Phase field model for crack propagation in outer coating layers of TRISO particle fuel

Authors: Mr. Lin Peng, Tang, Prof. Simiao, Li, Songyang, Zhu, Prof. Longxiang, LIAN, Dr. Qiang, Dr. Zhang Luteng, Pan, Prof. Liangming, Peng, Mr. Lin

Date: 2025-04-16T18:00:22+00:00

Abstract

As an advanced fuel form, TRISO particle fuel is relatively reliable due to the excellent capability of its thin coating layers to contain fission products, but it is still prone to cracks or pores in the coatings during production, transportation, and usage. These irregular geometries can significantly impact their ability to maintain structural integrity. Therefore, in order to advance the use of TRISO particles in space reactors, analyzing and predicting the crack propagation in their coatings is crucial. This model introduces the material properties of TRISO particles, irradiation behavior, and fission gas release model, and establishes a phase field model to investigate the crack propagation characteristics of the outer three coatings of TRISO particles. The accuracy of this model for TRISO particle performance was verified through an IAEA benchmark problem and a comparison with BISON program results for TRISO particles. The reliability of the phase field model for crack simulation was validated by analyzing a notched tensile plate and Kalthoff experiment. The effects of a crack in the IPyC layer, a residual pore in the SiC layer, a crack on the outer side of OPyC, and the simultaneous presence of a crack in the IPyC layer and a residual pore in the SiC layer, were studied in succession. The calculation results reveal that cracks in the IPyC layer cause debonding between the IPyC and SiC layers, but they are insufficient to propagate into the SiC layer during the early stages of burnup. Residual pores in the SiC layer lead to the complete fracture of the coating layers, primarily due to excessive gas pressure from the inner IPyC layer rather than the weakening effect of the pores on the structure. Cracks in the OPyC layer cause concentrated tensile stress on the outer side of the SiC layer during the early stages of burnup, which alters the crack propagation path in the coating layers during the later stages of burnup. Therefore, in addition to using material detection techniques to screen out TRISO particles with excessive defects before the production of FCM pellets, it is essential to enhance the ability of coating layers to maintain structural integrity and implement funda-

mental measures such as expelling accumulated gases from the particles. These actions are crucial for the safe and stable operation of TRISO particle fuel in space reactors.

Full Text

Preamble

Phase Field Model for Crack Propagation in Outer Coating Layers of TRISO Particle Fuel

Lin Peng,[1,2] Simiao Tang,[1,2,†] Songyang Li,[1,2] Meiyue Yan,[3] Longxiang Zhu,[1,2] Qiang Lian,[1,2] Luteng Zhang,[1,2] and Liangming Pan[1,2]

[1]Key Laboratory of Low-grade Energy Utilization Technologies and Systems, Ministry of Education, Chongqing University, Chongqing 400044, China

[2]Department of Nuclear Engineering and Technology, Chongqing University, Chongqing 400044, China

[3]Department of Mechanical Engineering, College of Design and Engineering, National University of Singapore, Singapore 117575, Singapore

TRISO particle fuel represents an advanced fuel form that offers relatively high reliability due to the excellent capability of its thin coating layers to contain fission products. However, these coatings remain susceptible to cracks or pores during production, transportation, and service. Such irregular geometries can significantly compromise structural integrity. Therefore, advancing TRISO particle applications in space reactors requires analyzing and predicting crack propagation in their coatings. This study introduces material properties, irradiation behavior, and a fission gas release model for TRISO particles, establishing a phase field model to investigate crack propagation characteristics in the outer three coating layers. Model accuracy for TRISO particle performance was verified through an IAEA benchmark problem and comparison with BISON program results. The phase field model' s reliability for crack simulation was validated through analysis of a notched tensile plate and Kalthoff experiment. The effects of a crack in the IPyC layer, a residual pore in the SiC layer, a crack on the outer side of OPyC, and the simultaneous presence of a crack in the IPyC layer and a residual pore in the SiC layer were sequentially investigated. Results reveal that cracks in the IPyC layer cause debonding between IPyC and SiC layers but are insufficient to propagate into the SiC layer during early burnup stages. Residual pores in the SiC layer lead to complete coating fracture, primarily due to excessive gas pressure from the inner IPyC layer rather than pore-induced structural weakening. Cracks in the OPyC layer cause concentrated tensile stress on the SiC layer' s outer side during early burnup, altering crack propagation paths during later stages. Consequently, beyond using material detection techniques to screen out TRISO particles with excessive defects before FCM pellet production, enhancing coating structural integrity and implementing measures to expel accumulated gases are essential for safe and stable TRISO particle fuel operation in space reactors.

Keywords: TRISO particle, Phase field, Fracture mechanics, Nuclear engineering, Space reactor

Introduction

Driven by stringent requirements for reactor stability and safety, several Accident Tolerant Fuels (ATFs) have been developed and partially implemented [?, ?], aiming to maintain fuel structural integrity and ensure reactor safety under both normal and accident conditions. Among these, Fully Ceramic Microencapsulated (FCM) fuel stands out as a promising candidate [?, ?]. FCM consists of TRistructural-ISOtropic (TRISO) coated fuel particles dispersed within a Nano-Infiltration and Transient Eutectic-phase SiC (NITE-SiC) matrix. To ensure fuel pellet stability, investigation must focus on its fundamental unit: the TRISO particle.

A TRISO particle comprises a kernel surrounded by four consecutive coating layers, as illustrated in Fig. 1 [Figure 1: see original paper]. The kernel serves as the reactor heat source through nuclear reactions and can be made of UO_2, UN, or UCO. The first coating layer, known as the Buffer layer, is composed of low-density pyrocarbon (PyC). It acts as a cushion, providing space for gaseous fission products while alleviating stresses from kernel expansion on outer coating layers [?]. The second layer is the Inner Pyrolytic Carbon (IPyC) layer, made of dense PyC, which prevents internal structure corrosion during manufacturing and shields the SiC layer from damage caused by gaseous and solid fission products [?, ?]. The next layer, silicon carbide (SiC), is deposited on the IPyC layer using Chemical Vapor Deposition (CVD), referred to as CVD-SiC (to distinguish it from NITE-SiC). The SiC layer contains fission products and serves as the main pressure shell to maintain TRISO particle structural integrity [?]. Finally, the outermost layer is the Outer PyC (OPyC) layer, which acts as the final barrier for fission products and protects the CVD-SiC layer during manufacturing [?]. Owing to this multi-layered structure, TRISO particles effectively contain fission products and maintain structural integrity, exhibiting excellent irradiation stability and thermo-mechanical performance [?, ?].

Experimental and numerical studies of TRISO particles have established a solid foundation. After fabrication, residual stresses may exist in coating layers, significantly affecting mechanical performance. Experimental studies by A. J. Leide et al. identified tensile residual hoop stresses in pyrolytic carbon layers and compressive residual hoop stress in the silicon carbide layer [?]. Similarly, K. I. Montoya et al. quantified residual stresses at the SiC-OPyC interface, showing their influence on mechanical stability and fracture behavior [?]. Irradiation experiments demonstrate that buffer layer porosity causes volume shrinkage under neutron irradiation [?]. Due to thermal resistance between layers and the gas gap, significant temperature differences across TRISO particles may occur, with excessive thermal variations threatening nuclear fuel integrity [?]. At 800°C, the SiC layer experiences approximately 10 MPa thermal stress [?]. J. D. Hales et al. simulated TRISO particles using the BISON code [?], demonstrating numerical simulation feasibility and program effectiveness. C. Zhang et al. employed COMSOL software to develop simulation methods for TRISO particles and FCM pellets [?, ?], concluding that TRISO particles are relatively reliable under normal HTGR conditions.

However, increasing demands for space exploration and deep-sea missions have made space reactor research and development increasingly urgent [?]. Previous studies [?] revealed that space reactor requirements for higher fuel temperatures, greater fission rates, and longer operational lifetimes cause significant increases in internal gas pressure on the IPyC layer's inner side during mid-to-late burnup stages. This results in higher tensile stresses in the SiC layer, greatly increasing failure probability. Cracks may even develop in outer coating layers, potentially leading to TRISO particle collapse, as shown in Fig. 2 [Figure 2: see original paper] [?]. The stability of nuclear fuels, cladding, and other structural components plays a critical role in reactor operation [?, ?]. Therefore, studying crack propagation characteristics in TRISO particle outer coating layers is paramount. Only by exploring and predicting crack initiation and propagation mechanisms and influencing factors can safe and stable application of TRISO particles and FCM fuel in space reactors be advanced.

When experimental investigation of crack phenomena is difficult, researchers must rely on numerical simulation methods to predict complex crack paths [?], particularly under TRISO particles' intricate operating conditions. Consequently, numerical simulation methods for crack propagation have developed significantly. The discrete crack model introduces new boundaries for crack surfaces through adaptive mesh reconstruction [?]. The eXtended Finite Element Method (XFEM) enhances cracked elements by integrating discontinuous shape functions into the conventional Finite Element Method (FEM) framework [?, ?]. Similarly, the Cohesive Zone Model (CZM) simulates crack propagation by allowing displacement jumps along element boundaries, effectively modeling debonding and interfacial fractures, with cracks confined to predefined paths such as element edges [?]. The phantom-node method models cracks independently of the mesh by overlapping elements at crack locations, enabling discontinuous displacement without enrichment functions [?]. Furthermore, element-erosion methods address fracture surfaces by setting stresses of elements meeting fracture criteria to zero, providing an alternative approach for simulating crack growth [?]. In summary, these complex crack simulation methods present challenges for practical engineering applications.

