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Review

A review of TRISO fuel performance models

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ABSTRACT

Several advanced reactor designs incorporate tristructural isotropic (TRISO) fuel particles to achieve high coolant temperature and high fuel burnup levels and thus require reliable and robust fuel performance models (FPMs) to evaluate reactor performance. This manuscript provides a detailed and concise review of the numerous published TRISO FPMs. The article begins with a brief review of TRISO fuel particles, before describing the important fuel behavior and failure mechanisms of TRISO fuel. Suggested material property correlations for use in TRISO fuel performance modeling are summarized with an emphasis on the limits of validity for those correlations and notes regarding their use and origin. A review of the major historical and current TRISO FPMs assesses each model's capabilities and origin and provides a systematic comparison of the codes to document similarities and differences in their features. Finally, areas of improvement and unsolved problems are discussed that may limit the accuracy of TRISO fuel performance modeling.

Contents

1. Introduction

Tristructural isotropic (TRISO) fuel particles represent the chosen fuel technology for various nuclear reactor design projects that involve goals of high coolant temperatures or high burnup performance of nuclear fuel. TRISO fuel was originally developed and used in Germany for the AVR reactor, a 46 MW_{th} (15 MW_e) prototype pebble bed reactor, and the Thorium High Temperature Reactor (THTR-300), a 750 MW_{th} (300 MW_e) reactor; both of these reactors were high-temperature gas-cooled reactors (HTGRs) [1–4]. China currently uses TRISO fuel in its 10 MW_{th} prototype pebble bed High Temperature Reactor (HTR-10), and Japan uses TRISO fuel in its 30 MW_{th} prismatic core High Temperature Test Reactor (HTTR) [5–7]. TRISO fuel programs currently exist in the United States (US), France, the United Kingdom, Russia, and South Africa. The Next Generation Nuclear Plant (NGNP) program in the US, along with other projects in the US and around the world, plans to use TRISO fuel [8].

TRISO particles typically consist of five distinct regions. At the center of the particle is the fuel kernel, typically an oxide, carbide or oxycarbide, which contains the nuclear fuel: uranium, plutonium, thorium, or transuranic elements (TRU). A porous carbon buffer surrounds the kernel, with the objective to attenuate recoiling fission fragments and to accommodate internal gas buildup and particle dimensional changes. The outer layers

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consist of an inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer. The PyC layers are relatively dense pyrolytic carbon, typically at about 90% of their theoretical density (TD) of 2.2 g/cm^3 [9]. The SiC layer acts as the main pressure vessel for the particle, withstanding the stresses from internal gas pressure buildup and other sources, and also provides a diffusion barrier to prevent the release of gaseous and metallic fission products (FPs). The possibility of replacing the SiC layer with ZrC has been suggested and is currently being evaluated [10–13]. The PyC layers protect the SiC layer from chemical attack during TRISO particle operation, act as additional diffusion barriers to FPs, and the IPyC protects the fuel kernel from corrosive gases used to deposit the SiC layer [9].

Table 1 provides typical dimensions and densities for a UO_2 TRISO particle, based upon a German 500 μm kernel [9]. The actual dimensions and densities vary according to design purposes and manufacturing processes. Recent studies have shown that variations in manufacturing methods and processes can yield drastic differences in the quality and capabilities of the TRISO particles produced [14].

While the TD of the kernel is not listed, exercising careful controls of kernel manufacturing processes generally yields nearly full density (about 97% TD) fuel.

Fig. 1 provides a simple illustration of a TRISO particle, as reproduced from Ref. [15]. Fig. 2 shows a micrograph of an actual TRISO particle, taken from Ref. [16], in which the porous nature of the buffer and some cracking in the coating layers are visible.

Liu et al. [17] performed a brief review of TRISO fuel performance models (FPMs) that heretofore was the only such survey in the literature; however, it failed to document or describe significant aspects of the various FPM codes, nor did it assess their similarities and differences. A more significant and complete survey of the numerous published FPMs is needed to both identify the strengths and weaknesses of existing TRISO fuel performance modeling and identify areas that require improved sub-models or additional data.

Table 1
Nominal parameters for a German UO_2 TRISO particle [9].

Layer	Density (g/cc)		Outer radius (μm)
	Actual	Theoretical	
Kernel	10.96	–	250
Buffer	1.1	2.2	345
IPyC	1.7	2.2	385
SiC	3.2	3.2	420
OPyC	1.7	2.2	460

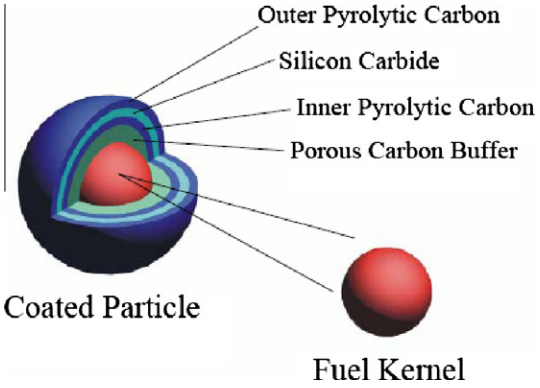

Fig. 1. Illustrative cutaway drawing of a TRISO fuel particle, as reproduced from Ref. [15].

