\text{Xe}}-0.142\times M_{\text{Kr}})}{(M_{\text{Xe}}+M_{\text{Kr}})^2} \right) \times \Phi_{\text{XeKr}} \]  

\( M_{\text{Kr}} (83.8 \text{ g/mol}) \) and \( M_{\text{Xe}} (131.3 \text{ g/mol}) \) are the molecular weights of the gas mixture components and the “\( \Phi \)” functions are given by:

\[ \Phi_{\text{KrXe}} = \left( 1 + \frac{\sqrt{k_{\text{Kr}}}}{\sqrt{k_{\text{Xe}}}} \frac{\sqrt{M_{\text{Kr}}}}{\sqrt{M_{\text{Xe}}}} \right)^2 \]  

\[ \Phi_{\text{XeKr}} = \left( 1 + \frac{\sqrt{k_{\text{Xe}}}}{\sqrt{k_{\text{Kr}}}} \frac{\sqrt{M_{\text{Xe}}}}{\sqrt{M_{\text{Kr}}}} \right)^2 \]

### 3.1.5. SiC

The Young’s modulus of the SiC, \( E \) (GPa), is given in Table 1 [10] as a function of its temperature, \( T \) (°C). Values in-between table entries are linearly interpolated.

| \( T \) (°C) | \( E \) (GPa) | \( T \) (°C) | \( E \) (GPa) |
|--------------|--------------|--------------|--------------|
| \( \leq 25 \) | 428          | 1215         | 340          |
| 940          | 375          | \( \geq 1600 \) | 198          |

The Poisson’s ratio of the SiC, \( \mu \), is given by [10]:

\[ \mu = 0.13 \]  

The thermal conductivity of the SiC, \( k \) (W/m-K), is given by [10]:

\[ k = \frac{17885}{T+273} + 2 \]  

where \( T \) (°C) is the temperature of the SiC.

The specific heat capacity of the SiC, \( c_p \) (J/kg-K), is given by [15]:

\[ c_p = 925.65 + 0.3772 \times T - 7.9259 \times 10^{-5} \times T^2 - 3.1946 \times 10^7 \times T^{-2} \]  

where \( T \) (K) is the temperature of the SiC.

The coefficient of thermal expansion of the SiC, \( \alpha \) (\( \times 10^6/°C \)), is given by [10]:

\[ \alpha = 4.9 \]  

SiC is a brittle material and, as such, its probability of failure is calculated using Weibull statistics. The Weibull characteristic strength, \( \sigma_0 \) (MPa-m\(^3\)/m), and modulus, \( m \), of the SiC are given by [10]:

\[ \sigma_0 = 9.64 \]  

\[ m = 6 \]

### 3.2. Physical Models

#### 3.2.1. Strain-Displacement and Stress-Strain Constitutive Relationships

In BISON, displacements can be calculated by application of either small strain or finite strain [16] theories. For TRISO fuel calculations, the small strain theory is used and the strain-displacement constitutive equations in any coating layer of a spherical TRISO particle are given by:

\[ \varepsilon_r = \frac{\partial u}{\partial r} \]  

\[ \varepsilon_t = \frac{u}{r} \]
where \( \varepsilon_r (-) \) and \( \varepsilon_t (-) \) are the radial and tangential components of the strain, respectively, and \( u (m) \) is the radial displacement. In the absence of shear strains in axisymmetric solids, all the other components of the strain tensor are zero. The total strain tensor, \( \{ \varepsilon \} \), and stress tensor, \( \{ \sigma \} \), are related by the constitutive relationship:

\[
\sigma \{ \sigma \} = [E] \times \{ \varepsilon \} = [E] \times (\{ \varepsilon \} - \{ \varepsilon_C \} - \{ \varepsilon_{I\text{IDC}} \} - \{ \varepsilon_{\text{TE}} \})
\]

(46)

where \([E]\) is the elastic matrix and \(\{ e_E \}\) is the elastic strain tensor consisting of creep strain, \(\{ \varepsilon_C \}\), irradiation-induced shrinkage/swelling strain, \(\{ \varepsilon_{I\text{IDC}} \}\), and thermal expansion strain, \(\{ \varepsilon_{\text{TE}} \}\).

Stress equilibrium is enforced by solving the so-called weak form of the following partial differential equation:

\[
\nabla \sigma = 0
\]

(47)

In BISON, the displacement is the field variable being solved for by the mechanics models. It is iteratively updated, along with other field variables, until convergence is achieved. During each iteration, the strains are computed from the displacements (eq. 44 and eq. 45), after which the stresses are obtained from the strains (eq. 46). The stresses are then integrated over the finite elements to get the nodal forces, which must be in equilibrium (eq. 47) for the solution to be considered converged.

