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Revision 1

Fuel Performance Modeling Plan to Support the Advanced Gas Reactor Program

March 2024

William F. Skerjanc
Idaho National Laboratory

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Idaho National Laboratory
Advanced Reactor Technologies
Idaho Falls, Idaho 83415

http://www.art.inl.gov

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Technical Reviewer:

Adriaan A. Riet AGR PIE Analyst	3/7/2024 Date

Approved by:

Paul A. Demkowicz AGR Fuels Technical Director	3/14/24 Date
Travis R. Mitchell ART Program Manager	3/12/2024 Date
Michelle T. Sharp INL Quality Assurance	3/12/2024 Date

ABSTRACT

This report documents the current status of the fuel performance modeling initiative to support the Advanced Gas Reactor (AGR) Fuel Development and Qualification Program in the development of tristructural isotropic (TRISO)-coated fuel particles. It includes a brief summary of the codes that have been developed to support TRISO modeling along with a summary of the behavior of fuel particles during irradiation and the modeling used to capture these effects. In addition, this report identifies further modeling and material property needs for further development based on experience from previously performed AGR experiments.

The remaining activities to support fuel performance modeling for the AGR program include continued AGR experiment support for AGR-3/4 and AGR-5/6/7 as well as modeling improvements identified throughout the course of the program. These modeling improvements can be summarized as capturing multidimensional thermomechanical particle behavior and fission product transport.

Additional modeling needs may be identified while processing the data collected during the AGR post-irradiation examination effort which may lead to further improvements that are not included in this report.

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ACRONYMS

AGR	Advanced Gas Reactor
ATR	Advanced Test Reactor
DOE	Department of Energy
DTF	designed-to-fail
HTR	high-temperature reactor
HTGR	high-temperature gas-cooled reactor
INL	Idaho National Laboratory
IPyC	inner pyrolytic carbon
MHTGR	modular high-temperature gas-cooled reactor
MOOSE	Multiphysics Object-Oriented Simulation Environment
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NEUP	Nuclear Energy University Program
OPyC	outer pyrolytic carbon
PARFUME	PARticle FUel ModEl
PIE	post-irradiation examination
R/B	release-to-birth
SiC	silicon carbide
TRISO	tristructural isotropic
UCO	uranium oxycarbide

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Fuel Performance Modeling Plan to Support the Advanced Gas Reactor Program

1. INTRODUCTION

Fuel performance modeling assists in fuel design, fabrication, optimization, experiment design, and understanding of fuel behavior under normal and accident conditions. The predictive results from fuel performance modeling rely not only on the validity of the code, but also the material properties associated with the fuel type in question, both during reactor operation and transient analyses. The extreme environment to which the fuel is subjected, along with complex, coupled, multidimensional physiochemical and thermomechanical phenomena make modeling advanced fuel forms challenging.

This report documents the current status of the fuel performance modeling initiative to support the U.S Department of Energy (DOE) Advanced Gas Reactor (AGR) Fuel Development and Qualification Program in advancing tristructural isotropic (TRISO)-coated fuel particles. Included in this report outside of AGR Program objectives is a summary of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) activities to further TRISO development. A brief description of the codes that have been developed to support TRISO modeling is included, as is a summary of fuel particle behavior during irradiation and the models used to capture these effects. In addition, this report identifies modeling and material property needs for further development based on experience from past AGR Program experiments.

1.1 Background

The performance of the TRISO-coated fuel particle and the manufacturing quality level are critical to the success of modular high-temperature gas-cooled reactors (HTGRs). The TRISO-coated particle fuel design has existed since the 1960s and has been developed specifically for use in HTGRs. These fuel particles are characterized by a superior fission product containment capability at the high temperatures reached in the worst accident scenarios.

Coated particle fuel consists of spherical kernels—less than a millimeter in diameter—of oxide, carbide, or oxycarbide (a mixture of oxide and carbide) fuel encased in multiple coating layers: a porous carbon buffer, a dense inner layer of pyrolytic carbon (IPyC), a silicon carbide (SiC) layer, and an outer pyrolytic carbon layer (OPyC). The SiC layer is the most important component of the coating layer containment system. It is the primary load bearer of internal pressure from fission gas and carbon monoxide potentially created by the reaction of excess oxygen released from fission of uranium dioxide with the buffer, and it is the primary barrier to the release of fission products. The shrinkage of the dense PyC layers with increasing fast neutron fluence imparts a compressive stress on the SiC layer sandwiched between them, significantly reducing the peak tensile stress that can be attained in the SiC layer during irradiation. The PyC layers also act as retention barriers to fission gases. Finally, the buffer provides a void volume to accommodate fission gases and carbon monoxide, which helps reduce the deleterious pressure buildup. The buffer also attenuates fission product recoils, which protects the IPyC layer, and it accommodates kernel swelling during irradiation.

A multitude of phenomena have been historically observed in TRISO coated fuel particles undergoing irradiation, leading to the identification of failure mechanisms (i.e., failure of one or more coating layers). Models have been subsequently developed to accurately simulate these failure mechanisms with the intent of mitigating them through adequate fuel design (e.g., by optimizing particle geometry or coating layer properties) or careful choice of irradiation conditions.

1.2 AGR Program

The U.S. DOE AGR Fuel Development and Qualification Program was established to qualify TRISO-coated fuel for use in HTGRs. The primary goal of the program is to provide a baseline fuel qualification data set in support of the licensing and operation of an HTGR (Mitchell and Demkowicz 2022).

Seven fuel and material irradiation experiments were planned for the DOE AGR program. The overall objectives of these experiments were to:

- Develop fuel fabrication capabilities
- Perform fuels and materials irradiation
- Perform safety testing and post-irradiation examination (PIE)
- Refine fuel performance modeling
- Evaluate fission product transport behavior to support improved radionuclide source term analysis.

Fuel performance modeling is critical to the success of the AGR program. This program element addresses the structural, thermal, and chemical processes that can lead to TRISO-coated particle failures. This includes the effects of fission product chemical interactions with the coatings, which can lead to coating degradation. Fission product release from the fuel particles and transport in the fuel-compact matrix and fuel-element graphite during irradiation are also modeled. Computer codes and models will be further developed and validated as necessary to support fuel development (Mitchell and Demkowicz 2022).

Fuel performance modeling, as it relates to the AGR program, consists of the following:

- Improve the existing coated particle material property database to help develop constitutive relationships that describe the thermomechanical, thermophysical, and physiochemical behavior of coated particles.
- Develop a mechanistic fuel performance model for normal and off-normal HTGR conditions and benchmark these against relevant performance data.

2. FUEL PERFORMANCE MODELING CODES

As a key component of the AGR program's modeling capability, Idaho National Laboratory (INL) has developed PARticle FUel ModEl (PARFUME), a TRISO fuel performance modeling code. Subsequently, INL incorporated the theory and models developed for PARFUME into the modeling code BISON using the Multiphysics Object-Oriented Simulation Environment (MOOSE) finite element library. A brief description of the two codes follows.

2.1 PARFUME

PARFUME is an integrated, mechanistic computer code that evaluates the thermal, mechanical, and physicochemical behavior of coated-fuel particles and the probability for fuel failure given the particle-to-particle statistical variations in physical dimensions and material properties that arise during the fuel fabrication process (Miller, Petti and Maki, et al. 2023). PARFUME describes both the mechanical and physicochemical behavior of the fuel particle under irradiation and postulated accident conditions, while capturing the statistical nature of the fuel, and determines the failure probability of a population of fuel particles, accounting for the mechanisms that can lead to particle failure. In addition, PARFUME calculates fission product transport by determining the diffusion of fission products from the fuel through the particle-coating layers and their subsequent release through the fuel matrix to the coolant. The general solution procedure used by PARFUME consists of the basic processes depicted in the flow chart of Figure 1.

Coated particle fuel exhibits statistical variations in physical dimensions and material properties from particle to particle due to the nature of the fabrication process. Particle behavior is also inherently multidimensional, further complicating model development. The failure probability of a batch of fuel particles depends on statistical variations in the fuel design parameters as well as variation in the characteristic strengths of the coating layers in a batch. The calculation of fuel particle failures implemented in PARFUME samples the fuel design parameters from a Gaussian statistical distribution, and the layer strengths are sampled from a Weibull statistical distribution (Kovacs, Bongartz and Goodin 1985) (Martin 2002). PARFUME allows for statistical variations in kernel diameter, coating thicknesses, pyrocarbon densities, pyrocarbon anisotropy (as measured by the Bacon anisotropy factor), creep coefficient for the pyrocarbon, Poisson's ratio in creep for the pyrocarbon, bond strength between the IPyC and SiC layers, and particle asphericity (as measured by the aspect ratio).

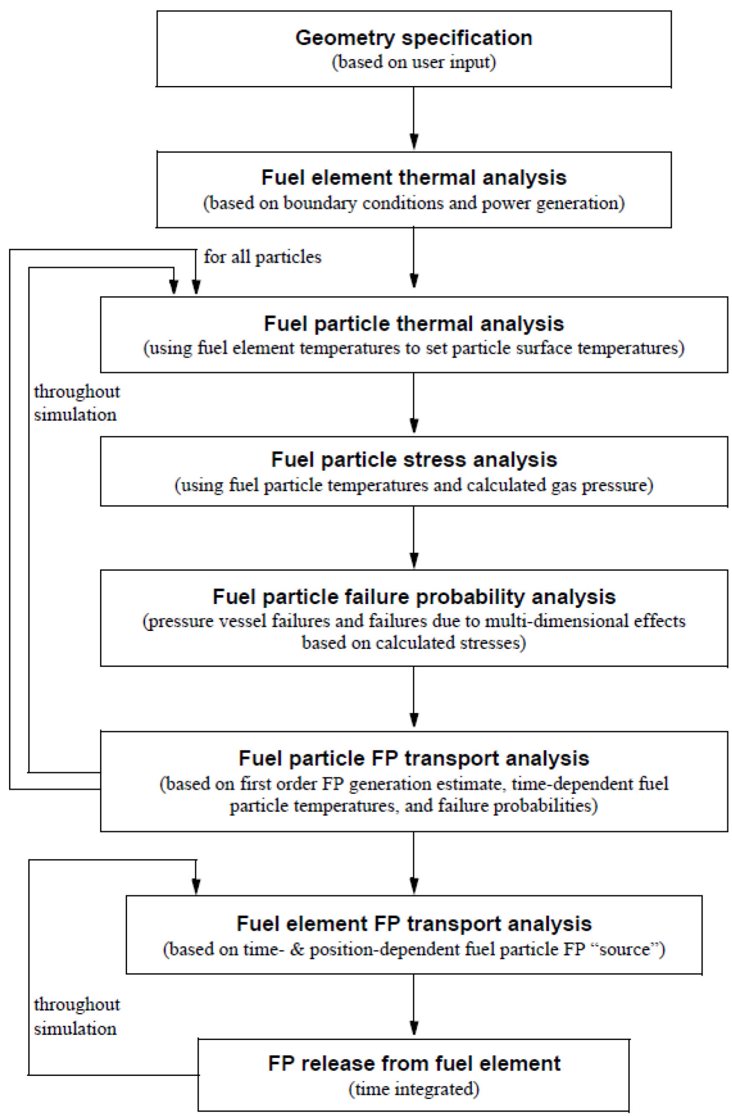

Figure 1. PARFUME calculation flow chart.