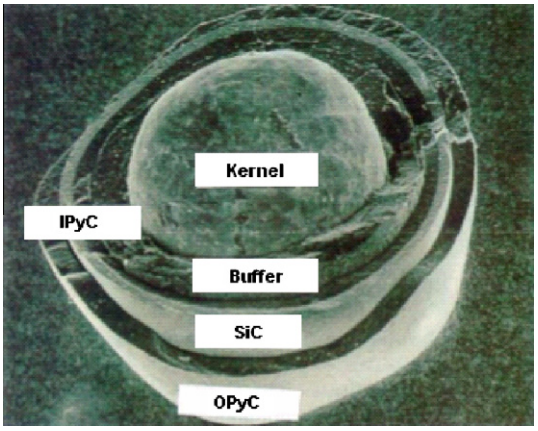

Fig. 2. Micrograph of an actual TRISO fuel particle, as reproduced from Ref. [16].

This manuscript focuses on reviewing the current state of TRISO fuel performance models (FPMs) and thus will not provide an extensive discussion of observed TRISO fuel behavior and failure mechanisms, which have been recently reviewed by Petti and co-workers at Idaho National Laboratory (INL) [9,14,18–23] and by others elsewhere [24,25]. The interested reader is also directed to the many excellent reviews of TRISO performance results [9,14,19,25–34]. To provide context for the review of the FPMs Sections 2 and 3 briefly summarize fuel behavior and failure mechanisms. Section 4 provides an assessment of the available materials databases and Section 5 then describes the available fuel performance models. Section 6 provides a critical assessment of the key challenges for fuel performance codes to predict TRISO fuel behavior at high temperature and high burnup. Section 7 presents the conclusions of this review.

Table 2 defines the symbols and nomenclature used throughout this article, following the convention established by Miller and co-workers at INL [9,35].

2. Fuel behavior

A multitude of phenomena observed in TRISO fuel particles undergoing irradiation and fission have been identified as important aspects to understand and accurately model. In particular, we will review the important mechanisms of heat transfer, fission product production and transport, oxygen release from the fuel

Table 2
Symbols and nomenclature used throughout this article, following from Refs. [9,35].

Nomenclature [9,34]	
α	Thermal expansion coefficient of a coating (K^{-1})
E	Modulus of elasticity of a coating layer (MPa)
c	Irradiation-induced creep coefficient of a PyC layer (MPa n/m^2, $E > 0.1$ MeV)
μ	Poisson's ratio of a coating layer
ν	Poisson's ratio in creep for a PyC layer
$\dot{S}$	Dimensional change rate ((n/m^2)$^{-1}$, $E > 0.1$ MeV)
Subscripts	
a, b	Inner or outer (radius)
kern	Fuel kernel
PyC	PyC layer of interest
SiC	SiC layer
t	Tangential direction
TD	Theoretical density

kernel, internal gas pressure buildup, irradiation effects on TRISO materials, and variability in TRISO particles due to manufacturing processes.

Heat transfer directly impacts any nuclear fuel due to the importance of conducting the heat generated by fission events out to the working coolant in the system. The resulting temperature distributions and gradients affect many other phenomena and material properties.

The simultaneous production, destruction (through radioactive decay or nuclear reactions with neutrons or gamma rays), and transport of fission products (FPs) represents another key behavior in TRISO fuel. Gaseous FPs, with Xe and Kr typically considered the dominant species, build up in the kernel and buffer of the particle and exert pressure on the PyC and SiC coatings. Some FPs migrate out of the kernel and can escape through the PyC and SiC layers to become radiological source terms in the matrix and coolant, impacting plant operational safety.

Oxygen atoms released from the fuel kernel to the buffer region, due to both thermal solubility and fission events consuming the heavy metal atoms in the kernel, can lead to the formation of CO or CO_2 gas via the reactions

$$O_2 + C = 2CO \quad (1)$$

and

$$2CO = CO_2 + C \quad (2)$$

and increase the internal pressure of the particle. The partial pressures or CO, CO_2, and O_2 are thermodynamically controlled and also impacted by the composition of the fuel.

Fission product, CO, and CO_2 gases accumulate in the buffer void volume and exert outward pressure on the coating layers. This internal gas pressure builds up over time and has traditionally been the dominant behavior suspected of causing TRISO fuel particle failures. Fission products diffuse through the fuel kernel, outward through the buffer and coating layers, and then through the graphitic matrix, which can produce mobile radioactive source terms.

PyC initially shrinks, and then later swells, when irradiated with fast neutrons (defined in this manuscript as neutrons with energies above 0.1 MeV). The seminal 1993 Combustion Engineering–General Atomics (CEGA) report [36] defined this as Irradiation-Induced Dimensional Change (IIDC) and provided a reasonable description of the process. More detailed descriptions exist elsewhere [37,38]. SiC undergoes a similar irradiation-induced volumetric change, though most FPMs ignore this because it is generally believed to be negligible compared to other degradation behavior in PyC and SiC [9].

Stresses and strains in the coating layers result from the phenomena described above, with additional contributions from irradiation creep and the differential thermal expansion of each region. Displacements of the layer interfaces occur due to these strains and solid fission product swelling in the fuel kernel. These stress–strain–displacement relationships must be well understood for reliable TRISO fuel design and performance since they directly impact the maximum stress predicted in the SiC pressure boundary. A viscoelastic model is often used for the IPyC–SiC–OPyC system [35], with the SiC layer treated as an isotropic elastic material since SiC is a ceramic and thus undergoes very little (if any) plastic deformation before failure.