In contrast, the Phase-Field Method (PFM), which has gained significant attention, offers a more convenient approach for fracture simulation. It represents discrete cracks using a scalar field that smoothly transitions between intact and fully fractured material without treating cracks as physical discontinuities. This eliminates the need for explicit fracture surface tracking, simplifying simulation of crack propagation, branching, and merging in complex geometrical models. Moreover, by directly solving Partial Differential Equations (PDE) to determine phase-field distribution, PFM adopts a numerical solution process similar to other physical fields, making crack simulation more convenient and accessible. Currently, several phase-field methods, including multi-physics coupling approaches, have been developed on software platforms such as ABAQUS [?], MOOSE [?], FEniCS [?], and COMSOL [?]. The phase field method has been applied in multiphysics coupled crack propagation analysis [?] and engineering problems including hydraulic fracturing [?], concrete cracking [?], coal seam fracturing [?], and hydrogen-induced cracking in pipelines [?]. However, studies on crack propagation in TRISO fuel particles remain limited. The microstructure of SiC in TRISO particles [?, ?] and its oxidation behavior [?] have been experimentally studied, and SiC fracture strength has been investigated [?]. A. M. Recuero et al. employed an interaction integral approach to calculate stress intensity factors for cracks in the inner pyrolytic carbon layer perpendicular to the silicon carbide layer [?]. Y. Li simulated micro-defect-induced cracking in the IPyC layer using XFEM [?]. J. Tan et al. simulated cracks within the IPyC layer and at the IPyC-SiC interface through phase field modeling, concluding that combined shrinkage and creep-induced stress relaxation effects play a crucial role in determining crack evolution and subsequent stress distribution in the SiC layer [?]. Overall, crack propagation characteristics in TRISO particle coating layers and their influencing factors require further investigation.

This paper develops a phase field model to simulate crack propagation characteristics in the outer three coating layers of TRISO particles. A 2D axisymmetric geometry model of the IPyC, CVD-SiC, and OPyC layers is constructed, incorporating material properties, irradiation behaviors, and fission gas pressure to simulate TRISO particle operating conditions. The mechanical model was validated against the IAEA Coordinated Research Program (CRP-6) Case 8 benchmark [?], and the complete TRISO particle model accuracy was confirmed through comparison with BISON simulation results from our previous study [?]. Subsequently, crack propagation characteristics in the outer three layers are investigated. First, the influence of prefabricated crack depth in the IPyC layer on crack propagation and maximum tensile stress in the SiC layer is analyzed. Then, the effect of residual pores of different sizes in the SiC layer on crack initiation and propagation in the pressure vessel is studied. The impact of prefabricated cracks in the OPyC layer is also examined. Finally, the study explores crack propagation characteristics caused by residual pores in the SiC layer following interface damage between IPyC and SiC layers due to prefabricated cracks in the IPyC layer during early burnup. Recommendations for limitations on crack and pore sizes and their impact on TRISO particle stability are provided as part of the conclusions.

II. Model Description

Fig. 3 [Figure 3: see original paper] illustrates the model components and their interactions, providing a basis for subsequent explanation of specific model construction steps.

A. Elastic Behavior

Experiments [?] and previous studies [?] have shown that during early burnup stages, the IPyC layer and buffer layer separate, forming a gap that eliminates significant interaction and stress transfer between the two layers. Consequently, this study focuses on constructing the geometric model for the outer three coating layers only. Moreover, previous studies demonstrated that the temperature gradient within the outer three layers is very small and temperature is nearly uniform, eliminating the need for temperature field calculation [?]. This study introduces solid mechanics governing equations to simulate mechanical behavior of TRISO particle outer coating layers, without considering thermal strain and residual stresses in the outer three layers. Additionally, due to high mesh refinement requirements for crack simulation, a 2D axisymmetric model was developed to reduce computational costs, as shown in Fig. 4 [Figure 4: see original paper].

Regarding material mechanical properties, Young's modulus of PyC is expressed by the following equations [?]:

$$E_r = E_0(0.384+0.324\rho)(1.463-0.463BAF_0)\cdot(2.985-0.0662L_c)(1+0.23\phi)(1+0.00015(T-20))$$

$$E_\theta = E_0(0.384+0.324\rho)(0.481+0.519BAF_0)\cdot(2.985-0.0662L_c)(1+0.23\phi)(1+0.00015(T-20))$$

where E_0 is 25.5 GPa, BAF_0 represents the initial degree of anisotropy (reasonable value: 1.03), L_c is the crystallite diameter size (value: 45 Å), and ρ, Φ, and T denote density (10^6 g/m^3), neutron flux (10^{25} n/m^2), and temperature (°C), respectively.

The Poisson' s ratio of IPyC is 0.21 [?], and its density is 1900 kg/m^3 [?].

The Young' s modulus of CVD-SiC is obtained experimentally [?]:

$$E = E_0 - B \cdot T \cdot e^{-T_0}$$

where E_0 is 460 GPa, B is 0.04 GPa/K, and T_0 is 962 K.

The Poisson' s ratio and density of SiC are set to 0.21 and 3210 kg/m^3, respectively [?].

B. Irradiation Behavior

Under neutron irradiation, PyC undergoes irradiation creep and irradiation-induced dimensional change, while SiC experiences creep and swelling. This section explains the corresponding strain models.

Burnup Burnup calculation in TRISO particles follows the model proposed by Olander [?], where burnup is defined as the ratio of fissions to initial uranium atoms:

$$\beta = \frac{\int_0^t \dot{F} dt}{N_f^0}$$

where $\dot{F}$ and N_f^0 represent the fission rate per unit volume (fissions/m^3/s) and initial uranium atom density (atoms/m^3) in the fuel, respectively. These quantities are calculated using:

$$\dot{F} = q\sigma_f N_f \Phi$$

$$N_f = \frac{D \cdot TD \cdot N_A}{MUO_2}$$

In these equations, q is enrichment (ratio of fissile to total uranium atoms), σ_f is the effective fission cross-section in the relevant neutron energy spectrum (barns), N_f is the total uranium atoms per unit volume, Φ is neutron fluence (n/m^2), D is the theoretical density ratio, TD is theoretical density (g/cm^2), N_A is Avogadro' s constant, and MUO_2 is the molar mass of uranium dioxide (g/mol). The relationship between burnup Bu (energy released in MWd/kgU) and β (in %FIMA) is:

$$Bu = 9.5\beta$$

Fast neutron flux is calculated using the BISON formula [?]:

$$\dot{\Phi} = c \cdot P$$

where $\dot{\Phi}$ is fast neutron flux, c is a conversion factor (typically 3×10^{13} (n/(m $\cdot$ s^2)/(W/m))), and P is linear heat rate (W/m).

Irradiation-Induced Dimensional Change, Creep, and Swelling During irradiation, both porous and dense PyC layers experience fast neutron fluence causing irradiation-induced dimensional changes. The irradiation strain rate for IPyC differs in radial and tangential directions, described by German' s formulas [?]:

$$\dot{\varepsilon}_r = -0.077e^{-\Phi} + 0.031$$

$$\dot{\varepsilon}_\theta = -0.036e^{-2.1\Phi} - 0.01$$

where $\dot{\varepsilon}$ and Φ denote irradiation strain rate in $1/(10^{25}\text{n/m}^2)/\text{s}$ and fast neutron fluence in 10^{25}n/m^2, respectively.

With prolonged neutron irradiation, radiation effects on material microstructure result in creep. The irradiation-induced creep rate of IPyC is described by [**?**]:

$$\dot{\varepsilon}_{cr,r} = K[\sigma_1 - v_c(\sigma_2 + \sigma_3)]\dot{\Phi}$$

$$K = 2K_0[1 + 2.38(1.9 - \rho_0)]$$

$$K_0 = 1.996 \times 10^{-29} - 4.415 \times 10^{-32}T + 3.6544 \times 10^{-35}T^2$$

where $\dot{\varepsilon}_{cr,r}$ is radial creep rate in 1/s (other directions follow similarly), K is creep constant in $\text{m}^2/\text{n/MPa}$, ρ_0 is initial density of porous or dense PyC in g/cm^3, σ_i denote principal stresses in three directions, v_c is Poisson' s ratio for creep (0.5), and T is temperature in °C.

Silicon carbide is also subject to irradiation creep, expressed by [**?**]:

$$\dot{\varepsilon}_{cr} = K\dot{\Phi}\sigma_e$$

where creep constant K is typically 0.4×10^{-31} $\text{m}^2/\text{n/MPa}$, $\dot{\Phi}$ and σ_e represent neutron flux in 10^{25} $\text{n/m}^2/\text{s}$ and effective stress in MPa, respectively.

SiC also undergoes irradiation swelling, with neutron-induced swelling between 1250°C and 1500°C expressed by [**?**]:

$$\varepsilon_V = 0.0018\left(1 - e^{-\frac{\phi}{\phi_0}}\right) + 1.297 \times 10^{-28}\phi$$

where ε_V is volumetric strain caused by swelling and ϕ_0 is 0.3396×10^{25} n/m^2.