2.2 BISON

BISON (Williamson, et al. 2021) is a nuclear fuel performance application built using the MOOSE finite element library (Permann, et al. 2020) developed at INL that is capable of modeling multiple fuel forms in a wide variety of dimensions and geometries. It solves coupled nonlinear partial differential equations, including heat conduction, mechanics, fission product species transport, etc., in a fully implicit manner. More detailed descriptions of the BISON fuel performance code as it relates to TRISO fuel modeling can be found in "BISON TRISO Modeling Advancements and Validation to AGR-1 Data" (Hales 2021), "Numerical Evaluation of AGR-2 Fission Product Release" (Hales, Toptan, et al. 2022), and "TRISO particle fuel performance and failure analysis with BISON" (Jiang, Hales, et al. 2021). The Monte Carlo methodology used in BISON to calculate the failure probability of a batch of fuel particles is summarized in Figure 2 (Jiang, Hales, et al. 2021). Recently, a more efficient statistical failure analysis, similar to the "fast" integration methodology in PARFUME, has been added to BISON (Jiang, Singh, et al. 2022).

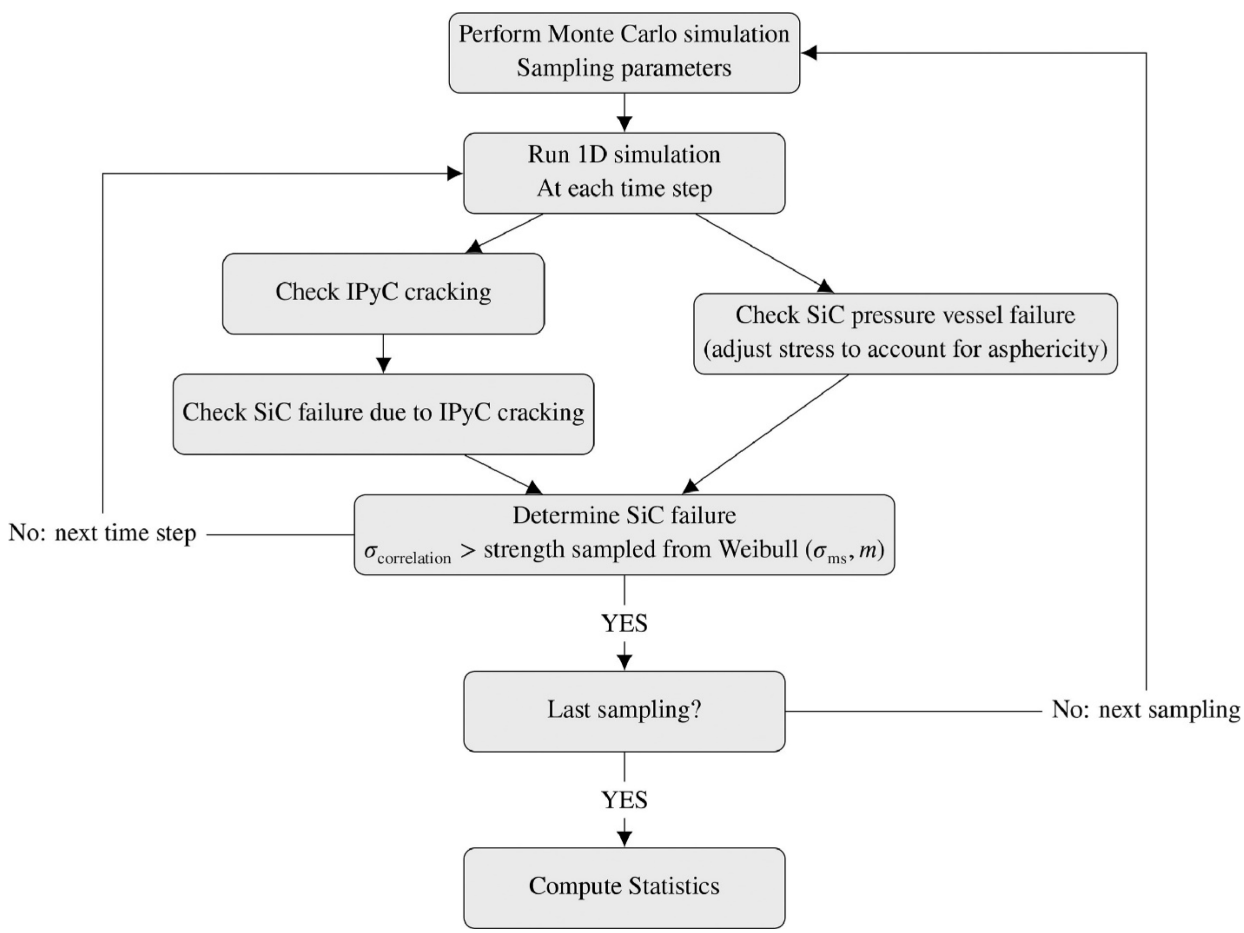

Figure 2. Monte Carlo methodology for calculating failure probability in BISON.

BISON can easily incorporate different irradiation conditions and run either very small analyses with a single processor or very large analyses on multiple processors on a supercomputer. For TRISO fuel, BISON supports spherically symmetric models, axisymmetric models, and fully three-dimensional (3D) models. Thermomechanical models for each material layer include elastic modulus, irradiation creep, irradiation-induced dimension change, thermal expansion, and thermal conductivity.

Fission product generation, diffusion, and release can also be modeled for TRISO particles with uranium dioxide (UO_2), uranium oxycarbide (UCO) and uranium nitride kernels. In addition, BISON has the ability to perform statistical failure analyses of large samples of fuel particles. This capability enables the evaluation of failure due to multidimensional failure phenomena by analyzing thousands of particles. This enables realistic calculations of the fission product release from the many particles in a TRISO-fueled reactor. Fuel particle behavior phenomena that impact fuel performance that have not previously been accounted for in the modeling codes will be implemented in BISON since many of these require multidimensional simulations.

3. TRISO-COATED FUEL PARTICLES

The AGR program has selected the UCO fuel kernel (as opposed to UO_2) due to its superior performance at high temperatures during irradiation and at high burnup (>12% fissions per initial metal atom). A brief description of a typical TRISO-coated fuel particle follows, along with the potential failure mechanisms under consideration for modeling purposes. A more detailed description of potential failure mechanisms is provided in the “Technical Program Plan for INL Advanced Reactor Technologies Advanced Gas Reactor Fuel Development and Qualification Program” (Mitchell and Demkowicz 2022).

3.1 Fuel Particle Behavior

A TRISO-coated particle is shown in Figure 3. Several physical phenomena influence particle behavior, including fission gas production and irradiation effects. For example, fission gas pressure builds up in the kernel and buffer regions while the IPyC, SiC, and OPyC act as structural layers to retain this pressure. The basic fuel behavior during irradiation is shown schematically in Figure 4, where the IPyC and OPyC layers both shrink and creep due to irradiation of the particle while the SiC response is essentially limited to elastic behavior. The pressure generally increases as the irradiation of the particle progresses, thereby contributing to a tensile hoop stress in the SiC layer. The shrinkage of the IPyC during irradiation counters the effect of the pressure load by pulling inward on the SiC. Likewise, OPyC shrinkage causes it to push inward on the SiC. Particle failure is expected if the stress in the SiC layer reaches its fracture strength. SiC failure results in an instantaneous release of elastic energy that should be sufficient to cause the simultaneous failure of the pyrocarbon layers. These effects are described using material, thermal, and physicochemical models.

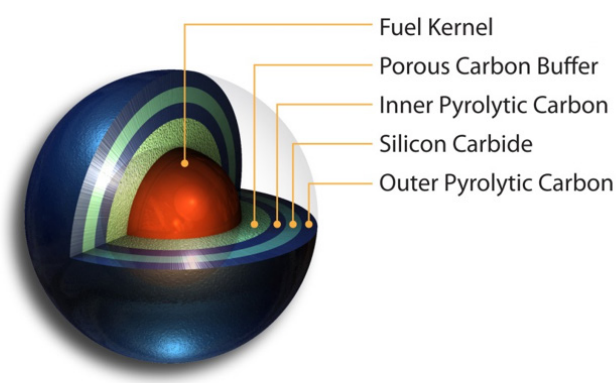

Figure 3. Typical TRISO-coated fuel particle geometry.

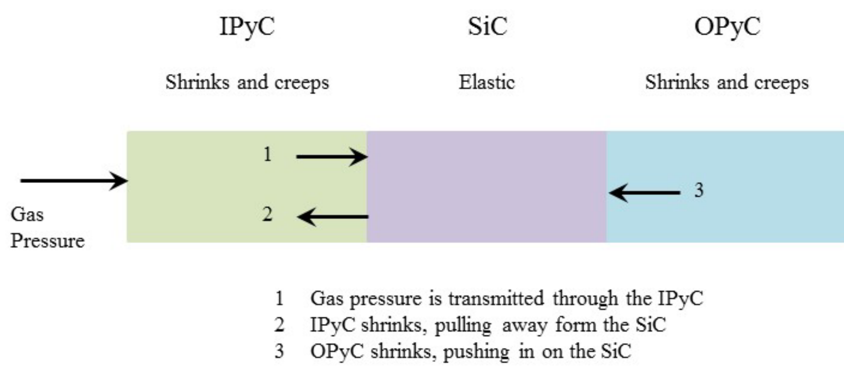

Figure 4. Behavior of coating layers in fuel particles.

3.2 Fuel Failure Mechanisms

Weibull statistical theory is used to determine whether particles fail using a mean strength for the SiC layer based on a stress distribution corresponding to the failure mechanism under consideration. The failure modes are implemented such that a particle fails only in the mode of failure that would occur first for that particle. The code retains the time at which the failures occur, allowing for the construction of a time evolution of the failure probability for a batch of fuel particles. Weibull parameters used to evaluate failures of the SiC layer and cracking of the IPyC layer are discussed in a CEGA Corporation report (CEGA 1993). SiC layer failure is assumed to lead to full TRISO particle failure.