The material properties (e.g., thermal conductivity and Young's modulus) of each layer vary during operation. The properties should vary with temperature, porosity, accumulated fast fluence, and fuel burnup level. While fully accurate materials property calculations would incorporate all of these parameters and yield precise knowledge, the material property correlations currently available fall significantly short of this. The best known correlations should be used for each property in fuel models, with flexibility designed into the models to allow future revisions.

Lastly, the dimensions and densities of each layer of a TRISO particle vary from particle to particle due to variability in the manufacturing processes. The expected manufacturing tolerances for a TRISO particle of a particular design using specific manufacturing methods and processes can be identified and accounted for in fuel models. The calculated failure fraction of a set of "real" particles based upon nominal parameters and their manufacturing tolerances determines the predicted performance of the fuel; if it is too high then the fuel design or reactor design must be changed or, alternatively, the manufacturing tolerances can be tightened. Adequate sampling of statistical variations in particle parameters (e.g., layer thicknesses and densities) for a representative population of particles requires a large number of calculations, and thus necessitates a computationally efficient fuel performance model. Wang [16] presents a detailed discussion about manufacturing uncertainties and quantifies the typical value ranges for several TRISO particle parameters, including layer thicknesses and densities.

3. Failure mechanisms

Fuel performance modeling for any fuel form directly depends upon identifying the possible failure modes for the fuel and which modes are limiting. Once the limiting failure modes are known, computational models can be constructed to assess how the fuel behaves relative to these criteria. For example, if a fuel is limited by creep rupture then creep rate calculations determine fuel performance. Likewise, detailed stress calculations are necessary to model and assess performance of a fuel limited by through-clad cracking due to stresses. TRISO fuel particles have been experimentally observed to possess multiple possible failure modes, which are categorized as being driven by either one-dimensional (1D) or three-dimensional (3D) effects [9,19].

The dominant 1D failure mechanism for TRISO fuel particles involves pressure vessel failure, where the SiC layer develops a through-thickness crack resulting from a tensile stress that exceeds the fracture strength of the material. This fracture stress for SiC varies significantly in the literature but is on the order of 350–400 MPa [9]. The classic definition for this pressure vessel failure assumes that the SiC layer fails catastrophically once a crack initiates and that there is enough energy in the system released upon SiC cracking that the PyC layers crack in the same location. More modern approaches to pressure vessel failure explicitly calculate separate stresses and through-layer crack probabilities for the SiC layer and each PyC layer; models using this approach require that all three layers must fail for the particle to be considered "failed". The tangential stress at the IPyC/SiC interface usually represents the limiting stress in the SiC layer and depends upon multiple phenomena, as illustrated in Fig. 3. More rigorous fracture

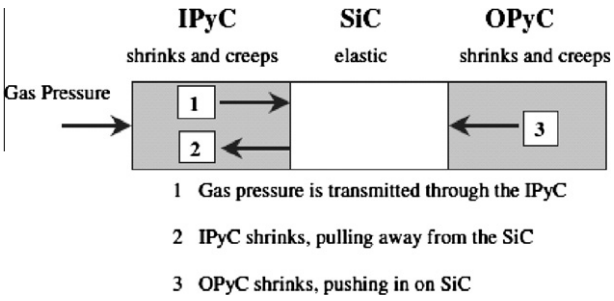

Fig. 3. Illustration of the different fuel behaviors driving SiC stress, as reproduced from Ref. [9].

mechanics approaches have generally not been performed in TRISO fuel performance modeling.

Both PyC layers initially experience irradiation-induced radial shrinkage; during this phase, the outward stress due to gas pressure and irradiation creep of PyC is counteracted by an inward stress from PyC shrinkage. However, after an initial densification stage, PyC begins exhibiting irradiation-induced swelling. This produces a situation where internal gas pressure, the PyC IIDC, and PyC irradiation creep all act outward on the coating layers. Thus, the tangential stress in the SiC layer has a beginning of life (BOL) stress level determined by manufacturing and system stresses (usually about 0 MPa), decreases to a maximum compressive stress (nominally on the order of −100 MPa at a fast fluence of roughly 0.5×10^{25} n m^{-2}), and then increases until end of life (EOL). If the stress becomes tensile (positive) before EOL it may exceed the presumed failure, or fracture, strength.

3D failure modes observed in TRISO fuel particles include shrinkage cracks within the IPyC layer, IPyC/SiC debonding, particle asphericity, kernel migration (the so-called "amoeba effect"), and SiC coating thinning. A brief description of each mechanism is given below, while Refs. [9,19] each provide more detailed descriptions.

Irradiation-induced shrinkage of the IPyC can cause a partial or through-coating crack to form in the IPyC [16]. Partial or full debonding of the IPyC and SiC layers at their interface can occur if the differential radial stress exceeds the IPyC/SiC interfacial bond strength [22]. Particle asphericity refers to a TRISO particle's geometric deviation from a perfect sphere [9,22]. Kernel migration, the movement of the center of mass of the fuel kernel away from the center of the TRISO particle, results from CO gas migration down the thermal gradient in a TRISO toward the cold side of the particle and subsequent formation of CO_2 and solid-phase carbon due to the combination of two CO molecules. Over time, solid carbon builds up on the cold side of the buffer and "pushes" the kernel to migrate toward the hot side of the TRISO particle, as shown in Fig. 4. Each of these mechanisms cause changes in temperature or stress distributions and may lead to particle failure.