At a neutron flux of 5×10^{17} $\text{n/m}^2/\text{s}$ and temperature of 1500 K, irradiation-induced dimensional change (IIDC), swelling, and creep constants are shown in Fig. 5 [Figure 5: see original paper]. As burnup progresses, PyC undergoes radial contraction followed by expansion, while the tangential direction continuously contracts. In contrast, SiC swelling and creep are relatively small compared to PyC irradiation behavior.

C. Fission Gas Behavior

In actual nuclear fuels, fission gas atoms are generated within uranium dioxide grains through nuclear fission reactions. These atoms can form intragranular bubbles or diffuse to grain boundaries, where they may coalesce into intergranular bubbles. When gas atom concentration exceeds a critical threshold (influenced by temperature and other factors), they are released into free volume through Fission Gas Release (FGR) [?]. After release, fission gases interact with layers beyond the kernel and generate internal pressure on the IPyC layer. Accurately constructing the fission gas release model is critical, as gas does not immediately release into free space and can dramatically affect TRISO particle coatings, significantly influencing simulation accuracy for TRISO particle fuel performance and failure assessments.

The fission gas model established in this study incorporates several key effects: gas dissolution, atom diffusion, bubble growth, boundary concentration saturation, and the influence of grain growth and external pressure. These factors are modeled using equations and conditions to account for gas atom coalescence, migration, and resulting internal pressures on the IPyC inner side. This model has been validated and refined in previous studies [?]. Since previous calculations are comprehensive and sufficient, this study directly uses gas pressure values calculated under typical HTGR and more stringent space reactor conditions from prior research, as shown in Fig. 6 [Figure 6: see original paper].

D. Phase Field Model for Fracture

Brittle Fracture Theory Consider a domain Ω with a pre-existing crack Γ, where Dirichlet and Neumann boundary conditions are applied at boundaries. For instance, one side has fixed constraint while the other applies given traction $\mathbf{f}$ or displacement $\mathbf{u}$, as shown in Fig. 7 [Figure 7: see original paper].

According to Griffith' s theory [?], the energy required to create a fracture surface per unit area equals the critical fracture energy density G_c, also referred to as the critical energy release rate. Therefore, total potential energy can be expressed as:

$$\Pi = \int_\Omega \psi_\varepsilon(\varepsilon) d\Omega + \int_\Gamma G_c dS - \int_\Omega \mathbf{b}\cdot\mathbf{u} d\Omega - \int_{\partial\Omega} \mathbf{f}\cdot\mathbf{u} dS$$

Total potential energy consists of four components: elastic energy, fracture energy, body force energy, and external force energy. Elastic energy can be written in terms of the elastic energy density function. Assuming isotropic linear elasticity, the elastic energy density is defined by Miehe et al. [?]:

$$\psi_\varepsilon(\varepsilon) = \frac{\lambda}{2}\cdot \mathrm{tr}^2[\varepsilon] + \mu \cdot \mathrm{tr}[\varepsilon^2]$$

where λ and μ are Lamé constants derived from Young' s modulus and Poisson' s ratio, and $\mathrm{tr}[A]$ represents the trace of matrix A. The strain tensor ε used here is the standard linear strain tensor in solid mechanics, given by:

$$\varepsilon = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

Phase Field Approach to Fracture Energy In Eq. (14), the fracture energy term involves integration over the crack surface, which is difficult to accurately capture during crack propagation. To address this challenge, the concept of a crack surface density function is introduced to approximate the fracture surface Γ. This requires defining a new field variable, distinct from the displacement field, to represent the crack surface. This field variable is the phase field, a scalar function $p(\mathbf{x}, t) \in [0, 1]$, where $p = 1$ represents the fully cracked state and $p = 0$ indicates an intact body (as shown in Fig. 7). This phase field naturally represents a diffusive crack situation, allowing smooth approximation of crack propagation.

With the phase field introduced, the crack surface density per unit volume of the solid can be calculated, as given by Miehe et al. [**?**]:

$$\gamma(p, \nabla p) = \frac{G_c}{2l_0}(p^2 + l_0^2(\nabla p)^2)$$

where l_0 is a parameter governing the phase field transition region from 0 to 1. This length scale parameter represents crack width.

With Eq. (17), the originally complex surface integral for fracture energy is transformed into a volume integral, facilitating numerical implementation. Thus, fracture energy is approximated as:

$$\int_\Gamma G_c dS = \int_\Omega \gamma(p, \nabla p) d\Omega = \int_\Omega \frac{G_c}{2l_0}\left(p^2 + l_0^2(\nabla p)^2\right) d\Omega$$

Crack surface energy is driven by elastic energy, which controls phase field evolution. To ensure crack propagation is only influenced by tensile loading, the elastic energy must be decomposed, with the compressive component having no contribution [**?**]. The spectral decomposition method is as follows:

$$\varepsilon = \varepsilon^+ + \varepsilon^-$$

$$\varepsilon^+ = \sum_{i=1}^{d} \langle \varepsilon_i \rangle^+ \mathbf{n}_i \otimes \mathbf{n}_i$$

$$\varepsilon^- = \sum_{i=1}^{d} \langle \varepsilon_i \rangle^- \mathbf{n}_i \otimes \mathbf{n}_i$$

where ε^+ and ε^- are tensile and compressive strain tensors; $\{\varepsilon_i\}_{i=1\dots d}$ are principal strains and $\mathbf{n}_i$ is the direction vector. The bracket operators mean $\langle x \rangle^+ = \frac{x+|x|}{2}$ and $\langle x \rangle^- = \frac{x-|x|}{2}$.

In Eq. (14), the elastic energy density function ψ_ε represents energy stored per unit volume in the bulk solid. Without considering damage, applying the decomposed strain tensor from Eqs. (19) and (20), the reference energy function associated with the undamaged elastic solid ψ_0 is similarly decomposed [**?**]:

$$\psi_\varepsilon^0 = \psi_\varepsilon^{0+} + \psi_\varepsilon^{0-}$$

$$\psi_\varepsilon^{0+} = \frac{\lambda}{2} \cdot \langle \mathrm{tr}[\varepsilon] \rangle^2 + \mu \cdot \mathrm{tr}[\varepsilon^{+2}]$$

$$\psi_\varepsilon^{0-} = \frac{\lambda}{2} \cdot \langle \mathrm{tr}[\varepsilon] \rangle^2 + \mu \cdot \mathrm{tr}[\varepsilon^{-2}]$$

Considering crack propagation and assuming only the tensile part of elastic energy density is influenced by the phase field, degradation due to fracture is incorporated, and the elastic energy density function is expressed to model stiffness reduction [**?**]:

$$\psi_\varepsilon(\varepsilon, p) = g(p)\psi_\varepsilon^{0+}(\varepsilon) + \psi_\varepsilon^{0-}(\varepsilon)$$

The monotonically decreasing degradation function $g(p)$ describes degradation of the positive (tensile) part of stored energy with evolving damage. It must satisfy: $g(0) = 1$, $g(1) = 0$, $g'(1) = 0$. A common form is the power function:

$$g(p) = (1-p)^2$$

At this point, all potential energy terms can be expressed. For a domain with kinetic energy, kinetic energy can be represented as:

$$\psi_{\mathrm{kin}} = \int_\Omega \frac{1}{2}\rho \left(\frac{\partial \mathbf{u}}{\partial t} \right)^2 d\Omega$$

The total Lagrange energy function is the sum of fracture energy from Eq. (18), elastic energy from Eq. (23), kinetic energy from Eq. (25), and external potential energy due to applied loads:

$$\mathcal{L} = \int_{\Omega} \left[\frac{G_c}{2l_0} (p^2 + l_0^2 (\nabla p)^2) + \frac{1}{2}\rho \left(\frac{\partial \mathbf{u}}{\partial t} \right)^2 + (1-p)^2 \psi_\varepsilon^+ + \psi_\varepsilon^- \right] d\Omega + \int_{\Omega} \mathbf{b}\cdot\mathbf{u} d\Omega + \int_{\partial\Omega} \mathbf{f}\cdot\mathbf{u} dS$$

Applying the variational principle to function $\mathcal{L}$, the first variation must be zero [**?**], resulting in governing equations:

$$\nabla \cdot \sigma + \mathbf{b} = \rho \frac{\partial^2 \mathbf{u}}{\partial t^2}$$

$$\frac{G_c}{l_0}(p - l_0^2 \nabla^2 p) = 2l_0 \psi_\varepsilon^+$$

where σ_{ij} is the Cauchy stress tensor component, which can be similarly decomposed as:

$$\sigma_{ij} = (1-p)^2 \frac{\partial \psi_\varepsilon^+}{\partial \varepsilon_{ij}} + \frac{\partial \psi_\varepsilon^-}{\partial \varepsilon_{ij}}$$

The Cauchy stress tensor can be rewritten as:

$$\sigma = (1-p)^2 \left(\lambda \langle \mathrm{tr}(\varepsilon) \rangle^+ \mathbf{I} + 2\mu \varepsilon^+ \right) + \lambda \langle \mathrm{tr}(\varepsilon) \rangle^- \mathbf{I} + 2\mu \varepsilon^-$$

where $\mathbf{I}$ is the unit tensor $\in \mathbb{R}^{d \times d}$.