3.2.2. Failure probability

Pyrocarbon and silicon carbide are brittle materials. The fracture strength of a brittle material is typically represented by a statistical distribution expressed in terms of Weibull parameters (characteristic strength \(\sigma_0 (\text{MPa}\cdot\text{m}^{3/2}) \) and modulus \( m (-) \)) that are indicative of the flaw distribution in a given volume of the material. When a maximum stress, \(\sigma_{\text{max}} (\text{MPa})\), is applied to the material, its failure probability, \(P_f (-)\), is given by [10]:

\[
P_f = 1 - e^{-\left(\frac{\sigma_{\text{max}}}{\sigma_{\text{ms}}}\right)^m}
\]

(48)

where the mean strength, \(\sigma_{\text{ms}} (\text{MPa})\), is related to the characteristic strength and to the normalized integration of the tensile stress distribution over the volume of the material, \(I (\text{m}^3)\):

\[
\sigma_{\text{ms}} = \frac{\sigma_0}{I^{1/m}}
\]

(49)

3.2.3. Heat Equation

The general heat conduction equation is given by:

\[
\rho \times c_p \times \frac{\partial T}{\partial t} - k \times \nabla^2 T - E_f \times \dot{F} = 0
\]

(50)

where \(\rho (\text{g/cm}^3)\) is the density, \(c_p (\text{J/kg-K})\) is the specific heat capacity, \(T (\text{K})\) is the temperature, \(k (\text{W/m-K})\) is the thermal conductivity, \(E_f (3.204 \times 10^{-11}\text{ J} = 200\text{ MeV})\) is the average energy released per fission, and \(\dot{F}\) (fission/cm$^3$-s) is the volumetric fission rate.

3.2.4. Fission Yields

The numbers of fission product atoms created per fission, or fission yields, depend on the neutron spectrum in each core using TRISO fuel. Default values, \(\gamma (-)\), are included in BISON for Ag, Cs, Sr, and noble gases (Kr + Xe) [10]:

For \(^{235}\text{U}\) enrichment lower than 17.5%:

\[
\gamma_{\text{Ag}} = 1.31625 \times 10^{-3} \times (B_u \lor 1)^{0.55734}
\]

(51)

\[
\gamma(\text{Cs}) = 0.14
\]

(52)

\[
\gamma(\text{Sr}) = 0.11754 \times (B_u \lor 0.6)^{-0.21762}
\]

(53)

\[
\gamma(\text{Kr} + \text{Xe}) = 0.297
\]

(54)
For $^{235}$U enrichment higher or equal to 17.5%:

$$p_{f} \gamma_{Ag} = 8.24492 \times 10^{-4} \times (B_{u} \vee 1)^{0.53853}$$

(55)

$$\gamma(Cs) = 0.16$$

(56)

$$\gamma(Sr) = 0.11819 \times (B_{u} \vee 0.6)^{-0.15778}$$

(57)

$$\gamma(Kr + Xe) = 0.297$$

(58)

where $B_{u}$ (%FIMA) is the burnup and $\vee$ is the “max” function.

3.2.5. Fission Gas Release of Long-Lives Isotopes

The release of long-lived fission gases from the kernel is modeled as a two-step process: first, the gas atoms are driven through the grain towards the grain boundary; second, the gas atoms migrate from the grain boundary to the free surface of the fuel where they are instantaneously released into the free volume of the TRISO particle. The model includes both direct recoil and diffusion to grain boundaries. The release fraction, $RF (-)$, which corresponds to the fraction of the gas generated by fission that is released by the kernel is given by:

$$RF = (RF)_{R} + (1 - (RF)_{R}) \times (RF)_{B}$$

(59)

where $(RF)_{R}$ is the fraction of fission gas released by recoil and $(RF)_{B}$ is the fraction of the remaining fission gas released by diffusion.