Lastly, experimental observations indicate that chemical attack of the SiC by species such as palladium (Pd) can thin the coating. Erosion rates are low but can be appreciable for high stress environments or long irradiation times [14,39]. Chemical attack rates have been shown to accelerate in the presence of defects such as cracks in the IPyC layer or IPyC/SiC debonding. Accurate modeling of fission product diffusion allows estimates of SiC thinning rates due to chemical attack by Pd or other species.

It should be noted that while the above failure mechanisms represent the dominant known failure modes for TRISO fuel particles, additional failure mechanisms likely exist.

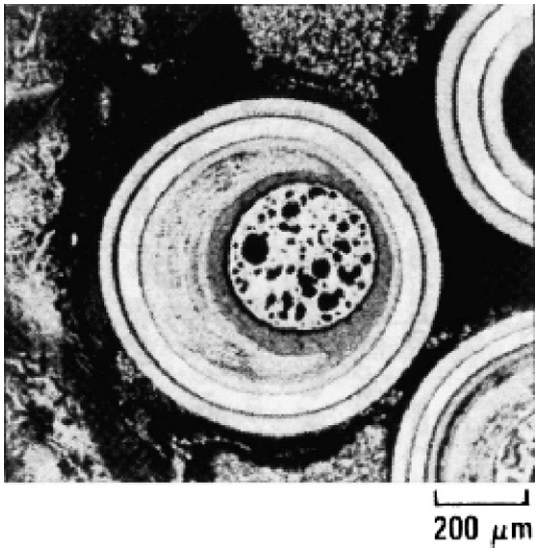

Fig. 4. Micrograph showing kernel migration in a TRISO particle, as reproduced from Ref. [19].

4. Material properties

Several literature reviews have identified and discussed the best available correlations and values for material properties to model fuel [9,40,41], PyC [9,26,36], and SiC [9,26,36] in TRISO FPMs. In particular, Snead [42] provides a review and handbook of SiC properties for fuel performance modeling containing especially useful information and further resources. A summary of the important findings can be found below, but the interested reader can find more details in the references cited throughout this section.

Table 3 summarizes the key material properties for a UO_2 fuel kernel. Modifications or additions to these properties would be necessary for hypostoichiometric fuel forms (e.g., $UO_{1.7}$) or non-uranium fuels (e.g., PuO_2). τ represents the fuel burnup in units of % FIMA and P is the fractional porosity of the fuel kernel. Though not included in the table below, it is important to note that Ref. [41] provides diffusion coefficients for several fission products in UO_2 or ThO_2 fuel kernels; and Ref. [47] documents diffusion coefficients for fission products in UO_2 or UCO fuel kernels.

Recommended correlations and values for the key material properties of PyC are summarized in Table 4. P is the fractional porosity of the PyC layer being analyzed, Φ represents the neutron fluence in units of 10^{25} n m^{-2}, and BAF_0 is a measure of the anisotropic grain orientation (nominally 1.02–1.05 [9]). The buffer PyC is assumed to have isotropic grain orientation. $M_{Irr.Creep}$ is a user-specified PyC irradiation creep constant multiplier with a value of 2.0 based upon Idaho National Laboratory (INL) recommendations [9]. The radial (parallel) and tangential (normal) directions are sometimes denoted by the subscripts 1 and 3, respectively. It must be noted that the UK correlation for PyC thermal conductivity shown below yields significantly higher thermal conductivities for the PyC buffer layer than German correlations recommend [9]; since the magnitude of the temperature gradient across a TRISO fuel particle is almost entirely determined by the temperature drop across the buffer layer, this could have a large impact on fuel performance calculations. Ref. [47] provides diffusion coefficients for several fission product species in the carbon buffer layer and dense PyC layers, as well as matrix graphite.

The recommended material properties for SiC (β-CVD SiC in particular) are summarized in Table 5, and come from multiple sources as previously noted. P represents the fractional porosity and Young's modulus has units of GPa instead of MPa. Much more detailed information, as well as experimentally measured material property data, can be found in Snead's SiC handbook [42]. Ref. [47] provides diffusion coefficients for several fission product species in SiC.

5. Existing fuel performance models

Numerous TRISO FPMs have been developed over the years. Different organizations and projects generally each created their own model due to the unavailability of other models, and/or the developers desire to either customize the code to their specific needs or to address improvements in knowledge. Most TRISO FPMs involved projects using either thorium or uranium oxide fuel kernels. Furthermore, most of these fuel kernels were stoichiometric (e.g., UO_2) rather than hypostoichiometric (e.g., $UO_{1.7}$).

Table 3
Summary of recommended material properties for TRISO fuel kernels.