However, direct application of the above phase-field model would cause the phase field to recover or even vanish after load removal, contradicting the irreversibility of real material cracks. To ensure a monotonically increasing phase field, an irreversibility condition must be imposed. Therefore, a strain-history field $H(\mathbf{x}, t)$ is introduced to record the maximum elastic energy density [**?**]:

$$H(\mathbf{x}, t) = \max_{s \in [0,t]} \psi_\varepsilon^+ [\varepsilon(\mathbf{x}, s)]$$

Replacing ψ_ε^+ with $H(\mathbf{x}, t)$ in Eq. (27) yields the second-order PDE in the strong form of the phase field model:

$$\frac{G_c}{l_0} (p - l_0^2 \nabla^2 p) = 2l_0 H$$

E. Weak Form for FEM and Solution Strategy

The phase field model in this work involves a coupled multiphysics problem with displacement and phase field as the two primary fields, along with the strain-history variable H. The displacement field is solved using COMSOL’ s “Solid Mechanics” module, while the phase field is governed by the energy conservation equation. To apply the finite element method, governing equations must be reformulated into weak form [?, ?]:

$$\int_{\Omega} \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} \cdot \delta \mathbf{u} d\Omega - \int_{\Omega} \sigma : \delta \varepsilon d\Omega + \int_{\Omega} \mathbf{b} \cdot \delta \mathbf{u} d\Omega + \int_{\partial\Omega} \mathbf{f} \cdot \delta \mathbf{u} dS = 0$$

$$\int_{\Omega} \left[l_0 H g'(p) \delta p + G_c \left(l_0 \nabla p \cdot \nabla(\delta p) + \frac{p}{l_0} \delta p \right) \right] d\Omega = 0$$

where δ represents the test function in FEM.

Since the phase field model does not require tracking the crack surface but instead directly solves weak form equations to obtain phase field distribution, it can be unified with other PDE problems and solved numerically using the finite element method. To avoid unacceptable computational costs of fully coupled calculations, this study adopts a decoupled solver to sequentially solve for the displacement field, history strain field, and phase field (as shown in Fig. 3), enabling reasonable crack simulation.

Finally, regarding phase-field parameters for the outer three TRISO particle coatings, length scale parameters for PyC and SiC are assumed to be $l_1 = 3$ µm and $l_2 = 1$ µm, respectively. The critical energy release rate G_c can be derived using Borden et al.’ s formula [?]:

$$G_c = \frac{9E\sigma_c^2}{32}$$

where σ_c is tensile strength (critical fracture stress), experimentally tested as 200 MPa for PyC [?] and 667 MPa for SiC [?]; E is Young’ s modulus, dynamically calculated from Eq. (1) and Eq. (2). For anisotropic PyC, E in this formula is represented by the average value in three directions.

III. Verification

The code was validated against an IAEA HTGR benchmark, specifically the Case-8 scenario from the IAEA Coordinated Research Program (CRP-6) [?]. This case was selected to verify computational method accuracy by modeling the outer three TRISO particle coatings, where each layer material has distinct properties. These layers were subjected to ten time cycles, each lasting 100 days. In each cycle, fuel temperature increases linearly from initial 873 K to 1273 K, followed by immediate drop back to 873 K. Meanwhile, gas pressure on the IPyC layer' s inner side also increases and decreases linearly within each cycle. Due to different material properties and irradiation behaviors, the PyC layer exerts pressure on the SiC layer, creating different stress states across layers. As shown in Fig. 8 [Figure 8: see original paper], maximum tangential stresses at IPyC and SiC inner surfaces were compared with results from other programs, demonstrating good agreement. This indicates the software in this study can accurately simulate TRISO particle mechanical performance.

To validate the phase-field calculation method, two typical test cases were selected. First, for a square plate with an initial notch under static tension loading (Fig. 9 [Figure 9: see original paper]), vertical displacement u_y is applied to the plate' s upper boundary. Material parameters are: $E = 210$ GPa, $\nu = 0.3$, $G_c = 2700$ J/m^2, and length scale parameter $l_0 = 1.5 \times 10^{-2}$ mm. Maximum element size h is set to $l_0/2$. A displacement increment of $\Delta u = 1 \times 10^{-5}$ mm is applied for initial 450 time steps, followed by smaller increment $\Delta u = 1 \times 10^{-6}$ mm for remaining steps until full fracture.

Computational results for this test case are presented in Fig. 10 [Figure 10: see original paper]. As tensile displacement increases, stress concentrates at the notch, and the crack gradually forms and propagates. Results show excellent agreement with S. Zhou et al. [?].

To further verify transient calculation accuracy and phase-field modeling under shear forces, this study also selected the Kalthoff dynamic fracture experiment for comparison [?]. In this experiment, a steel plate with pre-existing cracks is placed freely on an adjustable workbench. A stress wave generated by edge impact loading causes edge cracks and initiates brittle fracture. Based on the Kalthoff experiment, a computational problem for numerical simulation is constructed, as shown in Fig. 11 [Figure 11: see original paper].

The specified velocity ν is set as:

$$\nu = \begin{cases} \nu_0 \frac{t}{t_0} & t \leq t_0 \\ \nu_0 & t > t_0 \end{cases}$$

where ν_0 is 16.5 m/s and t_0 is 1 µs. Material properties are: $\rho = 8000$ kg/m^3, $E = 190$ GPa, $\nu = 0.3$, $G_c = 22130$ J/m^2, $l_0 = 3.9 \times 10^{-4}$ m. The simulation is computed up to 90 µs, with phase field results at several time points shown in Fig. 12 [Figure 12: see original paper]. The crack appears at 24.84 µs and gradually extends upward toward the plate top. The crack angle relative to the horizontal axis is approximately 65 degrees, consistent with conclusions in [?] (ranging from 63° to 67°) and similar to experimental results in [?]. Additionally, cracks simulated using XFEM [?] and the phantom nodes method [?] from other studies are shown in Fig. 13 [Figure 13: see original paper]. The crack obtained using the phase field model in this study is very similar to these results, demonstrating that the phase field approach developed for brittle fracture is reliable.

IV. Demonstration Problems

Cracks may be introduced during manufacturing or generated during use in the PyC layer [?, ?], while residual pores are prone to exist in the SiC layer [?, ?]. These irregular geometries can lead to stress concentration, significantly affecting TRISO particles and potentially causing coating fracture. Therefore, studying these features is crucial for practical TRISO particle applications. This study analyzes four scenarios: (1) a crack on the IPyC layer inner side, (2) a residual pore in the SiC layer, (3) a crack on the OPyC layer outer side, and (4) the combined effect of a crack on the IPyC layer inner side and a residual pore in the SiC layer. Since IPyC and SiC are not monolithic, debonding may occur between them. When a crack reaches their interface, it tends to deflect in both directions [?]. Therefore, in the geometric model, a thin layer of 0.8 μm is defined on the IPyC outer side and SiC inner side, with their critical energy release rate G_c set to 0.8 times that of PyC, to simulate interfacial damage between the two layers. Geometric models for these features are shown in Fig. 14 [Figure 14: see original paper].

Irradiation behavior is incorporated into the model, with the IPyC layer subjected to fission gas pressure. To ensure both accuracy and convergence, pressure is linearly removed once the crack reaches the OPyC layer outer side; otherwise, separated materials would move too far apart. It should be noted that due to 2D axisymmetric simplification, notches and pores are effectively modeled as fully circumferential ring-shaped defects. Although these shapes differ from real defects, the resulting stress concentrations are more pronounced, leading to conservative estimates that satisfy engineering design margin requirements. Moreover, this simplification does not alter crack propagation characteristics, making the method reasonable.

To investigate sensitivity of crack propagation characteristics in TRISO particle outer three coatings to geometric parameters and provide recommendations for required limitations on pre-existing crack sizes in practical engineering applications, this study parameterized crack depth and pore radius in scenarios 1 and 2. Parameters for this analysis are listed in Table 1 . Because SiC layer reliability is high under normal operating conditions, scenarios 1 and 3 are modeled using typical HTGR conditions [?, ?], while scenarios 2 and 4 use more stringent space reactor conditions [?]. Corresponding parameters are listed in Table 2 .

Table 1. Parameters used for geometric models in four scenarios.

Geometric parameters	Scenario 1 (IPyC)	Scenario 2 (SiC)	Scenario 3 (OPyC)	Scenario 4 (IPyC & SiC)
Crack depth (μm)	1, 3, 5, 5.6, 5.7, 5.8, 5.9, 6, 8, 10	–	–	–

Geometric parameters	Scenario 1 (IPyC)	Scenario 2 (SiC)	Scenario 3 (OPyC)	Scenario 4 (IPyC & SiC)
Pore radius (μm)	–	0.1, 0.2, 0.4, 0.6, 0.7, 0.75, 0.8, 0.85, 0.9, 1	–	–

Table 2. Parameters for the two conditions used in simulations [?, ?, ?].