Direct recoil is accounted for by geometrical considerations using the respective molar fractions of Kr and Xe, $f_{Kr}$ (-) and $f_{Xe}$ (-):

$$(RF)_{R} = f_{Kr} \times (RF)_{R,Kr} + f_{Xe} \times (RF)_{R,Xe}$$

(60)

$$(RF)_{R,i} = 0.25 \times \frac{r_{Kr}^3 - (r_{i} - r_{Kr})^3}{r_{Kr}^3}$$

(61)

$$r_{i} = 10 \times \frac{r_{i,U} + 0.5 \times r_{i,O} + 0.5 \times r_{i,C}}{\rho_{K}(1 + \frac{u}{U})}$$

(62)

where $r_{i}$ ($\mu$m) is the radius of the kernel, $\rho_{K}$ (g/cm$^3$) is the density of the kernel, $r_{i,U}$, $r_{i,O}$, and $r_{i,C}$ are the mean ranges (mg/cm$^2$) of Kr and Xe in uranium, oxygen, and carbon, respectively ($r_{Kr,U} = 11.7$ mg/cm$^2$, $r_{Kr,O} = 3.3$ mg/cm$^2$, $r_{Kr,C} = 3.1$ mg/cm$^2$, $r_{Xe,U} = 8.3$ mg/cm$^2$, $r_{Xe,O} = 2.3$ mg/cm$^2$, $r_{Xe,C} = 2.2$ mg/cm$^2$) [17], and O/U (-) and C/U (-) are the oxygen to uranium and carbon to uranium atomic ratios.

Diffusive release to the grain boundaries is estimated by the Booth equivalent sphere diffusion model [18]:

$$(RF)_{B} = 1 - \frac{6}{\pi^2n^2t} \times \sum_{n=1}^{\infty} \left( \frac{1-e^{-n^2 \pi^2 n^2 D x^2}}{n^2 \pi^2 n^2} \right)$$

(63)

which corresponds to the fraction diffused out of a sphere of radius a (m) with diffusivity D (m$^2$/s) during time t (s). In the case of a fuel kernel, the effective radius for diffusion is taken equal to the average radius of a kernel grain (~10 $\mu$m). The diffusivity is an effective diffusion coefficient which accounts for intrinsic, radiation-enhanced, and thermal diffusion [19]:

$$D = 7.6 \times 10^{-10} \times e^{-\frac{35225}{T}} + s^2 \times j_{v} \times \sqrt{K'/j_{v}^2 + 2 \times 10^{-40} \times R_{f}}$$

(64)

$$j_{v} = 10^{13} \times e^{-\frac{27778}{T}}$$

(65)

$$K' = \frac{K \times B_{u}}{t}$$

(66)

where T (K) is the temperature of the kernel, $s (=3 \times 10^{-10}$ m) is the atomic jump distance, $j_{v}$ (s$^{-1}$) is the cation vacancy jump rate, K’ is the rate of defect production per atom and is obtained from the damage
rate \( K (=10^4 \text{ defects/fission}) \) and the burnup \( B_u (\text{FIMA}) \), \( Z (=2) \) is the number of sites around a point defect where recombination is inevitable, and \( R_f (\text{fission/m}^3\text{-s}) \) is the fission rate density.

### 3.2.6. Internal Gas Pressure

Fission gas released from the kernel accumulates in the void volume of the particle (porosities in the kernel and buffer plus the volume of the buffer-IPyC gap) where it builds up the internal pressure. The pressure, \( P (\text{Pa}) \), is calculated using the ideal gas law whose equation of state is given by:

\[
P = \frac{n_{fg} \times R \times T}{V}
\]

where \( n_{fg} (\text{mol}) \) is the inventory of fission gas (Kr+Xe) occupying the void volume \( V (\text{m}^3) \) at temperature \( T (\text{K}) \) and \( R (8.3145 \text{ J/K}\cdot\text{mol}) \) is the ideal gas constant. The inventory of krypton and xenon is obtained from fission gas release, while the void volume is obtained by calculating the variation in density of the kernel, buffer, and IPyC, which determines the porosities and volume of the buffer-IPyC gap. The temperature is averaged over the void volume.

### 3.2.7. Palladium Penetration

The fission product palladium is known to attack SiC at localized reaction sites. Based on the international historical database, the penetration rate of palladium into SiC, \( \dot{P}_{\text{Pd}} (\mu\text{m/day}) \), has been found to have an Arrhenius temperature dependence given by [20]:

\[
\dot{P}_{\text{Pd}} = 38.232 \times e^{-11342.3/T}
\]

where \( T (\text{K}) \) is the temperature of the SiC. The SiC layer is conservatively considered failed when the penetration reaches 50% of its thickness.

### 3.2.8. Fission Product Transport

The transport of mobile fission products through a TRISO particle is modeled by Fick’s laws of diffusion using effective diffusion coefficients:

\[
\frac{\partial C}{\partial t} + \nabla J - S = 0
\]

\[
J = -D \times \nabla C
\]

where \( C (\text{atom/m}^3) \) is the concentration of the diffusing species, \( t (\text{s}) \) is the diffusing time, \( J (\text{atom/m}^2\cdot\text{s}) \) is the diffusive flux, \( S (\text{atom/m}^3\cdot\text{s}) \) is the production rate of the diffusing species (fission products), and \( D (\text{m}^2/\text{s}) \) is the diffusivity of the diffusing species in the diffusing medium.