Parameter (units)	Recommended correlation or value	Source and notes
Thermal conductivity, k (W/m K)	$k_{\text{fuel}} = K_{1d}K_{1p}K_{2p}K_{4r}k_{0,\text{fuel}}$ $K_{1d} = \left(\frac{1.09}{\tau^{3.265}} + \frac{0.0643}{\sqrt{\tau}}\sqrt{T_{\text{kern}}}\right)\arctan\left(\frac{1}{\frac{1.09}{\tau^{3.265}} + \frac{0.0643}{\sqrt{\tau}}\sqrt{T_{\text{kern}}}}\right)$ $K_{1p} = 1 + \frac{0.019}{3 - 0.019\tau}\frac{1}{\left(1 + \exp\left(-\frac{T_{\text{kern}} - 1200}{100}\right)\right)}$ $K_{2p} = \frac{1-P}{1+2P}$ $K_{4r} = 1 - \frac{0.2}{1+\exp\left(\frac{T_{\text{kern}} - 900}{80}\right)}(1 - \exp(-\tau))$	Based on UO_2 work from Ref. [9]
Solid FP swelling rate, $\dot{S}_S$ (%/GWd/t_{HM})	$\dot{S}_S = \frac{d\left(\frac{\Delta V}{V}\right)}{d\tau} = 0.06$	Ref. [9]

Table 4
Summary of recommended material properties for porous (e.g., buffer) and dense PyC.

Parameter (units)	Recommended correlation or value	Source and notes
Thermal conductivity, k (W/mK)	$k_{PyC} = 10.98222\left(\frac{1-P}{1+2P}\right) + 0.00444$	UK correlation, Tables 1–9 of Ref. [9]
Anisotropic orientation parameters	$R_3 = \frac{2}{2+\text{BAF}_0}$ and $R_1 = \frac{1-R_3}{2}$	Ref. [35]
Young's modulus, E (MPa)	*Buffer*: $E = 34{,}500\exp(-2.03P)$ *Dense PyC*: $E_1 = k_\rho k_{\text{Lc}} k_\Phi k_{\text{T}} k_{\text{BAF01}} E_{01}$ $E_3 = k_\rho k_{\text{Lc}} k_\Phi k_{\text{T}} k_{\text{BAF03}} E_{03}$ $E_{01} = E_{03} = 25{,}500$ $k_\rho = 0.384 + 0.324\rho$ $k_{\text{Lc}} = 2.985 - 0.662\text{Lc}$ $k_\Phi = 1 + 0.23\Phi$ $k_{\text{T}} = 1 + 0.00015([T\,^\circ\text{C}] - 20)$ $k_{\text{BAF01}} = 0.481 + 0.519\text{BAF}_0$ $k_{\text{BAF03}} = 1.463 - 0.463\text{BAF}_0$	Tables 1–11 of Ref. [9]. Lc is the user-specified crystallite size, currently assigned a value of 3.0 based upon the suggested range in Ref. [9]
Poisson's ratio, μ (/)	*Buffer:* $\mu = 0.23$ *Dense PyC:* $\mu_{12} = 0.766R_3 - 0.275$ $\mu_{13} = -0.884R_3 + 0.825$ $\mu_{31} = \frac{\mu_{13}E_3}{E_1}$	US correlations from Tables 1–12 of Ref. [9]
Coefficient of thermal expansion, α ($10^{-6}\,\text{K}^{-1}$)	*Buffer:* $\alpha = 3.5$ *Dense PyC:* $\alpha_1 = 40(R_1 - 1)^2 + 1.11$ $\alpha_3 = -41.67R_3 + 33.33$	US correlations from Tables 1–8 of Ref. [9]
IIDC rates, $\dot{\varepsilon}$ $(10^{25}\,\text{nm}^{-2})^{-1}$	*Buffer:* $\dot{\varepsilon}_r = \dot{\varepsilon}_t = -0.176\exp(-1.75\Phi)$ *Dense PyC:* $\dot{\varepsilon}_r = -0.077\exp(-\Phi) + 0.031$ $\dot{\varepsilon}_t = -0.036\exp(-2.1\Phi) - 0.01$	German correlations from Tables 1–15 of Ref. [9]
Irradiation creep parameters, K (MPa nm^{-2})$^{-1}$ ν (/)	$K = K_0(1 + 2.38(1.9 - \rho))M_{\text{Irr,Creep}}$ $K_0 = 1.996\times10^{-29} - 4.415\times10^{-32}([T\,^\circ\text{C}])$ $+3.6544\times10^{-35}([T\,^\circ\text{C}])^2$ $\nu = 0.4$	Based on US correlations from Tables 1–14 of Ref. [9] but modified to have a multiplier and $\nu = 0.4$ per Ref. [9]

The existing FPMs can be categorized in various ways. One method divides them into models that use closed-form analytical solutions for the stress–strain–displacement relationships and those that use numerical approaches, such as finite element analysis or methods (FEA or FEM). The various techniques used for heat transfer solutions, internal gas generation, and pressure calculations can greatly affect the predicted results; however, such differences generally do not represent as fundamental difference in solution technique and code capabilities as selecting between closed-form or numerical methods for solving the stress–strain–displacement equations.

The dominant approach to calculating the stresses, strains, and displacements necessary in a TRISO FPM to predict fuel performance has been a closed-form analytical solution developed at INL [9,35,43]. This approach reduces the problem to a 1D symmetric sphere and then solves the system of equations from the center of the fuel kernel radially outward to the OPyC/matrix interface boundary. This is a simplification in that it ignores asphericity, temperature gradients across a TRISO particle, and other factors; however, it enables the model to calculate failure fractions for large sets of possible TRISO particles within reasonable time frames. Miller at INL laid the groundwork for such a closed-form

Table 5
Recommended material properties for SiC.