Five potential failure mechanisms are currently considered. The first is a pressure vessel failure caused by a buildup of gases (e.g., fission gas and carbon monoxide). Stresses for this failure mechanism are determined using the one-dimensional (1D) solution for a three-layer (IPyC-SiC-OPyC) particle. Fuel particle asphericity results in an increase in SiC stress that requires additional modeling using the finite element analysis code Abaqus (Abaqus 2021) for this multidimensional behavior to implement into PARFUME. Abaqus generates the multidimensional input required by PARFUME to correlate the stresses of an aspherical particle to a perfectly spherical particle using the PARFUME statistical methodology (Miller, Petti and Maki 2004). Because BISON is a finite element code, it is capable of modeling the two-dimensional (2D) and 3D nature of this failure mechanism without the aid of an additional Abaqus calculation.

The second mechanism considered is SiC layer failure caused by the partial debonding of the IPyC from the SiC. Debonding, if it occurs, results from the IPyC shrinking inward away from the SiC during irradiation. PARFUME first determines whether debonding between the layers occurs by comparing the radial stress between layers with the bond strength between layers. If debonding has occurred, the code estimates the stress in the SiC layer and accounts for the multidimensional effects using a previously documented methodology (Miller, Petti and Maki 2004). The implementation of the IPyC-SiC debonding phenomenon is currently under development in BISON. Because AGR particle fabrication is based on German processes, the bond strength is assumed to be representative of German particles (i.e., 100 MPa). At this bond strength, IPyC-SiC debonding is generally not predicted and therefore does not contribute to particle failures.

The third mechanism is fuel kernel migration into the SiC layer under the influence of a temperature gradient (or the "amoeba" effect). This effect is driven by the production of carbon monoxide and therefore is primarily restricted to particles with UO_2 kernels. Given the suppression of CO formation, kernel migration is not typically observed in UCO kernels.

The fourth mechanism is a SiC layer failure caused by irradiation-induced shrinkage and the subsequent cracking of the IPyC layer. The presence of a crack creates a stress concentration in the SiC layer (Miller, Petti and Vracalle, et al. 2001) that may or may not lead to total fuel particle failure.

Because PARFUME is a 1D fuel performance code, and the effects of an IPyC crack on a TRISO fuel particle are multidimensional, Abaqus (Abaqus 2021) is used to generate the required PARFUME input to estimate the stresses in the particle using the PARFUME statistical methodology (Miller, Petti, et al. 2003). In evaluating failures caused by IPyC cracking, PARFUME first determines whether the IPyC layer cracks using the Weibull statistical theory. If the IPyC layer cracks, the particle is evaluated for SiC layer failure due to the presence of the crack. Similar to particle asphericity, BISON does not need the additional Abaqus analysis to perform the 2D modeling of this phenomenon (Jiang, Singh, et al. 2022).

The fifth mechanism is chemical attack of the SiC layer by palladium (Pd), which is modeled in PARFUME and BISON by calculating the Pd penetration into the SiC layer. The penetration rate is calculated by an Arrhenius function fitted to in-reactor data for Pd penetration in SiC published between 1981 and 1990 (Miller, Petti and Maki, et al. 2023). SiC layer failure is not explicitly calculated as a function of the degree of Pd corrosion (i.e., “thinning” of the SiC layer), but rather calculates the depth of Pd corrosion and the user can apply a predetermined thinning criteria (e.g., 50%) at which the SiC layer is assumed to fail. This failure phenomenon has also been developed in BISON.

4. AGR PROGRAM SUPPORT

The AGR program—including irradiation experiments and collection of PIE data—has been an integral part of the TRISO-coated fuel qualification for use in high-temperature reactors (HTRs). Further, the data collected during these experiments have been used for the verification and validation of the codes that analyze the performance and integrity of these fuels. Comparisons between previous AGR experiments and modeling codes have been completed to both improve their modeling capabilities and identify gaps between the actual performance and analytic models. This work will continue for the last two AGR irradiation campaigns, AGR-3/4 and AGR-5/6/7, using both PARFUME and BISON, to create a high level of confidence in both fuel performance codes for further use in the qualification of TRISO fuel. The following is a summary of the planned work for the continued support of the AGR program.

4.1 AGR-3/4 Experiment

AGR-3/4 combined the third and fourth in this series of planned experiments to test TRISO-coated, low-enriched uranium UCO fuel. As defined in the technical program plan for the INL Advanced Reactor Technologies AGR fuel program (Mitchell and Demkowicz 2022), the objectives of the AGR-3/4 experiment are to:

1. Irradiate fuel containing UCO designed-to-fail (DTF) fuel particles that will provide a known source of fission products for subsequent transport through compact matrix and structural graphite materials
2. Assess the effects of sweep gas impurities (such as CO, H_2O, and H_2) typically found in the HTGR primary coolant circuit on fuel performance and subsequent fission product transport
3. Provide irradiated fuel and material samples for PIE and safety testing
4. Support the refinement of fuel performance and fission product transport models with online PIE, and safety test data.

4.1.1 As-run Irradiation Test Predictions

BISON was used to model three compacts in the AGR-3/4 experiment using the manufactured TRISO-coated fuel particle and compact data using the as-run irradiation conditions (Skerjanc and Jiang 2021). Using irradiation conditions determined from as-run physics and thermal calculations, the fuel particle failure probability and fission product release from the driver fuel and DTF particles were analyzed for the selected compacts. This study identified that further modeling improvements were needed in BISON to accurately model both the failure probability and fission product transport across the gas gaps into the capsule rings. Experimental data from past and future AGR experiments will be used to refine and improve the current models used in the codes to predict fuel particle behavior and fission product diffusion more accurately.

4.1.2 In-pile Irradiation PIE Comparison

PARFUME has previously been used to compare measured in-pile fission product release behavior, as determined during PIE of the fuel and irradiation capsules, to the as-run modeling results (Collin 2014b) (Skerjanc 2020). Due to the complexity of the experimental configuration of AGR-3/4, BISON was used along with PARFUME in a more recent study to compare the models with the experimental data (Skerjanc and Jiang 2022).

The fuel performance codes modeled the AGR-3/4 irradiation experiment using the fuel compact time-averaged volume-averaged daily temperatures to predict the release fraction of the fission product silver (Ag-110m) from a representative TRISO-coated fuel particle. Post-irradiation gamma scanning was performed on all 32 of the 48 fuel compacts to measure the retained Ag-110m inventory. The ratio of the measured Ag-110m inventory to the calculated (using as-run coupled neutronics and depletion models) inventory (M/C) was used as an estimate of the fraction of Ag-110m retained in each compact. This did not account for any bias that could be present in the calculated inventory (e.g., if the calculated inventory is biased high, it would bias the M/C value low which therefore would underrepresent the fraction of retained Ag-110m. An Ag-110m release fraction was then calculated as 1-[M/C] and these data were compared to the predicted release fraction by both PARFUME and BISON. The results showed good agreement between PARFUME and BISON, but both codes underpredicted the silver release fraction for all the compacts (Skerjanc and Jiang 2022).

In addition, BISON was used to model and predict the fission product concentration radial profile outside of the compacts in capsules' inner and outer rings. These rings were comprised of matrix or structural graphite. To obtain the concentration profiles of silver, cesium, and strontium, a sorption isotherm methodology was developed in BISON to capture the effects of fission product transport across the gaps between the concentric rings. BISON predictions were then compared to experimental measured data obtained from destructive PIE. The general shapes of the concentration radial profiles as calculated by BISON were similar in the inner ring but varied in the outer ring depending on the fission product of interest or capsule temperature. Using this methodology and model, BISON can now aid in developing new fission product diffusion coefficients for matrix or structural graphite materials (Skerjanc and Jiang 2022).

Modeling efforts to predict the diffusion of fission products from the driver fuel and DTF particles through the compact matrix, and eventually collected in the capsule components outside of the compacts in each AGR-3/4 capsule, are currently being investigated (Riet and Stempien 2022) (Riet 2023) and are discussed in greater detail in Section 5.8. The results of this effort will aid in producing new fission product diffusion coefficients to improve fission product modeling capabilities.

4.1.3 Heating Tests of Irradiated and Re-Irradiated Compacts

The fuel performance modeling codes PARFUME and BISON were used to predict the release of fission products silver, cesium, and strontium from as-irradiated fuel compacts containing TRISO-coated particles during heating tests after irradiation. The measured fission product release fractions from the heating tests were compared to modeling predictions calculated by PARFUME and BISON (Skerjanc 2023).The results indicate that that both modeling codes overpredict the fission product release fractions of silver, cesium, and strontium, which demonstrates that the diffusivities used in the codes are overestimated.

In addition, select compacts from the AGR-3/4 irradiation were chosen to be re-irradiated and then subjected to isothermal heating tests. The re-irradiation will provide inventory of short-lived isotopes (primarily I-131 and Xe-133) available to be released during the heating test. BISON will be used to model the re-irradiation and ensuing heating test to compare the predicted release of the short-lived isotopes to the measured data.

4.2 AGR-5/6/7 Experiment

As defined in the technical program plan for the AGR Fuel Development and Qualification Program (Mitchell and Demkowicz 2022), the objectives of the AGR-5/6/7 experiment are:

1. Irradiate reference design fuel containing low-enriched UCO TRISO fuel particles to support fuel qualification
2. Establish the operating margins for fuel beyond normal operating conditions
3. Provide irradiated fuel performance data and irradiate fuel samples for PIE and safety testing.

Similar to the previous AGR experiments, PARFUME will be used to model the AGR-5/6/7 irradiation experiment and subsequent data comparison with the PIE results. BISON will also be used in conjunction with PARFUME to continue the development and identify modeling needs.

4.2.1 In-Pile Fuel Failure Predictions

PARFUME was used to predict the fuel particle failure probability and fission product release from all 194 AGR-5/6/7 fuel compacts using the as-run neutronics and thermal analysis as input (Skerjanc 2021). Fuel particle failures in two of the five capsules were predicted and were caused by localized stress concentrations in the SiC layer due to cracking of the IPyC layer. The higher IPyC cracking probability leading to higher failure probabilities in these compacts was directly related to the low pyrocarbon creep rate at lower temperatures. The pyrocarbon creep rate at low temperatures used in both PARFUME and BISON needs further evaluation and is discussed in Section 5.1.