An international database has been assembled by the International Atomic Energy Agency (IAEA) and serves as a reference for fission product transport in TRISO modeling codes [21]. The diffusivities are available for Ag, Cs, Sr, and Kr and are expressed as temperature-dependent Arrhenius functions:

\[
D = D_1 \times e^{-Q_1/RT} + D_2 \times e^{-Q_2/RT}
\]

where \( R (8.3145 \text{ J/K}\cdot\text{mol}) \) is the ideal gas constant and the pre-exponent coefficients, \( D (\text{m}^2/\text{s}) \), and activation energies, \( Q (\text{kJ/mol}) \), are provided by the IAEA [21]. Diffusion coefficients for the kernel are values derived from experimental data with UO\(_2\) fuel. These values are used due to lack of data for UCO kernels.
4. UCO TRISO Fuel Performance Methodology
The purpose of the BISON TRISO model is to assess the structural integrity and leak-tightness to fission products of TRISO-coated UCO fuel particles under neutron irradiation. The calculation flow chart is shown in Figure 2 and summarized below:

- The fission rate density (code input) is used to calculate the heat generation rate in the TRISO particle and the fission product inventory (including fission gas that contributes to internal pressure); combined with the boundary temperature, the fission rate is used to solve the heat equation in the TRISO particle and determine its temperature profile.
- The temperature in a TRISO particle is used to calculate the internal gas pressure corresponding to its fission gas inventory; combined with the input fast neutron fluence, the temperature also drives the material properties used to compute the stress levels in the coating layers and the diffusivities used in fission product diffusion calculations.
- Using Weibull statistics, the stress levels determine the failure probability of the TRISO particles.
- Combined with diffusivities, obtained from the thermal analysis, the failure probability is used to calculate the diffusion and release of fission products from the intact and potentially failed TRISO particles.

Figure 3 depicts the methodology used to calculate the failure probability of a population of TRISO particles. The methodology relies on a Monte Carlo approach where each particle corresponds to a set of statistically sampled parameters from the distributions of as-fabricated fuel characteristics (e.g., dimensions, densities, etc.) that can be found amongst the particles in a pebble. For each sample, BISON runs a 1D model of the particle over the required time steps of the simulation. The 1D approach allows a fast determination of the stress distributions in the coating layers if the particle is spherical. For particles with localized flaws (i.e., aspherical particles and particles with cracked IPyC), an adjustment of the stress distributions is necessary to account for increased stress caused by these flaws. This adjustment is provided through so-called “2D stress factors”. The 2D stress factors are obtained by running 2D simulations aimed at developing correlation functions that maps the stress in an aspherical particle or a particle with cracked IPyC as a function of its dimensions, aspect ratio, and irradiation conditions. The 1D simulation then uses these correlations to calculate the required correction factors for asphericity or IPyC cracking and determine whether or not the flawed particle fails.

Figure 2. BISON flow chart for calculation of TRISO performance.
At each time step, the following failure mechanisms are checked:

- Pressure vessel failure of a spherical or aspherical particle – Failure is assumed when the maximum tangential tensile stress induced in the SiC layer by internal gas pressure is greater than the fracture strength of the SiC.
- IPyC cracking – Cracking of the IPyC is assumed when the maximum tangential tensile stress in the PyC layer is greater than its fracture strength. A cracked IPyC induces additional stress in the SiC layer.
- SiC failure is assumed when the maximum tangential tensile stress induced in the SiC layer by the cracked IPyC is greater than its fracture strength.
- Pd penetration – Failure is assumed when Pd penetration exceeds half the thickness of the SiC layer. In this case, the SiC layer loses its structural integrity and leak-tightness to fission products and is assigned a non-retentive diffusivity. Pd penetration is still to be implemented in the failure probability calculation scheme.

In all cases, the maximum stress ($\sigma_{\text{max}}$) is compared to a strength that is sampled from a Weibull distribution (mean strength $\sigma_{\text{m}}$ and modulus $m$) to determine whether or not failure (i.e., IPyC cracking, SiC failure) occurs.