Parameter (units)	Recommended correlation or value	Source (Refs.)
Thermal conductivity, k (W/m K)	$k_{SiC} = k_{0,SiC}(3.91112 \times 10^{-2} \cdot \exp(2.24732 \times 10^{-3} \cdot T_{SiC}))(1-P)$ $k_{0,SiC} = 42.58 + \frac{-1.5564 \times 10^4}{T_{SiC}} + \frac{1.2977 \times 10^7}{(T_{SiC})^2} + \frac{-1.8458 \times 10^9}{(T_{SiC})^3}$	[9]
Coefficient of thermal expansion, α (10^{-6} K^{-1})	if $T_{SiC} \leq 1273$ K $\alpha = -1.8276 + 0.0178T_{SiC} - 1.5544 \times 10^{-5}T_{SiC}^2 + 4.5246 \times 10^{-9}T_{SiC}^3$ if $T_{SiC} > 1273$ K : $\alpha = 5.0$	[42]
Young's modulus, E (GPa)	$E_1 = E_0 \exp(-3.57P) - 0.04T_{SiC} \exp(\frac{-962}{T_{SiC}})$ $E_0 = 460$	[26]

solution [43], which was then utilized by many organizations and projects throughout the world. Subsequent research observed that assuming a constant Poisson's ratio of 0.5 for PyC during irradiation was likely inaccurate, so Miller generalized the solution to allow for time-dependent values [35]. This updated method, which serves as the basis for much of the current work in TRISO FPMs using closed-form solution approaches, is described in further detail in Boer's doctoral thesis [44]. Boer also includes matrix notation formulation of Miller's technique. A closed-form solution is limited to 1D effects and thus can only predict pressure vessel failure; 3D effects such as cracking or debonding must be accounted for in other ways, as will be discussed later when describing the PARFUME code.

Using numerical methods to solve the full 3D stress–strain–displacement equations for a TRISO particle has been demonstrated as an alternate approach to avoid the simplifications involving a closed-form solution. The ATLAS code developed by the Commissariat à l'Énergie Atomique (CEA) in France uses finite element analysis (FEA) to reach numerical solutions. Comparisons of ATLAS and PARFUME results show reasonable agreement, as discussed in Ref. [9]. It is important to note that while FEA approaches to TRISO fuel performance modeling are very good at modeling 3D effects, they typically are much more computationally intensive than analytical, closed-form approaches and therefore are not as well suited to evaluate statistical variations in particle parameters.

The PARFUME code [9,18,45–47] developed at INL stands out as the state of the art TRISO FPM in the United States. PARFUME uses Miller's closed-form solution approach but incorporates multi-dimensional effects by using fully 3D ABAQUS calculations to aid the 1D model. As described more fully in Ref. [9], a suite of ABAQUS calculations account for 3D effects such as shrinkage cracks in the IPyC or particle asphericity; these effects feed back into the overall fuel performance predictions by using correlations derived to show the impact on 1D symmetric particle calculations. PARFUME accounts for almost all of the known behavior and failure mechanisms in TRISO particles and allows the user to specify the stress boundary condition to model external stresses on a TRISO particle. Recent development efforts in the PARFUME code have involved modeling fission production transport across each layer.

TIMCOAT [16] and PASTA [44,48,49] are extremely similar to PARFUME, since both were based upon the PARFUME code itself. TIMCOAT, developed at MIT, provides a particle/element model for pebble bed or prismatic block geometries [17]. It includes pebble refueling effects, such as temperature swings, and the description of the code notes that future efforts aim to improve calculations of FGR and incorporate chemical attack of the SiC layer [16]. The PASTA code, developed by Boer during his doctoral thesis at TU Delft in The Netherlands, provides 1D stress analysis for TRISO fuels. It models the kernel and buffer as a single effective region and accounts for stresses due to particle–particle and particle–matrix interactions as well as the contributions of helium gas to internal gas pressure in the TRISO.

CEA's ATLAS code, described in Section 2.2 of Ref. [9], represents the leading FPM using numerical 3D solutions. ATLAS provides a particle/element model that incorporates larger scale effects at the element level, explicitly represents and accounts for PyC and SiC layers, takes a thermomechanical approach to fuel performance modeling by tracking pressure and deformation effects, and uses an external stress boundary condition to model particle–matrix interaction effects [17]. As described above, an FEA numerical solver approach to fuel performance modeling explicitly accounts for 3D effects in the TRISO. ATLAS accounts for most of the known behavior and failure mechanisms of TRISO fuel, including pressure vessel failure of the SiC layer, IPyC cracking, debonding, and asphericity. One unique feature of ATLAS is that its FGR calculations explicitly account for fuel structure changes at burnup levels above 10% FIMA.

STRESS3 [50], a UK TRISO FPM, focuses on stresses in the coating layers. It accounts for fission product and CO_2 gases, kernel swelling, residual stresses introduced by kernel sintering during fabrication, mismatches in coefficients of thermal expansion, dimensional changes due to irradiation, and particle–matrix surface effects [17]. STRESS3 addresses pressure vessel, IPyC cracking, and debonding failure mechanisms and uses an internal void volume that changes during irradiation.