4.2.2 Heating Test Predictions

PARFUME and BISON will be used to predict fuel particle failure probability and diffusion of fission products during the planned isothermal heating tests as part of the AGR-5/6/7 PIE effort. Similar predictions have been performed previously for AGR-1 and AGR-2 (Collin 2012) (Collin 2014a). Results from the AGR-5/6/7 heating test predictions will provide an *a priori* estimate of the TRISO fuel performance in the higher temperature environment simulating accident conditions. This will include fuel particle failure probabilities, palladium penetration, and fission product release.

4.2.3 In-Pile Fission Product Release Predictions

The modeling performed to support the AGR-5/6/7 PIE effort will be similar to that described above for AGR-3/4 and previously completed for AGR-1 and AGR-2. This will include modeling fission product diffusion and comparing it to experimental data obtained from nondestructive (gamma scanning) and destructive (deconsolidation-leach-burn-leach) examination of fuel compacts. The isotopes analyzed will include Ag-110, Cs-137, and Sr-90.

It is anticipated that the fission product release modeling from AGR-3/4 will result in updated diffusion modeling parameters that can be implemented in PARFUME and/or BISON. The implementation of these new parameters can be used for future modeling analyses and compared to experimental data.

4.2.4 Fission Product Release Predictions for Post-Irradiation Heating Tests

Post-irradiation safety tests will be performed on selected compacts at various temperature ranges to determine fission product release at temperatures that bound accidents conditions. PARFUME and BISON will be used to calculate the fission product release of Ag-110, Cs-137, and Sr-90 using the isothermal heating tests conditions. These modeling predictions have been previously performed for both

AGR-1 (Collin 2014b) and AGR-2 (Skerjanc 2020). If available, the updated fission product diffusion parameters derived from the AGR-3/4 experiment for the compact matrix will be used in this analysis.

4.3 TRISO Particle Kernel and Buffer Volume Fraction Margin

TRISO fuel is being considered for HTGR designs that deviate significantly from the prismatic or pebble-bed modular high-temperature gas-cooled reactors (MHTGRs) that were considered at the outset of the AGR program. These designs include microreactors with compact core designs that can benefit from increasing the core fissile density beyond that conventionally required in an MHTGR using TRISO fuel. One means of increasing the fissile density in an HTGR core is to adjust the coated particle design to increase the ratio of kernel volume to total particle volume, which would increase the volume of fissile phase in a fuel compact with no increase in particle packing fraction beyond that used in fuel compacts tested by the AGR program.

Previous studies have identified the critical manufacturing limit for the design of the AGR TRISO particle buffer layer thickness such that it can adequately absorb fission product gases and carbon monoxide (Skerjanc, Maki, et al. 2016). It was determined that the minimum buffer layer thickness in the AGR TRISO particle with a 425 μm kernel before experiencing an increase in fuel particle failure is approximately 50 μm. The current AGR TRISO particle has a buffer layer thickness of approximately 100 μm, leaving sufficient design margin before fuel particle failure is expected.

PARFUME was used to model a typical AGR-5/6/7 425 μm TRISO fuel particle with a 100 μm thick buffer layer to establish a baseline for fuel performance for comparison to a modified TRISO particle (Skerjanc 2023) (Skerjanc and Youinou 2023). The buffer layer thickness was then decreased in 10 μm increments while the kernel diameter increased in 20 μm increments thus maintaining the same overall TRISO particle diameter. Using this methodology, the overall TRISO fuel performance was assessed using current modeling capabilities and material properties. In general, increasing the kernel/buffer volume fraction increased the SiC stress and, subsequently, the failure probability of a fuel particle when compared to the AGR-5/6/7 particle design. There was little impact on fission product diffusion through the particle as the kernel/buffer volume fraction increased.

5. FUEL PERFORMANCE MODELING IMPROVEMENTS

Throughout the evolution of the AGR Program, phenomena and material properties have been identified for inclusion in fuel performance codes to predict the behavior of TRISO-coated fuel particles more accurately during irradiation and under accident conditions. To capture these effects and properties, the fuel performance codes PARFUME and BISON will require improvements in their respective modeling capabilities. The following sections identify potential areas of improvement to more accurately complete fuel performance simulations and aid in fuel failure probability and fission product diffusion predictions. An assessment of these modeling improvements—including data availability and significant impacts to the modeling results—is summarized in Appendix A. Along with the modeling improvements identified below, the NEAMS BISON TRISO development team are also aware modeling advances that meet their stakeholders' needs and complement those identified by the AGR program. These modeling improvements are detailed in Section 6.1, and together, resources between the two programs will be leveraged to expand INL's TRISO modeling capabilities.

Over the last twenty plus years, PARFUME has been under development by the AGR program and has become a valuable resource for benchmarking other TRISO fuel performance modeling codes as a basis for comparison. The fundamental principles established and the expertise gained in the development of PARFUME and the corresponding models developed over the years have since been implemented in BISON as a foundation for its fuel performance modeling capabilities. The AGR irradiation experiments and subsequent PIE of TRISO-coated fuel has identified fuel behavior that requires implementation of models beyond PARFUME's 1D capability. As a result, the new modeling improvements identified below will be implemented in BISON and only updated in PARFUME, where it is applicable to a 1D solution scheme (e.g., PyC creep rate, fission product diffusivities, release-to-birth (R/B) models, etc.)

5.1 Pyrocarbon Creep Rate

The irradiation-induced pyrocarbon creep consists of transient creep and steady-state creep. Due to the lack of established data and its minimal effect on particle stresses, transient creep is not included in PARFUME or BISON; only the steady-state creep is considered. The correlations used in the two fuel performance codes are only valid between 600 and 1350°C. If the irradiation temperature is below 600°C, the creep correlation is set to the value at 600°C. Similarly, if the temperature is above 1350°C, the coefficient is set to the value at 1350°C. The creep correlation used in PARFUME and BISON is illustrated in Figure 5 for various pyrocarbon densities (ρ).

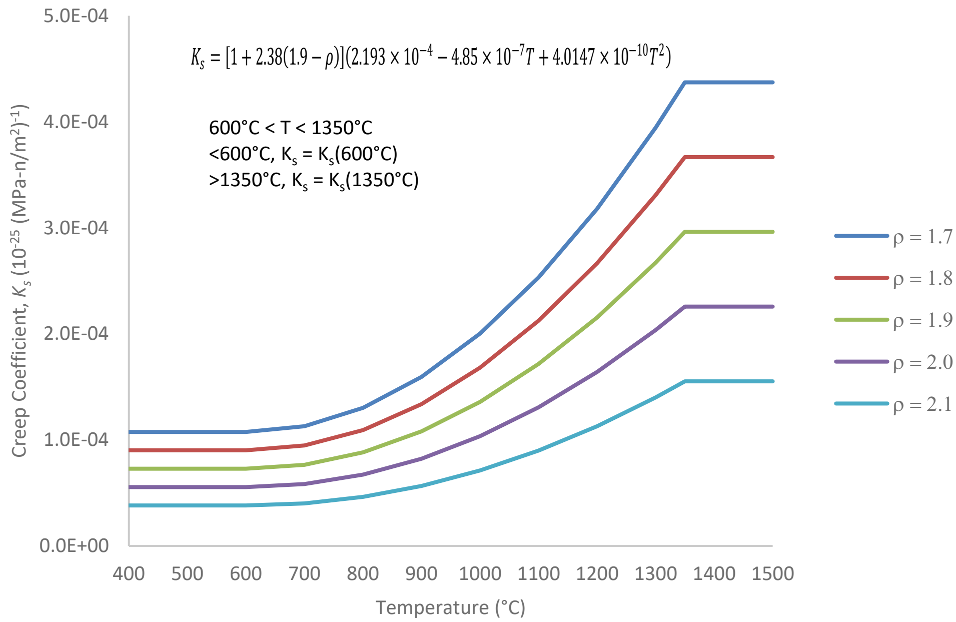

Figure 5. Irradiation-induced pyrocarbon creep correlation coefficients.

The irradiation-induced creep correlation is based on experimental data as derived in the CEGA Corporation report, first published in 1993 (CEGA 1993). Since then, the AGR program has performed graphite irradiation experiments and TRISO particle irradiations at lower temperatures that have shown that perhaps the creep correlation coefficients used in the two fuel performance codes may not be accurate at low temperatures. Although the creep coefficients used in the codes produce predictive results that are higher than those that have been experimentally observed, an updated creep correlation could potentially improve the accuracy of predicting fuel particle failures associated with IPyC cracking. This was demonstrated when predicting fuel particle failures during the AGR-5/6/7 irradiation using PARFUME (Skerjanc 2021). As summarized in Table 1, PARFUME overpredicted the number of fuel particle failures based on the average capsule failure fraction at lower temperatures. These fuel particle failures are caused by localized stress concentrations induced by cracks in the IPyC layer owing to shrinkage in the layer and the creep not relieving the stresses early during the irradiation. Informed irradiation-induced creep coefficients at temperatures below and above the current range of the applicability of the CEGA correlations have the potential to more accurately reflect the physical behavior of TRISO particles during irradiation.

Table 1. AGR-5/6/7 predicted fuel particle failure using PARFUME.

Capsule	5	4
Average compact temperature (°C)	741	839
Average compact predicted failure fraction	2.60E-04	1.14E-04
Total number of TRISO particles	81432	52728
Predicted number of TRISO particle failures	21	6
Observed number of TRISO particle failures[1]	0	0

1. Per AGR-5/67 irradiation as-run report (Pham, Palmer, et al. 2021) based on the data currently available.

5.2 IPyC Failure Prediction Validation

As discussed in Sections 3.1 and 5.1, the behavior of the IPyC layer during irradiation and its ability to retain structural integrity is an important function that is integral to the performance of the SiC layer. Irradiation-induced pyrocarbon shrinkage results in tensile stresses in the IPyC layer that can ultimately lead to cracking, compromising the integrity of the SiC layer. Failure of the SiC layer due to irradiation-induced IPyC cracking is the primary contributor to the total calculated failure probability in UCO fuel.

In some of the AGR irradiation capsules, the IPyC failure fraction, both predicted and observed, is sufficiently high that it is possible to meaningfully compare and validate the codes to empirical data. For example, during PIE of AGR-1 baseline fuel, it was observed that approximately 3% of the IPyC layers failed during irradiation (Demkowicz, et al. 2015). In some of the AGR-5/6/7 capsules the IPyC failure fraction predicted with PARFUME exceeded 50%. Because this predicted failure fraction is so high, analysis of only a few dozen particles from several AGR-5/6/7 compacts would be sufficient to compare the experimental data to the predicted irradiation induced IPyC failure from the fuel performance codes and assess the accuracy of the prediction. While past studies of coating layer failure were primarily performed on many particle cross sections, x-ray computed tomography will be used in the future to nondestructively determine the extent of layer fracture and avoid the inaccuracies inherent in viewing only a single plane of the particle.