Parameter	Applied scenarios	Value
Kernel power	1 and 3	50 mW
Lifetime of fuel	1 and 3	76 Ms (About 2.4 yrs.) (Scenario 1 calculated up to 15 Ms only)
TRISO particle temperature	1 and 3	1500 K
Fast neutron flux	1 and 3	5×10^{17} $n/m^2/s$
Fast fluence at the end of irradiation	1 and 3	3.8×10^{25} n/m^2
Fission rate per unit volume	1 and 3	3.03×10^{19} $fission/m^3/s$
Burnup at the end	1 and 3	10.45% FIMA
Gas pressure	1 and 3	As shown in Fig. 6
Kernel power	2, 3 and 4	70 mW
Lifetime of fuel	2, 3 and 4	1700 K
TRISO particle temperature	2, 3 and 4	7×10^{17} $n/m^2/s$
Fast neutron flux	2, 3 and 4	15×10^{25} n/m^2
Fast fluence at the end of irradiation	2, 3 and 4	4.24×10^{19} $fission/m^3/s$
Fission rate per unit volume	2, 3 and 4	42.35% FIMA
Burnup at the end	2, 3 and 4	–

V. Results and Discussion

A. Effect of a Crack in the IPyC Layer

Irradiation behavior is most active before 1.5×10^7 s (as shown in Fig. 5), and maximum tangential stress in the IPyC layer also occurs before this time. After this point, stress gradually relaxes as burnup progresses [?]. Therefore, crack formation and propagation primarily occur during early burnup stages. If no cracks form by this time, none will appear subsequently. Consequently, maximum calculation time is set to 1.5×10^7 s.

Figs. 15, 16, and 17 show the phase field at selected time points for pre-existing cracks of 1 µm, 6 µm, and 10 µm depth on the IPyC inner side. With a 1 µm deep crack, stress distribution within the IPyC layer remains relatively uniform with no significant crack effect, and the maximum phase field value at calculation end is only 0.17, indicating no crack propagation. However, with a 6 µm deep crack, propagation toward the SiC layer begins at 0.80×10^7 s. Compared to a complete spherical shape or shallower crack, a deeper crack causes significant non-uniform deformation within the IPyC layer during irradiation-induced radial shrinkage, with large stress concentrations at the crack tip. Under tensile stresses on both notch sides, a crack initiates from the notch tip. Subsequently, with ongoing irradiation shrinkage, the IPyC layer shows increasing tendency to debond from the SiC layer, with the interface damage zone expanding and partial separation occurring. In the case of a 10 µm deep crack, propagation starts earlier at 0.43×10^7 s. The crack expands more rapidly after reaching the interface, and by 1.50×10^7 s, most of the region on the IPyC layer outer side has separated from the SiC layer. This result is consistent with J. Tan et al. predictions [?]. While this may not exactly match real system behavior due to factors such as thermal expansion [?], corrosion [?], constraints from the FCM matrix under real operating conditions, and 2D axisymmetric simplification effects, it provides good prediction of IPyC-SiC debonding, demonstrating phase field method feasibility for studying crack propagation in coating layers.

Fig. 18 [Figure 18: see original paper] shows maximum phase field values at 1.5×10^7 s and crack propagation initiation times for different pre-crack depths. When crack depth is smaller than 5.8 µm, no propagation occurs. However, when crack depth is sufficient, the crack propagates, with initiation time becoming earlier as pre-crack depth increases.

Fig. 19 [Figure 19: see original paper] presents tangential stress (hoop stress) distribution at 1.5×10^7 s for pre-existing cracks with depths of 5 µm, 6 µm, and 10 µm. When the crack does not propagate, the notch induces significant tensile stress in the IPyC layer while the SiC layer remains under compressive stress. For a 6 µm pre-existing crack, local debonding between IPyC and SiC layers caused by crack propagation results in strong compressive stress concentration in the SiC layer beyond the crack tip due to IPyC layer constraint. In contrast, the region near the crack front experiences tensile stress. Fortunately, this tensile stress concentration is primarily confined within the IPyC layer, and localized tensile stress is insufficient to cause SiC layer fracture.

Regarding IPyC crack and interface debonding effects on SiC stress, Fig. 20 [Figure 20: see original paper] shows debonded area proportions and maximum tangential (hoop) stress in the SiC layer at calculation end for different pre-crack depths. Overall, IPyC layer cracks increase tensile stress experienced by the SiC layer. When crack propagation does not occur, the SiC layer remains under compressive stress at burnup end. Once a crack forms, stress concentration caused by interface debonding and the crack tip causes SiC to experience tensile stress simultaneously. Deeper pre-cracks lead to further crack propagation along the interface, and while more interface debonding can alleviate tensile stress in SiC, stress remains significantly higher than when crack propagation does not occur.

For a 10 μm pre-crack, behavior throughout fuel lifetime has been simulated, and Fig. 21 [Figure 21: see original paper] compares maximum tangential stress on the SiC layer inner surface with and without pre-existing crack. When the crack approaches the SiC inner side, it induces sudden tensile stress increase within the SiC layer. Since SiC has significantly higher strength than pyrolytic carbon and stress concentration occurs in a very localized region, no immediate cracking occurs in early burnup stages. However, at 7.6×10^7 s, maximum tangential stress in the SiC layer becomes significantly higher than in the case without an initial IPyC crack. This could have considerable impact in long-lifetime applications such as space nuclear reactors.

To investigate interface bonding strength effects on crack propagation, a sensitivity analysis was performed on the critical energy release rate factor at the IPyC-SiC interface. As shown in Fig. 22 [Figure 22: see original paper], coating layer mechanical behavior differs significantly depending on interface bonding strength, represented by varying the factor from baseline PyC energy release rate. When bonding is strong (factor > 0.7), fewer local debonding areas are observed at IPyC outer surface and SiC inner surface at the same time point (1.5×10^7 s), and strong bonding generally induces tensile stress in the SiC layer early in burnup. In contrast, when bonding is weak (factor < 0.5), cracks initiated in IPyC can quickly damage the interface and lead to layer debonding. Due to irradiation-induced shrinkage, IPyC may fully separate from SiC early in burnup. Unlike strong bonding scenarios, this full separation means IPyC no longer transfers stress to SiC, leaving SiC under compressive stress and thus reliable. However, as burnup increases, internal gas pressure may cause IPyC to expand again and reapply pressure on SiC, or IPyC may fracture due to excessive internal pressure, directly exposing SiC to fission gases. These outcomes could significantly reduce TRISO particle behavior predictability.

B. Effect of a Residual Pore in the SiC Layer

SiC with residual pores of 0.1 μm and 1 μm radii at different time points are shown in Figs. 23 and 24, respectively. When a 0.1 μm pore is present, no significant stress concentration occurs around the pore, and no individual crack forms. Instead, the SiC layer is pulled apart by excessive internal pressure from the IPyC layer, leading to coating failure. In contrast, with a 1 μm pore, this geometric defect' s impact on SiC stress is more pronounced, causing cracks to form on both pore sides and propagate inward and outward, eventually resulting in complete fracture of all three coatings.

Fig. 25 [Figure 25: see original paper] shows complete fracture time of the outer three coatings and gas pressure on the IPyC layer inner side at fracture for different residual pore sizes in SiC. With larger pore radius, complete fracture occurs slightly earlier. When pore radius exceeds 0.2 μm, the pore begins impacting SiC overall structure. However, residual pore impact on TRISO particle structural strength is not very significant. Even with a 1 μm residual pore, the outer three coatings still fracture after more than five and a half years. Therefore, SiC fracture is primarily due to excessive fission gas pressure rather than residual pores. In this study' s model, TRISO particles can withstand gas pressure not exceeding 139 MPa.

C. Effect of a Crack in the OPyC Layer

HTGR conditions were first applied to simulate this crack type' s impact. Figs. 26 and 27 present phase field and tangential stress distribution at 7.6×10^7 s for a 10 μm deep pre-crack on the OPyC layer outer side, plus comparison of tangential stress on the SiC layer inner surface. Although this pre-crack induces stress concentration at its tip, the maximum phase field value remains only 0.28 at fuel lifetime end. Tangential stress on the SiC layer inner surface is higher than in the no-crack case throughout the entire lifetime, but its impact is weaker compared to IPyC layer inner side pre-cracks. However, as shown in Fig. 26(b), due to pyrolytic carbon radial shrinkage under irradiation, tensile stress transmitted to the SiC layer outer surface may cause fracture initiation from the outer side. Therefore, this crack type' s potential impact on TRISO particles under space reactor conditions is further investigated.

Under space reactor operating conditions, phase field with a pre-crack on the OPyC layer outer side is shown in Fig. 28 [Figure 28: see original paper]. Unlike IPyC layer inner side cracks, this crack type remains highly stable throughout early and mid-burnup stages. Although the crack slightly expands, OPyC inward shrinkage is supported by the SiC layer, which does not lead to crack propagation until 18×10^7 s. At 18.155×10^7 s, due to tensile stress concentration at two locations on the SiC layer outer surface (as shown in Fig. 26(b)), two corresponding cracks first initiate and propagate inward through the SiC layer. This crack propagation path is similar to those observed in ceramic laminates [**?**]. By 18.200×10^7 s, both cracks fully penetrate the SiC and IPyC layers, leading to complete fracture of the TRISO particle' s outer coating layers. This occurs earlier than in the case with a 1 μm radius residual pore in the SiC layer, but both scenarios result in complete outer coating layer failure only at the very end of the burnup process.