Germany's FZJ model [17] and JAERI's model in Japan [17,51] both offer pressure vessel failure only models; the FZJ model only accounts for the SiC layer, while JAERI's model incorporates PyC shrinkage/swelling and independent failures for each PyC and SiC layer. The FZJ model is similar to the jointly-developed GA/KFA model [52], which offers a simple pressure vessel failure prediction without accounting for effects from the PyC layers. The GA/KFA model accounts for a shrinking void volume during irradiation while the JAERI model assumes a fixed void volume that does not change.

The HEISHI code [53] developed by Young at SNL used 1D finite difference calculations to estimate pressure vessel failure probabilities for pebble bed space reactors.

Most of the fuel performance models detailed above do not explicitly model the diffusion of gaseous fission products, but rather utilize more simplified diffusion-based models for fission gas release. PARFUME utilizes a finite difference approach for solving the diffusion equation, including chemical (Fickian) and thermal (Soret) diffusion, and is able to model fission produce diffusion of several species from the kernel outward through the TRISO coating layers and then through a graphite fuel matrix [47]. ATLAS includes a Fickian diffusion model, which can be

Table 6
Summary of several major TRISO fuel performance models.

Code	PARFUME	PASTA	ATLAS	STRESS3	TIMCOAT	GA/KFA	JAERI
Developer	INL (US)	TU Delft (NL)	CEA (FR)	BNFL/NS (UK)	MIT (US)	GA/KFA (US)/(DE)	JAERI (JP)
References	[9,18,45–47]	[44,48,49]	[9,17]	[9,17,50]	[16]	[17,52]	[17,51]
Mission	NPR/AGR, NGNP	PUMA (EU)	FBR MOX	None specified	HTRs	Multiple	HTTR
Assumed geometry	Pebble bed, prismatic	None	None?	None	Pebble bed, prismatic	None	None
Pressure calculation	R-K EOS	R-K EOS	R-K EOS	Unknown	IGL	R-K EOS	IGL
CO production method	HSC-based yield	Custom (Nabielek?)	unknown	Martin	Karsten (KFA)	None, LEU, HEU	Proksch
Heat transfer calculation	1D finite difference with buffer/IPyC gap	THERMIX calculation with buffer/IPyC gap	Finite element	Unknown	Full-core then particle	Single irr. temp. used	Single irr. temp. used?
Phenomena modeled	Pressure, PyC IIDC, PyC irr. creep, thermal expansion, SFP swelling, FP diffusion	Pressure, PyC IIDC, PyC irr. creep, Thermal expansion	Pressure, PyC IIDC, PyC irr. creep, SFP swelling, GFP swelling	Pressure, PyC IIDC, PyC irr. creep, SFP swelling, SiC elasticity	Pressure, PyC IIDC, PyC irr. creep	Pressure, PyC IIDC, PyC irr. creep, SFP swelling	Pressure, PyC IIDC
Failure mechanisms modeled	PV, IPyC cracking, debonding, asphericity, SiC thinning, SiC thermal decomposition, kernel migration	PV, IPyC cracking	PV, IPyC cracking, debonding, asphericity	PV, IPyC cracking, debonding	PV, IPyC cracking via fracture mechanics	PV	PV
PyC shrinkage correlation	Custom	FZJ	Unknown	Custom	Unknown	Unclear	Unknown
PyC irr. creep coefficient $(\text{MPa n m}^{-2})^{-1}$	$c = 5 \times 10^{-29}$/ $\nu = 0.5$ or $c = 4 \times 10^{-29}$/ $\nu = 0.4$	3.0×10^{-29}	Unknown	4.9×10^{-29}	CEGA function	2.0×10^{-29}	Unknown
Fission gas release model (s)	Recoil + booth	Modified booth (cyclic situation)	Unknown	Unknown	UT/KFA (booth-based?)	Booth	Booth (single species)
Displacement calculations?	Yes	Yes	Yes	Yes	Yes	No	No

used for several species, and notes that further expansion of the diffusion model may occur as new information from irradiation experiments becomes available [9]. The available documentation and descriptions for TIMCOAT indicate that fission product diffusion modeling was planned for future code development efforts [16], but has evidently not yet been implemented. Documentation for the PASTA code discusses boundary conditions and a numerical solution approach to the diffusion equation for fission products, but does not clearly indicate which species are included or whether the diffusion model includes fission product release from the TRISO particle as a whole, or just the fuel kernel [44]. It has been noted that thermal (Soret) diffusion appears to be relatively unimportant for most operating conditions due to the relatively small thermal gradients in operating fuels, but it may be much more important for highly accelerated irradiations conducted for materials testing and fuel qualification [9].

Many of these fuel performance codes (PARFUME, ATLAS, STRESS3, PASTA, and TIMCOAT) include the ability to perform statistical analysis to predict failure fractions by evaluating the strength and strength distribution of the PyC and SiC layers through Weibull statistics. These models, which are based on weakest link statistics, predict failure fractions by considering a range of flaw sizes and locations amongst a particle population. The most important parameters in these Weibull distribution models are the Weibull mean fracture strength and the Weibull Modulus in the PyC and SiC layers, and suggested values for these parameters have been published [9,36,37]. In particular, Ref. [9] contains a more detailed description of Weibull theory and the use of Weibull statistics to predict fuel failure fractions. These statistical-based failure models can either be used to determine the allowable Weibull stress for a pre-determined fuel failure fraction or to determine the predicted fuel fraction based on the maximum stress values obtained from the fuel performance model.