5.3 Thermomechanical Buffer Layer Modeling

5.3.1 Background

The ongoing AGR PIE has examined thousands of particle cross sections to observe irradiated kernel and coating morphologies (see the AGR-1 (Demkowicz, et al. 2015) and AGR-2 (Stempien, et al. 2021) final PIE reports for summaries of these results). The work also involved extensive effort to locate particles with lower-than-normal fission product retention and examine these particles to identify any coating anomalies (Hunn, et al. 2016). The particle characterization methods allow localized degraded regions of particles to be pinpointed and examined in detail; they have greatly advanced the understanding of coating behavior during irradiation and causes of layer failure. Some of these empirical observations of particle behavior differ from the predicted or assumed behavior in the fuel performance models.

5.3.2 Buffer-IPyC Debonding

The buffer layer in the existing models is presumed to exhibit no adhesion to the IPyC layer, such that it can immediately detach as it begins to experience shrinkage during irradiation and create a growing gap between the buffer and IPyC layers. This gap is assumed to be uniform in the models (i.e., the kernel-buffer sphere is located concentrically inside the IPyC layer). As a consequence of this behavior, the buffer layer does not exert any mechanical influence on the IPyC layer during irradiation in the models. PIE data indicate that in many particles a significant portion of the buffer-IPyC interface remains intact after hundreds of days of irradiation to burnup as high as ~19% fissions per initial metal atom and a fast neutron fluence of ~5×10^{25} n/m^2 (E ≥0.18 MeV). This results in an asymmetric buffer-IPyC gap (Figure 6), the impact of which has not been examined in the models. A more important consequence of this behavior is that the buffer-IPyC interaction appears to affect the IPyC and SiC coating layer behavior, which is discussed below.

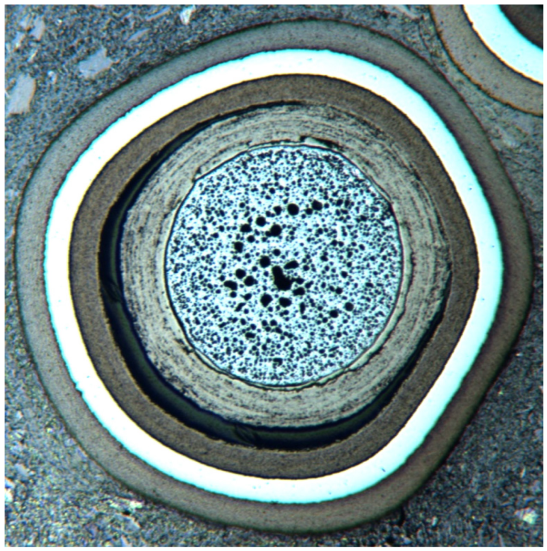

Figure 6. AGR-1 irradiated particle with an asymmetrical buffer-IPyC gap (Ploger, et al. 2012).

5.3.3 IPyC Cracking and SiC Failure

The extremely rare particles that experienced SiC layer failure during irradiation or during safety testing in the AGR-1 and AGR-2 experiments generally exhibited a similar failure mechanism, as described by (Hunn, et al. 2016) and summarized here. Mechanical failure of the IPyC layer can expose a small region of the inner surface of the SiC layer to a localized fission product (primarily Pd) attack (Figure 7). Subsequently, sufficient time and temperature can result in complete through-layer degradation, such that cesium retention is compromised. A key observation is that particles exhibiting IPyC failure are often those in which a significant portion of the buffer-IPyC interface remains intact, and the IPyC layer failure occurs at a location where the buffer-IPyC interface transitions from intact to separated, as in Figure 7. These observations strongly suggest that dramatic buffer shrinkage (measured to be between 26 and 40 volume percent in irradiated AGR-1 (Bower, et al. 2017) and AGR-2 particles (Stempien, Plummer, et al. 2019) and a relatively strong buffer-IPyC bond can increase the stress on the IPyC layer such that it promotes IPyC fracture and localized separation from the SiC layer. A second mode of IPyC fracture that has been observed is demonstrated in Figure 8, where a fracture in the buffer layer corresponds to a fracture in the IPyC layer in a region where the buffer-IPyC interface remains intact. In both cases, while the primary mode of SiC layer failure is fission product attack, the precursor to this is IPyC failure, which may be significantly influenced by an interaction with the buffer layer.

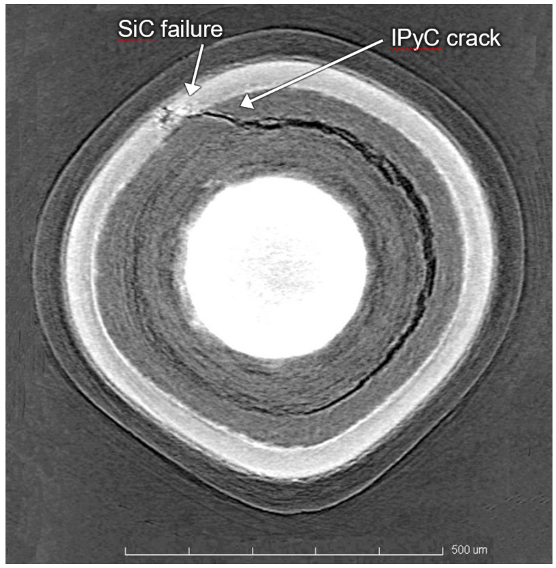

Figure 7. X-ray tomogram of an AGR-1 particle that experienced SiC failure, showing partial detachment of the buffer and IPyC layers and IPyC cracking at a point where the buffer-IPyC interface transitions from attached to separated (lower right), along with region of degraded SiC (Hunn, et al. 2016).

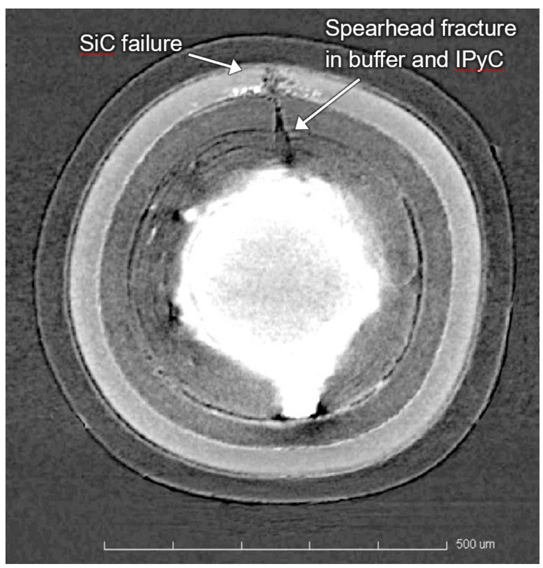

Figure 8. X-ray tomogram of an AGR-1 particle that experienced SiC failure, showing a buffer fracture aligned with an IPyC fracture in a region where the buffer-IPyC interface is intact (Hunn, et al. 2016).

Accurate modeling of this behavior will be challenging due to the complexity of the behavior and a lack of necessary material properties. Among these properties are the strength of the buffer-IPyC bond and the mechanical properties of the buffer layer itself. Complicating the analysis is the observation that the buffer and IPyC layers do not always cleanly separate at the observable interface, but that portions of the buffer layer are often left on the IPyC layer following separation (i.e., the fracture takes place in the buffer near the layer interface). Ongoing research projects at universities and national laboratories are currently investigating properties of as-fabricated and irradiated buffer and IPyC layers in TRISO particles. If sufficient data can be obtained from these studies, the results can be incorporated into the existing fuel performance models to add buffer behavior effect.

To accomplish capturing the complex 2D interaction between particle layers, the BISON team has been developing the models required to capture the thermomechanical behavior of the buffer layer observed in PIE for the AGR program. A new debonding model is currently being developed in BISON that will simulate the thermomechanical behavior of the buffer layer and buffer-IPyC debonding at different bonding states. Thermomechanical modeling capabilities will be enhanced by developing and applying models for SiC cracking and OPyC–SiC debonding. To model SiC cracking, a developed smeared cracking model will be calibrated to available data and coupled to the fission product transport models. Simulations highlighting the role of cracks as accelerated diffusion pathways for fission product transport will be analyzed. Studies will be conducted to examine the separate and combined effects of OPyC and IPyC failure on the stress state in and failure behavior of the SiC layer. The BISON predictions will be compared to existing simulation results and PIE data.

5.4 SiC-OPyC and OPyC-Matrix Bonding

Existing fuel performance models assume that the OPyC separates from the matrix layer, such that when it experiences shrinkage due to irradiation, it remains bonded to the SiC layer and contributes to the internal compressive stress. However, some experimental observations of irradiated particles (with and without additional post-irradiation safety testing) indicate a small gap between the SiC and OPyC layers. This suggests that the OPyC layer may, in fact, remain bonded to the matrix while at the same time having a relatively weak bond with the SiC layer, allowing the OPyC to separate from the SiC layer due to OPyC or matrix shrinkage during high-temperature irradiation. This is somewhat consistent with observations of the as-deposited SiC surface and SiC-OPyC interface, which indicate that the outer SiC surface is relatively smooth, with little topography that would allow the OPyC layer to interlock and form a strong bond, as occurs at the IPyC-SiC interface. This could have several implications for fuel performance models.

First, it suggests that the OPyC may not contribute significantly to SiC compressive stress or that the contribution to the SiC stress is unpredictable. Second, it suggests that, upon the mechanical failure of the IPyC and SiC layers (such that the OPyC remains the only intact layer to retain the pressure generated from fission gas buildup), it may not be appropriate to consider the stresses in the OPyC layer independent from the matrix. The existing models assume immediate failure of the OPyC layer in these cases because it does not have sufficient tensile strength to retain all of the stress previously retained by the SiC layer. However, if the OPyC layer is not coupled to the SiC layer and is, instead, attached to the matrix, the approach to evaluate layer failure would be considerably different.

5.4.1 Discussion

The experimentally observed failure rates of the AGR-1 and AGR-2 fuel particles are very low. Table 2 provides the measured failure fraction and upper bound on the failure fraction at 95% confidence for both SiC and TRISO failures for the AGR-1 and AGR-2 irradiations (additional details can be found in the respective final PIE reports (Demkowicz, et al. 2015) (Stempien, et al. 2021)). Note that “SiC failure” refers to a failure of the SiC layer such that it loses the ability to retain fission products (notably cesium) but with at least one PyC layer remaining intact to retain fission gases, while “TRISO failure” refers to the functional failure of all three dense coating layers such that fission gases are released from the particle.