D. Combined Effect of a Crack in the IPyC Layer and a Residual Pore in the SiC Layer

Simulated crack propagation results for an IPyC layer crack and SiC layer residual pore are shown in Fig. 29 [Figure 29: see original paper]. During early burnup stages, the IPyC layer crack extends and causes IPyC-SiC interface debonding. Stress generated on both sides of this main crack causes SiC to experience greater tensile stress, leading to complete fracture of the outer three coatings at an earlier time compared to the scenario with only a SiC residual pore. Therefore, in engineering applications, particular attention should be given to avoiding and limiting IPyC layer crack sizes. Complete fracture occurs at 18.18×10^7 s, the earliest among all studied scenarios.

Overall, these defects provide geometric conditions for stress concentration, serving as the foundation for further crack propagation. However, in early burnup stages, IPyC layer crack propagation (primarily irradiation-induced) only leads to IPyC-SiC layer debonding rather than complete coating failure. The primary cause of complete fracture is excessive internal gas pressure in the IPyC layer, resulting from high temperature and fission gas accumulation during later burnup stages due to prolonged operation. Therefore, before TRISO particle deployment in space reactors, it is crucial to screen for particles with minimal defects and implement measures to maintain coating structural integrity.

VI. Conclusions

This paper developed a phase field model for analyzing TRISO particle outer three coatings using COMSOL Multiphysics. The model fully considers variations in material properties and mechanical behaviors with environmental conditions, burnup, irradiation effects, and fission gas. Model reliability was validated by comparison with IAEA CRP-6 Case-8 benchmark results [?]. The phase field model was also validated using classic brittle fracture problems [?, ?], confirming its capability to simulate crack propagation. While the model does not account for residual stress and thermal strain, the conservative nature of axisymmetric simplification provides safety margins for engineering design, making conclusions practically applicable.

This study analyzed four defect scenarios: (1) a crack on the IPyC layer inner side, (2) a residual pore in the SiC layer, (3) a crack on the OPyC layer outer side, and (4) coexistence of an IPyC crack and SiC pore. Results show that when pre-existing crack depth on the IPyC inner side exceeds 5.8 µm, it propagates toward SiC and causes interface debonding. Separation between layers causes the SiC layer to experience tensile stress earlier, with deeper notches leading to earlier crack propagation and faster separation. Sensitivity analysis reveals that strong IPyC-SiC interface bonding (factor > 0.7) induces tensile stress in SiC during early burnup with limited local debonding. Weak bonding (factor < 0.5) leads to widespread interface damage and near-complete separation. Although this keeps SiC under compressive stress during early burnup, IPyC may not withstand increasing gas pressure alone and eventually fractures, exposing SiC to fission gas and causing higher failure risk.

For SiC pores, when radius exceeds 0.2 μm, cracks form at burnup end and propagate in both directions, eventually fracturing coatings. Even without defects, maximum tolerable gas pressure is 139 MPa. OPyC layer cracks have little effect early on but can redirect crack paths and cause coating failure at burnup end. When IPyC cracks and SiC pores coexist, coating failure occurs earlier than in the pore-only case.

Based on model results, before TRISO particle deployment, efforts should avoid these defects. If material detection techniques such as neutron radiography [?, ?] are available, IPyC cracks over 5.8 μm and SiC pores exceeding 0.2 μm should be screened out. OPyC cracks should also be minimized. Moreover, perfect coatings cannot withstand pressures beyond 139 MPa, so future work should explore strengthening the SiC layer, replacing it with stronger materials, or implementing methods to release internal gas. Additionally, PF-CZM methods [?, ?] can be developed to analyze interface debonding and matrix separation, and optimization approaches [?, ?] can help improve fuel design. Further research on pellet and rod cracking is also necessary for FCM fuel application in space reactors.

VII. Bibliography

[1] Zhuang, K., Wang, YZ., Deng, LN. et al. Steady-state and transient investigation of a small pressurized water reactor ACPR50S for different ATFs based on Bamboo-C code. *NUCL SCI TECH* 36, 11 (2025). doi:10.1007/s41365-024-01565-4.

[2] Zhang, BL., Liu, WG., Tu, MH. et al. Adhesion property of AlCrNbSiTi high-entropy alloy coating on zirconium: experimental and theoretical studies. *NUCL SCI TECH* 35, 141 (2024). doi:10.1007/s41365-024-01508-z.

[3] M. H. d. Toit, A. Mphofu, N. Mashilangako, Neutronic and thermal–hydraulic coupling of FCM and helium annular fuel as accident-tolerant fuel, *Nucl. Eng. Des.* 428, 113522 (2024). doi:10.1016/j.nucengdes.2024.113522.

[4] Liang, ZY., She, D., Wen, YT. et al. Chord length sampling correction analysis for dispersion fuel in Monte Carlo simulation. *NUCL SCI TECH* 35, 71 (2024). doi:10.1007/s41365-024-01409-1.

[5] C. Griesbach, T. Gerczak, C. McKinney, Irradiation-condition dependent mechanisms controlling buffer densification and fracture in TRISO nuclear fuel particles, *J. Nucl. Mater.* 605, 155565 (2025). doi:10.1016/j.jnucmat.2024.155565.

[6] Vrinda Devi, K.V., Dubey, J.N., Gupta, J. et al. TRISO fuel volume fraction and homogeneity: a nondestructive characterization. *NUCL SCI TECH* 30, 41 (2019). doi:10.1007/s41365-019-0555-1.

[7] Yin, CY., Gao, SX., Liu, SY. et al. Transient fuel performance analysis of UO_2-BeO fuel with composite SiC coated with Cr cladding based on multi-physics method. *NUCL SCI TECH* 34, 188 (2023). doi:10.1007/s41365-023-01344-7.

[8] R.L. Seibert, T.J. Gerczak, G.W. Helmreich, et al., AGR-2 irradiated TRISO particle IPyC/SiC interface analysis using FIB-SEM tomography, *J. Nucl. Mater.* 573, 154104 (2023). doi:10.1016/j.jnucmat.2022.154104.

[9] M. MW. Silicon Carbide Integrity in Triso Fuel Particles. Order No. 30714552 ed. University of Pretoria (South Africa); 2015.

[10] Q. Zeng, Z. He, X. Pan, et al., Effect of Coating Temperature on Microstructure and Properties of the SiC Layer in TRISO-Coated Particles, *J. Nucl. Mater.* 3 (2023). doi:10.1007/978-981-19-8899-8_{28}.

[11] A. Bratten, V. Jalan, M. Shi, et al., High-temperature oxidation behavior of the SiC layer of TRISO particles in low-pressure oxygen, *J. Am. Ceram. Soc.* 106(6), 3922-3933 (2023). doi:10.1111/jace.19032.

[12] Zhang, FY., Zhu, GF., Zou, Y. et al. Conceptual design and neutronic analysis of a megawatt-level vehicular microreactor based on TRISO fuel particles and S-CO_2 direct power generation. *NUCL SCI TECH* 33, 69 (2022). doi:10.1007/s41365-022-00633-8.

[13] P. A. Demkowicz, B. Liu, H. D. Hunn, Coated particle fuel: Historical perspectives and current progress, *J. Nucl. Mater.* 515, 434-450 (2019). doi:10.1016/j.jnucmat.2018.09.044.

[14] Alexander J. Leide, Thomas A. Haynes, Nassia Tzelepi, John Payne, Matthew Jordan, Steven Knol, Jan A. Vreeling, Mark Davies, David T. Goddard, Manuel J. Pfeifenberger, Markus Alfreider, Daniel Kiener, Dong Liu. Measurement of residual stresses in surrogate coated nuclear fuel particles using ring-core focussed ion beam digital image correlation. *Nuclear Materials and Energy*, Volume 36, 101470 (2023). doi:10.1016/j.nme.2023.101470.

[15] K. I. Montoya, E. G. Herbert, D. P. Schappel, et al., Micromechanical response of SiC-OPyC layers in TRISO fuel particles, *J. Nucl. Mater.* 606, 155654 (2025). doi:10.1016/j.jnucmat.2025.155654.

[16] G. R. Bower, S. A. Ploger, P. A. Demkowicz, et al., Measurement of kernel swelling and buffer densification in irradiated UCO-TRISO particles, *J. Nucl. Mater.* 486, 339-349 (2017). doi:10.1016/j.jnucmat.2017.01.006.

[17] Ji, WH., Cheng, JJ., Tao, HZ. et al. Numerical simulation of coupling heat transfer and thermal stress for spent fuel dry storage cask with different power distribution and tilt angles. *NUCL SCI TECH* 34, 26 (2023). doi:10.1007/s41365-023-01171-w.

[18] G.K. Miller, D.A. Petti, J.T. Maki, et al., PARFUME Theory and Model Basis Report, Idaho National Laboratory. INL/EXT-08-14497, 2009.

doi:10.2172/968587.

[19] J.D. Hales, R.L. Willianmson, S.R. Novascone, et al., Multidimensional multiphysics simulation of TRISO particle fuel, *J. Nucl. Mater.* 443(1-3), 531-543 (2013). doi:10.1016/j.jnucmat.2013.07.070.