Table 6 summarizes key modeling approaches, capabilities, and other important information for these TRISO FPMs as found in the available literature; specific aspects of FPMs that are unknown or unclear are marked accordingly and details indicated by a source but with some ambiguity have a question mark after the item. It should be noted that the above descriptions of each code provide additional information that may not be captured in the table.

6. Key challenges

Numerous major challenges remain unsolved in the pursuit of accurate TRISO fuel performance modeling. Most prominent of these are benchmarking the FPMs to reach the higher burnup levels currently proposed by projects such as Deep Burn [54], issues related to fundamental material properties and the phenomena exhibited by irradiated TRISO particles, manufacturing uncertainties, and modeling 3D effects.

While some data exists for TRISO fuel at high burnup levels [19,25], the results from these experiments vary significantly and have large uncertainties regarding how representative they are due to questions about the manufacturing processes used [14,19]. Thus, little or no data currently exists with which to benchmark TRISO fuel performance models up to the burnup levels (50% FIMA or even higher) needed to support high burnup reactor designs for actinide transmutation and efficient resource utilization.

Uncertainties and unknowns in fundamental material properties are also abundant, especially with regard to how properties vary as functions of temperature, fast fluence, and burnup. The response of SiC is understood fairly well for most properties up to about 10–30 dpa, but the databases for dense PyC material properties need refinement and expansion. The properties of porous carbon are marginally known at best and contain large uncertainties, although these properties may be less important to the overall fuel performance assessment. Fuel properties may be the least well known due to the rapid nature in which fuel designs evolve (e.g., changing the fuel material from UO_2 to ThCO or (Pu, Np, Am)$O_{1.7}$). Substantial work is required to improve our collective understanding of these materials in order to ensure high accuracy in fuel performance models. Examples of material properties with significant uncertainty include the irradiation creep constant, the value of Poisson's ratio in irradiation creep models, and the thermal conductivity of PyC. Accurate predictions for the chemical attack of SiC require effective diffusion coefficients of key fission products in various fuel materials (UO_2, UCO, PuO_2, ThCO, (TRU)$O_{1.7}$, and others) and PyC, which are currently either largely unknown or highly uncertain.

Expanding models to incorporate additional phenomena offers opportunities for better agreement between computational predictions and experimental observations of irradiated TRISO fuel particles. Recent efforts at INL highlight the importance of partial and full debonding between the IPyC and SiC layers and its impact on predicted TRISO fuel performance, including accurate estimates for the interfacial bond strength between the IPyC and SiC layers and possible approaches to increase this bond strength [14,22]. The use of fracture toughness based approaches to crack formation and propagation in TRISO coating layers, as implemented by MIT's TIMCOAT code, offers a path to incorporating fracture mechanics into TRISO fuel performance modeling to yield higher fidelity models that should produce more accurate predictions if the associated material properties are accurately known [16]. Fracture mechanics based approaches do, however, include additional uncertainties since the distribution of initial flaw sizes may not be well known. Thus it may be best to utilize fracture mechanics approaches for research to develop a detailed understanding of how particle layers fail but continue relying upon Weibull-based statistical models for predicting fuel failure fractions in a population of particles.

Manufacturing uncertainties, quantified as acceptable tolerances around specified dimensions and specified material properties such as density and grain orientation, further complicate TRISO fuel performance modeling. To make matters worse, relatively little is known about the precise ways in which changes in manufacturing processes (e.g., coating rates and temperatures) affect the dimensions and properties of the TRISO particles produced or their performance under irradiation [14]. Ongoing work in this area may enable more predictive and accurate material properties or performance models but will take some time.

Lastly, modeling three-dimensional effects such as cracking in coating layers, particle asphericity due to manufacturing, kernel migration, or other factors remains a substantial challenge in TRISO fuel performance modeling. While some approaches have been identified through the use of finite element calculations to inform 1D calculations as in PARFUME [9] or using a finite element calculation as in ATLAS [9], this remains one of the most challenging areas which requires additional research, especially considering that PyC cracking and other multi-dimensional effects are increasingly thought to be the limiting failure mode for TRISO fuel performance.

7. Conclusions

This paper summarizes a large body of literature that describes the behavior and failure mechanisms of TRISO fuel particles and, in particular, the available TRISO fuel performance models. Material property correlations for UO_2, PyC, and SiC exist; however, while SiC is fairly well characterized, considerable uncertainties and knowledge gaps remain in the material properties of PyC and fuel kernels. Numerous TRISO fuel performance models exist, in both a one-dimensional or three-dimensional framework, depending upon the assumptions made in deriving the model. These models seem to provide satisfactory prediction of fuel performance up to burnup levels around 20% FIMA for conventional uranium oxide fuel kernels. Little experimental data exists to benchmark model predictions at higher burnup levels or formulate material property correlations at the high levels of accumulated fast fluence characteristic of high burnup epithermal or intermediate spectrum nuclear systems. Additional research is needed to generate this experimental data to support development of TRISO fuel performance models capable of modeling non-traditional fuel forms (e.g., ThCO or (Pu, Np, Am)$O_{1.7}$) and multidimensional failure mechanisms, which may include chemical attack of the coating layers, and to fundamentally understand how manufacturing conditions affect the coating material properties and subsequent fuel performance.

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