Table 2. Measured failure fractions and upper bounds at 95% confidence for the AGR-1 and AGR-2 irradiation tests (Demkowicz, et al. 2015) (Stempien, et al. 2021).

Experiment	SiC Failures		TRISO Failures	
	Measured	Upper Bound at 95% Confidence	Measured	Upper Bound at 95% Confidence
AGR-1	1.3×10^{-5}	$\leq 3.1 \times 10^{-5}$	0	$\leq 1.1 \times 10^{-5}$
AGR-2	5.3×10^{-5}	$\leq 1.1 \times 10^{-4}$	$\leq 3.5 \times 10^{-5}$	$\leq 8.1 \times 10^{-5}$

Given the relatively low frequency of these coating layer failures and the large quantity of fuel tested in the AGR program to demonstrate fuel performance (over 400,000 UCO particles in the two tests represented in Table 2, with an additional ~570,000 particles from the AGR-5/6/7 experiment currently under PIE), an ample performance margin has been empirically demonstrated. As a result, capturing he nuanced impacts of coating performance in the models does not appear to represent a pressing concern with respect to AGR-spec UCO low-enriched uranium TRISO particles under the AGR Program's irradiation conditions. However, the impact of these particle behaviors for fuel designs that deviate significantly from the AGR program, using a significantly different performance envelope with little or no empirical data, remains to be determined. In these cases, model refinement may prove to be more crucial.

An initial goal of future code development efforts will be to determine the feasibility of refining the models to incorporate observed behaviors. This will likely be dependent on the availability of updated materials properties (see additional discussion in Section 6) or adequate experimental data for the failure modes to be incorporated based on empirical correlations (e.g., rate of localized Pd attack of SiC in the event of IPyC failure).

5.5 Particle Faceting

Aspherical particles have one or more flat facets created during fabrication, but are otherwise spherical, as illustrated in Figure 9. During irradiation, the faceted portion of the particle acts as a flat plate that restrains internal gas pressure. If the pressure reaches a high enough value, a local region of tensile stress develops in the central portion of the plate that can contribute to particle failures. Unlike failures caused by cracking of the IPyC, which is governed by shrinkage of the pyrocarbons, failures caused by asphericity are dominated by internal pressure. Therefore, while failures due to IPyC cracking are predicted to occur early during irradiation when shrinkage stresses are at their highest, failures due to asphericity are likely to occur later when the internal pressure is highest (Miller, Petti and Maki 2004).

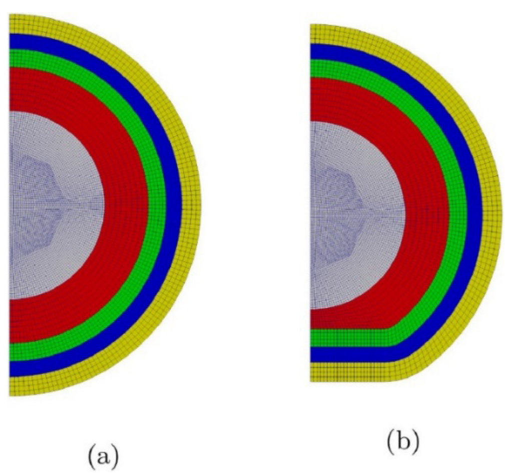

Figure 9. BISON mesh of a spherical particle (a) and an aspherical particle (b) (Dhulipala, et al. 2022).

The degree of asphericity for a particle is defined in terms of an aspect ratio, which is the ratio of major to minor radius. A reason for defining this parameter is that it is a commonly used measure of the severity of deformity in a particle and is thereby used as a criterion for particle acceptability. Image analysis can potentially improve information on faceting that could be used in the models instead of the relatively simple aspect ratio, which is more appropriate for characterizing oblate spheroids. Current fuel performance models identify the flat plate as the region with limiting tensile stresses and do not consider the higher stresses in regions with a high radius of curvature. Oak Ridge National Laboratory has developed new characterization methods that can provide statistical data on faceting that could be incorporated directly into the BISON models. This would also allow BISON to consider variations in coating layer thicknesses, which are typically observed in as-fabricated particles with facets.

5.6 Localized Pd Attack with IPyC Failure

Degradation of the SiC layer by the chemical interaction of Pd may provide pathways for fission product release. X-ray tomographs of AGR-1 particles indicate this phenomenon is accelerated in the presence of an IPyC layer crack, as illustrated in Figure 10 (Hunn, et al. 2016). The Pd accumulates at the IPyC crack tip because it provides a more rapid transport path. The chemical attack of the SiC by Pd compromises the structural integrity of the layer and its ability to retain fission products.

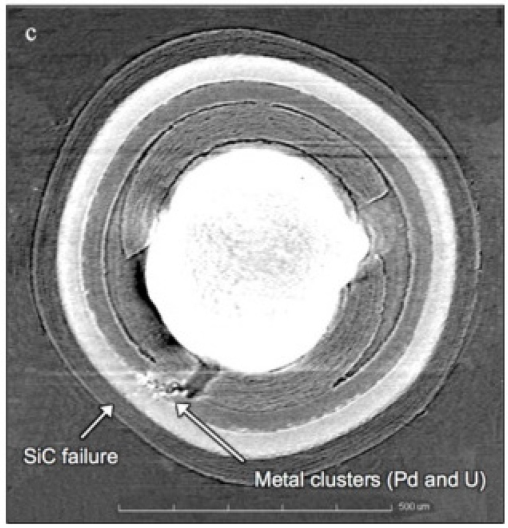

Figure 10. X-ray tomograph showing Pd accumulation at the IPyC crack tip (Hunn, et al. 2016).

The existing model for Pd corrosion (also called “thinning”) of the SiC layer is based on empirical correlations, all published prior to 1991, derived by measuring the depth of penetration in irradiated particles under a range of conditions. The level of thinning that results in SiC failure can be adjusted in the model (e.g., SiC is assumed failed after 50% Pd penetration). However, the SiC layer failures observed in the AGR tests are based on localized Pd attack that is promoted by IPyC failure. This is a different phenomenon compared to the thinning captured by the existing correlation.

Under typical AGR irradiation conditions, SiC failure due to Pd attack is not found to be a significant contributor to the total SiC failure probability. However, outside of the AGR Program, fuel vendors with various reactor designs are considering longer-life cores, in which the longer residence time of the fuel at high temperatures could promote more frequent particle failures due to SiC degradation from Pd attack. As a result, the BISON development team has begun implementing new Pd attack models to meet the fuel performance modeling demands of these long-life reactor core designs for their industry partners. This modeling task is discussed further in Section 6.1.

5.7 Kernel Migration in UCO Fuel

Kernel migration occurs at high temperatures due to the presence of a thermal gradient across the fuel particle and is a function of kernel composition and time. Current kernel migration models are based on historical data fit to an Arrhenius function to derive a kernel migration coefficient for UO_2 and UCO fuel. The phenomenon in UO_2 fuel is driven by the production of carbon monoxide. Since CO production is substantially suppressed in UCO fuel, only kernel migration in UO_2 fuel is considered to be of importance in the current models. However, evidence from AGR-5/6/7 PIE suggests that kernel migration occurred in

UCO fuel that was irradiated at very high temperatures in Capsule 3. Preliminary analysis suggests that this is consistent with the correlation for UCO used in PARFUME (which is based on UC_2 kernel migration behavior).

The current UCO kernel migration coefficient used in the models is based on experiment data (R. C. Martin 1993) and results in miniscule kernel migration. Using the AGR PIE data, it may be possible to generate a new kernel migration coefficient that more accurately predicts kernel displacement in UCO fuel.

5.8 Fission Product Transport Model

A main objective of the AGR-3/4 irradiation experiment is to provide fission product transport data following their migration throughout the fuel, graphitic matrix, and nuclear-grade graphite (Mitchell and Demkowicz 2022). Each AGR-3/4 compact contains driver fuel particles and 20 DTF particles placed along its axial centerline. The fuel compacts are surrounded by three concentric annular rings of test material, consisting of fuel-compact matrix material and fuel-element graphite. Figure 11 shows a BISON 2D axisymmetric model, with the 20 DTF particles placed in the center line and 1,793 randomly distributed driver particles hosted in the fuel compact. The four regions of the BISON model are fuel compact and inner, outer, and sink rings.

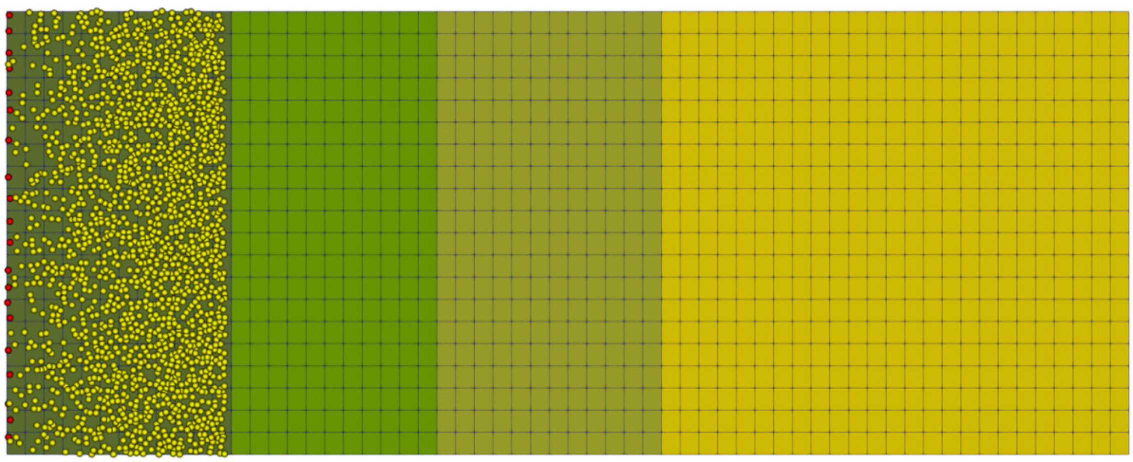

Figure 11. BISON 2D axisymmetric model of fission product transport. From left to right, the regions consist of a fueled compact (driver and DTF particles), inner ring, outer ring, and sink ring (Skerjanc and Jiang 2022).

To take advantage of radial symmetry and to reduce computational resources, the 2D BISON model illustrated in Figure 11 is simplified to generate a 1D finite-element method model, as illustrated in Figure 12. The temperature at the ring interfaces is obtained from the AGR-3/4 as-run thermal analysis report (Hawkes 2016) and applied as boundary conditions. The 1D finite-element model explicitly models the gas gaps between capsule rings and the transport across the gas gaps is accounted for using the Freundlich isotherm. A more detailed description of the finite-element method model can be found in (Riet and Stempien 2022) and (Riet 2023).