[20] C. Zhang, Y. Wu, S. Liu, et al., Multidimensional multiphysics modeling of TRISO particle fuel with SiC/ZrC coating using modified fission gas release model, *Ann. Nucl. Energy.* 145, 107599 (2020). doi:10.1016/j.anucene.2020.107599.

[21] C. Zhang, Y. Wu, Y. He, Investigation on thermo-mechanical performance of fully ceramic microencapsulated fuel, *J. Nucl. Mater.* 556, 153171 (2021). doi:10.1016/j.jnucmat.2021.153171.

[22] S. Tang, L. Zhu, Q. Lian, et al., Design and optimization of three segmented thermoelectric generator for nuclear reactor application, *Prog. Nucl. Energy.* 173, 105243 (2024). doi:10.1016/j.pnucene.2024.105243.

[23] Y. Wu, S. Tang, L. Zhu, et al., Transient analysis of megawatt-level space gas-cooled reactor coupled with He-Xe Brayton cycle system, *Appl. Therm. Eng.* 260, 124962 (2025). doi:10.1016/j.applthermaleng.2024.124962.

[24] S. Tang, Q. Lian, L. Zhu, et al., Thermal-electrical coupling analysis of the static heat pipe cooled reactor under heat pipe failure condition, *Nucl. Eng. Des.* 417, 112812 (2024). doi:10.1016/j.nucengdes.2023.112812.

[25] L. Peng, Y. Yang, S. Li, Investigation on irradiated-thermal-mechanical coupling performance and failure behaviors of TRISO particle fuel for space reactor applications, *Prog. Nucl. Energy.* 180, 105633 (2025). doi:10.1016/j.pnucene.2025.105633.

[26] D. A. Petti, J. T. Maki, J. Buongiorno, et al., Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, 2002. INEEL/EXT-02-00300.

[27] Yassin, K.M., Hassan, M.H., Ghoneim, M.M. et al. Multi-physics simulation of VVER-1200 fuel performance during normal operating conditions. *NUCL SCI TECH* 34, 28 (2023). doi:10.1007/s41365-023-01172-9.

[28] Y. Zhao, X. Gong, S. Ding, et al., A numerical method for simulating the non-homogeneous irradiation effects in full-sized dispersion nuclear fuel plates, *Int. J. Mech. Sci.* 81, 174-183 (2014). doi:10.1016/j.ijmecsci.2014.02.012.

[29] M. Klinsmann, D. Rosato, M. Kamlah, et al., An assessment of the phase field formulation for crack growth, *Comput. Methods Appl. Mech. Eng.* 294, 313-330 (2015). doi:10.1016/j.cma.2015.06.009.

[30] A. R. Ingraffea, V. Saouma, Numerical modeling of discrete crack propagation in reinforced and plain concrete, *Fract. Mech. Concr.: Struct. Appl. Numer. Calc.* 4, 171–225 (1985). doi:10.1007/978-94-009-6152-4_4.

[31] N. Moës, T. Belytschko, Extended finite element method for cohesive crack growth, *Eng. Fract. Mech.* 69(7), 813-833 (2002). doi:10.1016/S0013-7944(01)00128-X.

[32] L. Chen, T. Rabczuk, S.P.A. Bordas, et al., Extended finite element method with edge-based strain smoothing (ESm-XFEM) for linear elastic crack growth, *Comput. Methods Appl. Mech. Eng.* 209-212, 250-265 (2012). doi:10.1016/j.cma.2011.08.013.

[33] N.A. Collins-Craft, F. Bourrier, V. Acary, On the formulation and implementation of extrinsic cohesive zone models with contact, *Comput. Methods Appl. Mech. Eng.* 400, 115545 (2022). doi:10.1016/j.cma.2022.115545.

[34] Z. Song, B. Han, J. Zhang, et al., Numerical analysis of mesoscale fatigue cracking behavior in concrete based on cohesive zone model, *Struct.* 70, 107777 (2024). doi:10.1016/j.istruc.2024.107777.

[35] T. Metzler, E. Gaganidze, J. Aktaa, Prediction of fracture toughness of a reactor pressure vessel steel in the ductile-to-brittle transition region based on a probabilistic cohesive zone model approach, *J. Nucl. Mater.* 605, 155556 (2025). doi:10.1016/j.jnucmat.2024.155556.

[36] Z. Shirzadeh, M. Fakoor, Z. Daneshjoo, Simulating delamination in composite laminates with fracture process zone effects: A novel cohesive zone modeling approach, *Eng. Fract. Mech.* 315, 110834 (2025). doi:10.1016/j.engfracmech.2025.110834.

[37] Thanh Chau-Dinh, Goangseup Zi, Phill-Seung Lee, et al., Phantom-node method for shell models with arbitrary cracks, *Comput. Struct.* 92-93, 242-256 (2012). doi:10.1016/j.compstruc.2011.10.021.

[38] L. Yang, F. Vasilina, H. Nan, et al., A regularized phenomenological multiscale damage model, *Int. J. Numer. Methods Eng.* 99(12), 867-887 (2014). doi:10.1002/nme.4705.

[39] Z. Tian, A. Jiang, Modeling the Propagation of a Prefabricated Brittle Crack Using Phase-field Method within the Framework of ABAQUS, *KSCE J. Civ. Eng.* 28(7), 3042-3053 (2024). doi:10.1007/s12205-024-1944-0.

[40] P.C. Sidharth, B.N. Rao, An open-source moose implementation of phase-field modeling of fracture in functionally graded materials, *Procedia Struct. Integrity.* 58, 115-121 (2024). doi:10.1016/j.prostr.2024.05.019.

[41] Hirshikesh, D. Schneider, B. Nestler, Realization of adaptive mesh refinement for phase-field model of thermal fracture within the FEniCS framework, *Eng. Fract. Mech.* 293, 109676 (2023). doi:10.1016/j.engfracmech.2023.109676.

[42] Y. Wang, X. Hou, Y. Wang, Thermo-gaseous-mechanical coupling phase-field model for brittle crack propagation in tungsten, *J. Mater. Res. Technol.* 33, 7418-7433 (2024). doi:10.1016/j.jmrt.2024.11.145.

[43] Sana Shahoveisi, Mohammad Vahab, Babak Shahbodagh, et al., Phase-field modelling of dynamic hydraulic fracturing in porous media using a strain-based crack width formulation, *Comput. Methods Appl. Mech. Eng.* 429, 117113 (2024). doi:10.1016/j.cma.2024.117113.

[44] S. Zhou, T. Rabczuk, X. Zhuang, Phase field modeling of quasi-static and dynamic crack propagation: COMSOL implementation and case studies, *Adv. Eng. Softw.* 122, 31-49 (2018). doi:10.1016/j.advengsoft.2018.03.012.

[45] Y. Zhang, J. Sun, C. Liu, et al., Phase field modeling of coupling evolution of fracture and dielectric breakdown in ferroelectric materials, *Int. J. Mech. Sci.* 236, 107747 (2022). doi:10.1016/j.ijmecsci.2022.107747.

[46] X. Wu, M. Chen, L. Ke, An electro-thermo-mechanical coupling phase-field model of defect evolution induced by electromigration in interconnects, *Int. J. Mech. Sci.* 285, 109792 (2025). doi:10.1016/j.ijmecsci.2024.109792.

[47] W. Tang, S. Wen, H. Hou, et al., Phase-field simulation and machine learning of low-field magneto-elastocaloric effect in a multiferroic composite, *Int. J. Mech. Sci.* 275, 109316 (2024). doi:10.1016/j.ijmecsci.2024.109316.

[48] D. Yi, Z. Yang, L. Yi, J. Liu, et al., Phase-field model of hydraulic fracturing in thermoelastic–plastic media, *Int. J. Mech. Sci.* 283, 109750 (2024). doi:10.1016/j.ijmecsci.2024.109750.

[49] J. Luo, Q. Wang, W. Zhou, et al, A coupled phase-field model for sulfate-induced concrete cracking, *Int. J. Mech. Sci.* 283, 109694 (2024). doi:10.1016/j.ijmecsci.2024.109694.

[50] J. Liu, Z. Yang, L. Yi, et al., Cohesive phase-field model for dynamic fractures in coal seams, *Int. J. Mech. Sci.* 282, 109617 (2024). doi:10.1016/j.ijmecsci.2024.109617.

[51] J. Zhao, Y. Frank Cheng, A phase field method for predicting hydrogen-induced cracking on pipelines, *Int. J. Mech. Sci.* 283, 109651 (2024). doi:10.1016/j.ijmecsci.2024.109651.

[52] H. Zhang, E. López-Honorato, A. Javed, et al., A Study of the Microstructure and Vickers Indentation Fracture Toughness of Silicon Carbide Coatings on TRISO Fuel Particles, *J. Am. Ceram. Soc.* 95(3), 1086-1092 (2012). doi:10.1111/j.1551-2916.2011.05044.x.

[53] F. Cao, W. Hao, F. Guo, et al., Effects of water vapor on the oxidation and the fracture strength of SiC layer in TRISO fuel particles, *J. Am. Ceram. Soc.* 100(5), 2154-2165 (2017). doi:10.1111/jace.14723.