The methodology laid out in Figure 3 also includes the simulation of fission product diffusion, which is also evaluated at each time step for each Monte Carlo sample. The fission product diffusion calculations combine the release fractions (release normalized to calculated inventory) of all TRISO particles in the Monte Carlo sample. Coating layers that have been determined failed by stress analysis are assigned a large diffusivity (e.g., $10^6$ m$^2$/s) to model the loss of retention power of that layer. Release is calculated by Fickian diffusion, while inventory is obtained from fission rate density and fission yields.

5. Preliminary Results

BISON was compared to the Particle Fuel Model (PARFUME [10]) code that has been developed at INL since the early 2000’s to support the AGR program. A benchmark was developed using existing PARFUME results [22]. Both codes were used to predict the performance of a UCO TRISO particle with characteristics detailed in Table 2.
Table 2. Fuel parameters used in modeling.

| Category          | Parameter                  | Nominal Values ± Standard Deviation |
|-------------------|----------------------------|------------------------------------|
| Fuel Characteristics | $^{235}$U enrichment (wt%) | 15.5                               |
|                   | C/U (atomic ratio)         | 0.4                                |
|                   | O/U (atomic ratio)         | 1.5                                |
| Particle geometry | Kernel diameter ($\mu$m)   | 425±10                             |
|                   | Buffer thickness ($\mu$m)  | 100±10                             |
|                   | PyC thickness ($\mu$m)     | 40±3                               |
|                   | SiC thickness ($\mu$m)     | 35±2                               |
| Fuel properties   | Kernel density (g/cm$^3$)  | 11.0                               |
|                   | Kernel theoretical density(g/cm$^3$) | 11.4                              |
|                   | Buffer density(g/cm$^3$)   | 1.05                               |
|                   | Buffer theoretical density(g/cm$^3$) | 2.25                              |
|                   | PyC density(g/cm$^3$)      | 1.9±0.02                           |
|                   | IPyC/OPyC BAF              | 1.9±0.02                           |

The UCO fuel was modeled under three different sets of irradiation conditions, as shown in Table 3.

Table 3. Irradiation conditions.

| Case | EFPD | Burnup (%FIMA) | Fast fluence ($10^{25}$ n/m$^2$, E > 0.18 MeV) | Irradiation Temperature (°C) |
|------|------|----------------|-----------------------------------------------|-------------------------------|
| 1    | 500  | 13.5           | 5                                             | 700                           |
| 2    | 500  | 13.5           | 5                                             | 1000                          |
| 3    | 500  | 13.5           | 5                                             | 1300                          |

For each of the three cases of Table 3, the tangential stress in the SiC layer is plotted in Figure 4. Preliminary results show a good agreement between BISON and PARFUME. The slight under-prediction by BISON on the maximum compressive stress (negative stress values in Figure 4) early in irradiation seems to be partially compensated at higher fluence by the higher fission gas inventory calculated by PARFUME (see Figure 5) as release of these fission gases builds up internal pressure that results in increasing tensile stress in the SiC layer. Nevertheless, the discrepancies between both codes are still under investigation.

Figure 4. Tangential stress in SiC layer.

Figure 5. Internal gas pressure.
Finally, both codes were used to compute the probability of cracking of the IPyC layer. Results are reported in Table 4 and show decent agreement with BISON over-predicting PARFUME by 2% at 700°C and by 30% at 1000°C but under-predicting by 30% at 1300°C. Analysis is ongoing to explain these differences.

| Condition | PARFUME   | BISON   |
|-----------|-----------|---------|
| 1         | 8.94×10⁻¹ | 9.11×10⁻¹ |
| 2         | 5.48×10⁻² | 7.10×10⁻² |
| 3         | 1.16×10⁻³ | 0.80×10⁻³ |

6. Conclusion
A new TRISO model has been implemented in BISON to expand the code’s ability to model the fuel performance of TRISO particles, including its probability of failure.

Updated material properties were added to the code and a methodology was developed to allow Monte Carlo sampling of a population of TRISO particles to account for the particle-to-particle statistical variations in physical dimensions and fuel (e.g., density) and material (e.g., strength) properties that arise from the fuel fabrication process. The Monte Carlo sampling allows to properly capture the probability of failure of the fuel within that population of TRISO particles.

A benchmark was developed to compare BISON and AGR’s code PARFUME. Preliminary results show a decent agreement in stress level and failure probability, but BISON results are still being analyzed to find out the origin of the discrepancies.

Future work will involve developing the tables of 2D stress factors to allow 1D calculation of aspherical particles and particles with cracked IPyC layers and combine all stress analysis results into fission product release calculations. Additional developments will include accounting for pre-existing defects from fuel fabrication that contribute to increasing fission product release. Finally, Pd penetration will be implemented as part of the failure probability calculation scheme.

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