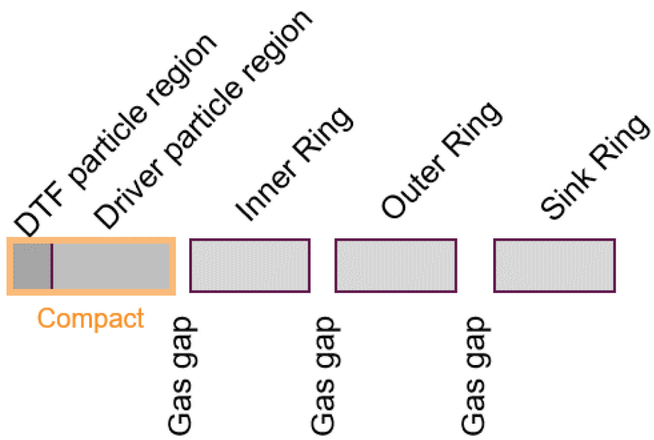

Figure 12. 1D finite-element method model geometry (Riet and Stempien 2022).

Much of the work to this point has been focused on implementing the 1D finite-element model to correctly model the AGR-3/4 experiment and compare the predicted fission product transport results to PIE experimental data (Riet and Stempien 2022) (Riet 2023). Several areas of uncertainty are being addressed including sorptivity of elements of interest, parameter estimation, and model improvements.

To better quantify the sorptivity of silver, strontium and europium, sorption experiments are being planned in collaboration with JRC Karlsruhe. Unfortunately, the detection limits of their Knudsen cell setup are 1–2 weight percent, well above the concentrations measured for any of the isotopes of interest in the AGR experiment. INL is currently working with an industry supplier to develop the samples for the analysis. After the supply is secured, loading the samples and running the experiment are expected to take several months.

Improvements to parameter estimation come from various techniques. Preliminary results using a parallel subset simulation Bayesian optimization technique are promising, so a full conditional parameter uncertainty evaluation will be performed using affine invariant sampling in a Bayesian framework. Applying the parameters found with 1D models in a 2D-model environment will be an additional gauge of model uncertainty. INL plans to model cesium transport based on fits to compacts and inner rings for multiple capsules, which will yield an effective diffusivity of the capsule. Multiple capsules will then be compared to estimate a general temperature dependence of diffusivity. Simultaneous fits with stochastic uncertainty quantification will also be attempted. For silver transport, a trapping model has been proposed which has led to preliminary results that are promising.

Several model improvements are currently planned. The plan to benchmark model performance across capsules and rings with verification against 2D models and observed concentration profiles has been mentioned previously. Also planned is a 1D+ODE (ordinary differential equation) short-circuit gap transport model, which may be a simple way to bound the contribution of unanticipated convection, if that contribution were to exist. Europium and strontium transport should also be evaluated using existing models and a dual diffusivity model, sometimes called a “dogleg.” The dogleg reflects a higher effective diffusivity at low temperatures and an alternate diffusion pathway. This dominates transport at lower temperatures but does not have a large temperature dependence; as such, it has limited effect at elevated temperatures.

It is estimated that the fission product modeling efforts from the AGR 3/4 experiment will be completed in FY-24. This includes incorporating the stochastic uncertainty quantification and developing the silver trapping model by the end of the second quarter of FY-24. Following the successful implementation of the silver trapping model, the stochastic uncertainty quantification for the cesium transport model will be completed shortly thereafter. The remainder of the time in the third quarter of FY-

24 will focus on implementing the 0D + 1D transport model to attain a rough approximation of short-circuit diffusion. This would be followed by benchmarking obtained fits using 2D models for the remainder of the fiscal year. Pending advances in source term modeling, these results may need to be revisited with a more accurate source term. Once the implementation of the fission product modeling effort using AGR-3/4 experimental data is complete, a comprehensive review of results will be attempted in FY-25.

5.9 Estimation of Fission Product Generation

The fission product inventory is an important input into the fission product transport model and is based on fission product generation, with inventory accumulated as a function of burnup. Currently, PARFUME and BISON use simple generation correlations based on burnup for each fission product species. These generation rates are elementally based, not distinguishing between individual isotopes. The basis for the generation rates currently used in the fuel performance codes are not documented, so the user is unable to ascertain if the correlations built into the models are appropriate for their application. For example, it is assumed that current fission product generation rates are based on an AGR fueled experiment using the Advanced Test Reactor (ATR) flux spectrum. In addition, it is unknown how many neutron groups were used in the development of these correlations. There are reactor and TRISO fuel designs that vary significantly from the base AGR fuel particle that fuel vendors and industry partners are currently exploring. These distinctions could potentially result in significant differences in fission product generation rates when compared to current models.

Using AGR experiment specific geometry and ATR flux spectra, new fission product generation rates can be developed and documented, leveraging the neutronic analyses that have already been performed. In addition, Griffin, the MOOSE-based neutronics depletion code, can be coupled to BISON so that users have the capability to input reactor and fuel specific flux spectra to perform detailed analyses on their current reactor design. The results of this effort would produce 1) documented, simple fission product generation rates based on AGR fuel and the ATR's neutron flux to use in PARFUME, 2) AGR experiment specific fission product generation rates (i.e. AGR-3/4 would have its own set of correlations) for use in BISON, and 3) a coupled BISON-Griffin capability to support outside fuel vendors and industry partners.

5.10 Release-to-Birth Ratios

The R/B ratios for short-lived fission gases (i.e., krypton and xenon) are a metric to evaluate the ability of the fuel kernel, particle layers, and compact matrix to retain fission gas species, preventing their release to the environment. The R/B ratio is a combination of fission gases released from defective and failed fuel particles (exposed kernels) and/or dispersed uranium contamination. The transport of short-lived fission product gases is primarily a function of a nuclide-specific effective diffusion coefficient, temperature, and radioactive decay constant.

The R/B ratios for short-lived fission product gases from failed particles and dispersed uranium contamination are accounted for in the fuel performance modeling codes for several prominent fission product isotopes. The correlations for these isotopes are based on historical experimental data using the Booth equivalent sphere model (Miller, Petti and Maki, et al. 2023). The total R/B ratio is then the sum of the R/B from exposed kernels, plus the contribution from dispersed uranium contamination.

Experimental R/B data from AGR PIE measurements is available to update the models used in the fuel performance codes (Pham, Einerson, et al. 2019). These measurement data have been used to develop an empirical model to predict the R/B ratios for the short-lived fission product gases. First, zero fuel particle failures were observed during the AGR-1 irradiation, so the release of fission product gases can be attributed to uranium contamination. This provided measured data to develop new correlations to model select krypton and xenon isotopes released from dispersed uranium. Second, the AGR-3/4 experiment contained 20 DTF fuel particles per compact, and the R/B data obtained from this experiment was used to develop a correlation for the R/B contribution from exposed kernels. Combined, the new empirical model can be implemented in the fuel performance codes to predict the R/B ratios of short-lived fission gas isotopes.

6. BEYOND THE AGR PROGRAM

There are several activities being performed outside of the AGR program that support the overall objective of developing fuel performance modeling tools for TRISO-coated fuel particles. A number of HTR vendors have been considering the use of TRISO-coated particles and rely on expertise and experimental data in the development of fuel performance models to support their potential application in the industry. However, because the scope of their work and variations in both reactor and fuel design fall beyond the AGR program, they will not be discussed further in this report.

6.1 NEAMS BISON TRISO Development

The BISON fuel performance code falls outside of the AGR program scope, but it is continuously under development for TRISO fuel performance modeling, whether it be by INL staff, fuel vendors, or university partnerships. This report attempts to capture the major activities directly related to the immediate support of the AGR program and is not all encompassing. Further, BISON is export-controlled software and many of the fuel vendors have developed their own version of the BISON code to meet their needs. Because many of these modifications are business sensitive, they too are not included in this report.

Planned BISON activities for the next two years are summarized in Table 3. These NEAMS BISON TRISO activities support industry partnerships to further fuel performance modeling and fission product transport. These activities will also support modeling improvements that have been identified in Section 5 to leverage resources between AGR staff and the BISON development team.

Table 3. NEAMS BISON TRISO planned activities.

Application	Estimated Complete	Task
BISON/Marmot/ Atomistic	FY-24	Model fission product transport and micro-structural behavior under irradiation in TRISO fuel • Simulate fission product release and diffusion in UCO, fission product diffusion through PyC and SiC layers, including effects of defects, and fission product effects on mechanical response of fuel kernel • Improve upon current models for behavior of layers through multiscale modeling by developing the following areas: Lower-length scale informed material models that vary as functions of temperature, fast fluence, density and anisotropy • Models at high burnup levels and high temperature to support high burnup/temperature reactor designs
BISON	FY-24	Particle fuel verification and validation • Sensitivity study and uncertainty quantification of material properties and particle dimensions • Develop comprehensive BISON TRISO assessment and validation (using AGR data)
BISON/Marmot	FY-24	Model statistical failure of TRISO particles across multiple temperature ranges • Eliminate 1D assumptions to allow full use within 2D and 3D simulations • Develop capability for modeling debonding at the buffer-IPyC interface • Develop fracture mechanics-based approach to yield more accurate prediction of cracking • Consider other failure mechanisms (e.g. kernel migration, Pd penetration in SiC layer) • Develop lower length scale models for penetration of Pd and other species through SiC layer • Improve and optimize Bison's existing capability to perform statistical fuel particle failure analysis
BISON/Marmot	FY-25	Model the relationship between IPyC adhesion during irradiation and IPyC degradation and SiC failure including localized Pd attack at the point of IPyC fracture/delamination
BISON/Marmot/ Atomistic	FY-25	Extend particle fuel-specific BISON modeling and simulation capabilities to include uranium nitride and SiC matrix
BISON/Marmot/ Atomistic	FY-25	Develop and demonstrate models for graphite and fuel compacts. • Development and early assessment of thermal and mechanical models for graphite • Material applications (e.g., graphite vs graphite-matrix) to identify and prioritize needed properties and models • Oxidation models in graphite • Capability development for anisotropic finite strain creep and plasticity models
BISON	FY-26	Model the heating of TRISO fuel under large moisture ingress events, such as multiple steam generator tube ruptures
BISON	FY-27	Correlate manufacturing conditions to TRISO material properties and fuel performance to improve understanding of how manufacturing process affects fuel performance and optimize manufacturing process.

Note: Shaded items are considered complete.