[54] H. M. Lee, K. Park, J. Park, et al., High-Temperature Fracture Strength of a CVD-SiC Coating Layer for TRISO Nuclear Fuel Particles by a Micro-Tensile Test, *J. Korean Ceram. Soc.* 52, 441-448 (2015). doi:10.4191/kcers.2015.52.6.541.

[55] A. M. Recuero, G. Singh, W. Jiang, Fracture mechanics approach to TRISO fuel particle failure analysis, *J. Nucl. Mater.* 596, 155083 (2024). doi:10.1016/j.jnucmat.2024.155083.

[56] Y. Li, Q. Wei, L. Li, Analysis of micro-defect-induced cracking in the IPyC layer of TRISO particle with the XFEM, *Eng. Comput.* 41, 1973-1986 (2024). doi:10.1108/EC-11-2023-0873.

[57] J. Tan, Y. Wu, Q. Li, et al., Phase field modeling of irradiation-induced shrinkage in TRISO fuel particle, *J. Nucl. Mater.* 592, 154963 (2024). doi:10.1016/j.jnucmat.2024.154963.

[58] INTERNATIONAL ATOMIC ENERGY AGENCY, *Advances in High Temperature Gas Cooled Reactor Fuel Technology*, Technical Report IAEA-TECDOC-1674, 2013.

[59] D. P. Schappel, *Improvements to the Predictive Capability of FCM Fuel Performance Modeling*, PhD diss., University of Tennessee, 2017.

[60] L. L. Snead, T. Nozawa, Y. Katoh, et al., Handbook of SiC properties for fuel performance modeling, *J. Nucl. Mater.* 371(1-3), 329-377 (2007). doi:10.1016/j.jnucmat.2007.05.016.

[61] D. R. Olander, *Fundamental aspects of nuclear reactor fuel elements: solutions to problems*, Technical information center, Energy research and development administration, 1976. doi:10.2172/7290222.

[62] J. D. Hales, R. L. Williamson, S. R. Novascone, et al., BISON Theory Manual: The Equations Behind Nuclear Fuel Analysis, Idaho National Laboratory, Fuel Modeling and Simulation Department, INL/EXT-13-29930 Rev. 3, 2016. doi:10.2172/1374503.

[63] D. Petti, P. Martin, M. Phelip, R. Ballinger, *Development of improved models and designs for coated-particle gas reactor fuels.* Technical Report, INL/EXT-05-02615, December 2004. doi:10.2172/911237.

[64] A.H. Booth, A method of calculating fission gas diffusion from UO_2 fuel and its application to the x-2-f loop test, Atomic Energy of Canada. AECL-496, September 1957.

[65] T. Kogai, Modelling of fission gas release and gaseous swelling of light water reactor fuels, *J. Nucl. Mater.* 244(2), 131-140 (1997). doi:10.1016/S0022-3115(96)00731-3.

[66] K. Forsberg, A.R. Massih, Diffusion theory of fission gas migration in irradiated nuclear fuel UO_2, *J. Nucl. Mater.* 135(2-3), 140-148 (1985). doi:10.1016/0022-3115(85)90071-6.

[67] Y. Cui, Y. Huo, S. Ding, et al., An analytical solution for simulation of the fission gas behaviors with time-dependent piecewise boundary resolution, *J. Nucl. Mater.* 424(1-3), 109-115 (2012). doi:10.1016/j.jnucmat.2012.02.010.

[68] A. A. Griffith. The Phenomena of Rupture and Flow in Solids, *Ser. A, Math. Phys.* 221, 163-198 (1921).

[69] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, *Comput. Methods Appl. Mech. Eng.* 199(45-48), 2765-2778 (2010). doi:10.1016/j.cma.2010.04.011.

[70] M. J. Borden, C. V. Verhoosel, M. A. Scott, et al., A phase-field description of dynamic brittle fracture, *Comput. Methods Appl. Mech. Eng.* 217-220, 77-95 (2012). doi:10.1016/j.cma.2012.01.008.

[71] C. Miehe, F. Welschinger, M. Hofacker, Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations. *Int. J. Numer. Meth. Eng.* 83, 1273-1311 (2010). doi:10.1002/nme.2861.

[72] K. Bongartz, E. Gyarmati, H. Schuster, K. Täuber, The Brittle Ring Test: A method for measuring strength and young' s modulus on coatings of HTR fuel particles, *J. Nucl. Mater.* 62(2–3), 123-137 (1976). doi:10.1016/0022-3115(76)90012-X.

[73] J.F. Kalthoff, Modes of dynamic shear failure in solids, *Int. J. Fract.* 101, 1–31 (2000). doi:10.1023/A:1007647800529.

[74] S. Liu, G. Fang, J. Liang, et al., A coupling model of XFEM/peridynamics for 2D dynamic crack propagation and branching problems, *Theor. Appl. Fract. Mech.* 108, 102573 (2020). doi:10.1016/j.tafmec.2020.102573.

[75] J. Song, P. M. A. Areias, T. Belytschko. A method for dynamic crack and shear band propagation with phantom nodes, *Int. J. Numer. Meth. Eng.* 67, 868-893 (2006). doi:10.1002/nme.1652.

[76] Z. M. Krajewska, T. Buchwald, A. Drożdżiel, Mechanical defects in the "p-TRISO" -particle covering layers obtained through the ion implantation process, *Ann. Nucl. Energy.* 190, 109897 (2023). doi:10.1016/j.anucene.2023.109897.

[77] S. Liu, Y. Li, P. Chen, et al., Effect of residual pore structure on the performance of TRISO particle fuel, *Front. Mater.* 9, 1072255 (2022). doi:10.3389/fmats.2022.1072255.

[78] A. Baux, S. Jacques, A. Allemand, et al., Complex geometry macroporous SiC ceramics obtained by 3D-printing, polymer impregnation and pyrolysis (PIP) and chemical vapor deposition (CVD), *J. Eur. Ceram. Soc.* 41(6), 3274-3284 (2021). doi:10.1016/j.jeurceramsoc.2021.01.008.

[79] T.A. Haynes, A. Battistini, A.J. Leide, et al., Peridynamic modelling of cracking in TRISO particles for high temperature reactors, *J. Nucl. Mater.* 576, 154283 (2023). doi:10.1016/j.jnucmat.2023.154283.

[80] J. T. Maki, D. A. Petti, D. L. Knudson, et al., The challenges associated with high burnup, high temperature and accelerated irradiation

for TRISO-coated particle fuel, *J. Nucl. Mater.* 371(1-3), 270-280 (2007). doi:10.1016/j.jnucmat.2007.05.019.

[81] Yassin, K.M., Hassan, M.H., Ghoneim, M.M. et al. Multi-physics simulation of VVER-1200 fuel performance during normal operating conditions. *NUCL SCI TECH* 34, 28 (2023). doi:10.1007/s41365-023-01172-9.

[82] Liu, H., Lei, GH. & Huang, HF. Review on synergistic damage effect of irradiation and corrosion on reactor structural alloys. *NUCL SCI TECH* 35, 57 (2024). doi:10.1007/s41365-024-01467-5.

[83] V. Carollo, J. Reinoso, M. Paggi, Modeling complex crack paths in ceramic laminates: A novel variational framework combining the phase field method of fracture and the cohesive zone model, *J. Eur. Ceram. Soc.* 38(8), 2994-3003 (2018). doi:10.1016/j.jeurceramsoc.2018.01.035.

[84] Sun, Y., Wang, QB., Li, PC. et al. Indirect neutron radiography experiment on dummy nuclear fuel rods for pressurized water reactors at CMRR. *NUCL SCI TECH* 35, 189 (2024). doi:10.1007/s41365-024-01534-x.

[85] Cheng, C., Xie, YJ., Xia, XR. et al. A single-pixel elemental imaging method using neutron-induced gamma-ray activation. *NUCL SCI TECH* 36, 2 (2025). doi:10.1007/s41365-024-01566-3.

[86] Dusane, A. R. Budarapu, P. R. Pradhan, et al., Simulation of bridging mechanisms in complex laminates using a hybrid PF-CZM method, *Mech. Adv. Mater. Struct.* 29(28), 7743–7771 (2022). doi:10.1080/15376494.2021.2006835.

[87] C. Zou, H. Yang, G. Chen, et al., Internal-interfacial cracking interaction: Combined phase-field and discontinuous Galerkin/cohesive zone modeling, *Int. J. Mech. Sci.* 273, 109211 (2024). doi:10.1016/j.ijmecsci.2024.109211.

[88] Liu, Y. Wang, W. Wu, A modified phase-field model for cohesive interface failure in quasi-brittle solids, *Int. J. Mech. Sci.* 252, 108368 (2023). doi:10.1016/j.ijmecsci.2023.108368.

[89] He, YF., Sun, B., Ma, MJ. et al. Topology optimization of on-chip integrated laser-driven particle accelerator. *NUCL SCI TECH* 33, 120 (2022). doi:10.1007/s41365-022-01101-2.

[90] Yu, GP., Cheng, YF., Zhang, N. et al. Multi-objective optimization and evaluation of supercritical CO_2 Brayton cycle for nuclear power generation. *NUCL SCI TECH* 35, 22 (2024). doi:10.1007/s41365-024-01363-y.

Note: Figure translations are in progress. See original paper for figures.