6.2 University Led Programs

The DOE's Nuclear Energy University Program (NEUP) supports university research and collaboration. Currently, there are two NEUP-funded projects that coincide with an application to fuel performance modeling. In an attempt to measure the material properties of TRISO layers and their interfaces, NEUP-19-17251 (Dunzik-Gougar 2019) was awarded to Idaho State University to develop strength characterization techniques via tensile testing for unirradiated and irradiated TRISO-coated fuel for deployment to other collaborators. If the characterization of the TRISO layers is successful, PARFUME and BISON can be updated with new material properties for further investigation and comparison to the experimental data obtained throughout the AGR program.

Additionally, NEUP-20-19556 (Zhang 2020) was awarded to the University of Wisconsin to develop a predictive model for the buffer layer performance during irradiation. In conjunction with data obtained from the AGR experiments and subsequent PIE, this research will help improve modeling capabilities in BISON when evaluating the buffer layer performance during irradiation. Because PARFUME is a 1D fuel performance code, the application of buffer layer behavior is not anticipated to be included in its modeling capabilities.

Finally, the DOE's Integrated Research Projects program awarded the University of Tennessee to develop computationally efficient multiphysics models in BISON for TRISO-coated fuel in advanced reactors (Wirth 2020). The results of this research can be utilized in future versions of BISON for TRISO fuel performance modeling.

7. SUMMARY

The remaining activities to support fuel performance modeling for the AGR program include the continued AGR experiment support for AGR-3/4 and AGR-5/6/7 as well as modeling improvements identified throughout the course of the program. These modeling improvements can be summarized as thermomechanical and thermochemical enhancements to predict fuel particle behavior as well as updating fission product transport models and diffusion parameters.

Fuel particle thermomechanical and thermochemical behavior includes the improved modeling of the buffer layer during irradiation, potentially updating pyrocarbon creep coefficients at lower temperatures, and localized Pd attack in the presence if an IPyC crack. The AGR program has accumulated substantial experimental data on the behavior of fuel particles, both during irradiation and under accident conditions, and processing these data may lead to the identification of further modeling improvements. For example, the physicochemical behavior of SiC layer corrosion by fission products has been observed and will need to be quantified for inclusion in fuel performance models.

Fission product transport modeling capabilities will be improved using empirical data obtained from the AGR-3/4 PIE campaign. This will include implementation of new fission product diffusion parameters for graphite and/or compact matrix in both PARFUME and BISON. The implementation of these new diffusion parameters must be compared with AGR-1 and AGR-2 data, as well as published fuel performance benchmarks.

Fuel performance modeling activities and improvements that have been identified in this report are summarized in Table 4, along with notional completion dates where applicable.

Table 4. Fuel performance modeling plan summary.

Activity	Modeling Code	Completion	Document
AGR Experiment Support			
AGR-3/4 As-run Irradiation Test Predictions	BISON	FY-21	INL/EXT-21-65160
AGR-3/4 In-pile Irradiation PIE Comparison	PARFUME/BISON	FY-22	INL/RPT-22-69003
AGR-3/4 As-irradiated Compacts Safety Test Comparison	PARFUME/BISON	FY-23	INL/RPT-23-74505
AGR-3/4 Re-irradiated Safety Test	BISON	FY-24	
AGR-3/4 Fission Product Transport Model	BISON	FY-25	INL/RPT-22-69040 INL/RPT-23-74853
AGR-5/6/7 As-run Irradiation Test Predictions	PARFUME	FY-21	INL/EXT-21-64576
AGR-5/6/7 Safety Test Predictions	PARFUME/BISON	FY-25	
AGR-5/6/7 In-pile Irradiation PIE Comparison	PARFUME/BISON	FY-25	
AGR-5/6/7 Safety Test Comparisons	PARFUME/BISON	FY-26	
AGR Kernel/Buffer Fraction Margin	PARFUME	FY-23	INL/RPT-23-71441
Modeling Improvements			
Pyrocarbon Creep Rate	PARFUME/BISON	TBD	
IPyC Failure Prediction Validation	PARFUME/BISON	TBD	
Thermomechanical Buffer Layer Modeling	BISON	FY-25	
SiC-OPyC and OPyC-Matrix Bonding	BISON	TBD	
Particle Faceting	BISON	TBD	
Localized Pd Attack with IPyC Failure	BISON	FY-25	
Kernel Migration in UCO Fuel	PARFUME/BISON	FY-24	
Fission Product Transport Model	BISON	FY-25	
Fission Product Generation Correlations	PARFUME/BISON	FY-24	
Release-to-Birth Ratios	PARFUME/BISON	FY-24	
Other Activities			
NEUP-19-17251	PARFUME/BISON	TBD	
NEUP-20-19556	BISON	TBD	
IRP-20-22094	BISON	TBD	

Note: Shaded items are considered complete.

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Appendix A
Modeling Improvements: Data Availability and Impact

The potential modeling improvements described in Section 5 are provided below along with a subjective assessment of the availability of experimental data to facilitate implementing the new model. Also included is the subsequent impact the model would have on the results from the fuel performance modeling codes. Unless otherwise noted, the impact is based on a typical AGR designed UCO fuel particle with irradiation conditions similar to those experienced by the AGR experiments. This assessment is also summarized in Table A1.

PyC Creep Rate

Data Availability – Low

Experimental data from the AGR irradiation program regarding the PyC creep rate does not exist. However, substantial experimental data are available from the ART Graphite program (Advanced Graphite Creep irradiations) in the low temperature regime. There is potential to utilize these data and apply a density correction to generate a new PyC creep rate model.

Impact to Model – High

The SiC failure probability for UCO fuel is primarily due to localized stress concentration from an IPyC crack, especially at low temperatures.

IPyC Failure Prediction Validation

Data Availability – Medium

The AGR-5/6/7 irradiation had a sufficient number of particles irradiated at low temperatures to be examined to determine the structural integrity of the IPyC layer. The IPyC failure fraction in these particles is sufficiently high (on the order of 10^{-1}) that only a few dozen particles would need to be examined.

Impact to Model – High

IPyC cracking and the resulting stress concentration on the SiC layer is the leading mechanism predicting particle failure in UCO fuel. Validating the IPyC cracking models in the fuel performance codes would provide greater confidence in applying a modified IPyC creep rate.

Thermomechanical Buffer Layer Modeling

Data Availability – High

Measured buffer failure fraction data is available from the AGR-1, 2, and 3/4 irradiations. In addition, AGR PIE has obtained a substantial number of micrographs that can be used to quantify buffer failure (cracking, buffer/IPyC bonding, etc.) that can be used to develop and validate thermomechanical buffer layer behavior models.

Impact to Model – Medium

The thermomechanical behavior of the buffer layer and its interaction with the IPyC layer has potential to compromise the structural integrity of the SiC layer and its ability to retain fission gas. The performance of the buffer layer is an important phenomenon to consider when assessing the overall performance of the particle and how it impacts other failure mechanisms (e.g. IPyC cracking, localized Pd penetration, "spearhead" SiC layer failures).

SiC-OPyC separation and OPyC-Matrix Interaction

Data Availability – Medium

Available PIE data would consist of examining micrographs of irradiated fuel and quantifying the impact of the separation of the SiC from the OPyC along with the OPyC-matrix interaction. An ample number of micrographs of irradiated AGR fuel have been obtained but would require a significant effort to categorize the behavior.

Impact to Model – Low

It is suspected that the behavior of the OPyC and its interaction with either the SiC or matrix would have minimal impact on the overall behavior of a TRISO fuel particle when considering all other phenomenon that occur during irradiation.

Particle Faceting

Data Availability – Medium

Oak Ridge National Laboratory has developed a new methodology to characterize particle faceting and can provide statistical data that can be utilized by the fuel performance models to evaluate a traditional "flat plate" facet geometry or a more realistic ovate shaped particle. The data furthermore include particle cross sections that provide quantitative assessment of coating layer thicknesses around facets, which can also be incorporated into the models.

Impact to Model – Low

Faceted particles are of particular concern in UO_2 fuel since the increase in fission gas pressure at the end of irradiation can lead to fuel particle failures that are typical of a pressure vessel failure magnified by aspherical shaped particles. However, since AGR fuel uses a UCO kernel and fission gas pressure at the end of irradiation is minimized, pressure vessel failures of this type are not considered to be a significant contributor to fuel particle failure.

Localized Pd Attack with IPyC Failure

Data Availability – Medium

Micrographs of irradiated AGR fuel would be used to quantify the extent and frequency of localized Pd attack of the SiC layer due to IPyC cracking, potentially correlating the extent of attack with temperature and burnup. This effort also requires an updated Pd yield as a source term for the model.

Impact to Model – Low/High

For AGR fuel under AGR irradiation conditions, Pd attack of the SiC layer is not a major contributor to the total fuel particle failure probability. However, proposed new HTR designs rely on a longer fuel residence time. This results in fuel being exposed to longer time-at-temperature conditions that are conducive to Pd attack of the SiC layer.

Kernel Migration in UCO Fuel

Data Availability – Medium

PIE data from AGR-5/6/7 could potentially be used to calculate an empirical kernel migration coefficient. Besides the data obtained from AGR-5/6/7, there is no other data available in the literature to develop an empirical kernel migration coefficient for UCO fuel.

Impact to Model – Low

Kernel migration is more prominent in UO_2 fuel where the partial pressure from fission gas generation results in the displacement of the fuel kernel. This is not the case for UCO fuel where the formation of carbon monoxide is limited. An updated kernel migration coefficient developed for

AGR UCO fuel would result in a more accurate representation of the fuel behavior. However, kernel migration is not observed in the AGR UCO fuel irradiations except at the highest irradiation temperatures (~1400 °C) and has not been observed to cause fuel particle failure in any of the AGR irradiation tests.

Fission Product Transport Model

Data Availability – High

Extensive fission product data has been collected from the AGR experiments up to this point. One specific objective of the AGR-3/4 experiment was to produce fission product transport modeling data to develop fundamental fission product diffusion models based on AGR fuel. The extensive amount of the data and its applicability to develop new fission product diffusivities presents a challenge.

Impact to Model – High

Correctly modeling the transport of fission products from the fuel kernel to the environment is important for safety and regulatory licensing. Updating the fundamental fission product diffusion models will enable the fuel performance codes to more accurately account for fission products.

Fission Product Generation

Data Availability – High

Neutronic analyses have already been performed for each AGR experiment and can be used to generate new models to create new fission product generation correlations as a function of burnup. These correlations would be AGR experiment specific to account for the different irradiation positions in the ATR, which produce different neutron flux profiles. The MOOSE-based neutronics code Griffin has already been developed and can be coupled to BISON.

Impact to Model – Medium

The fission product generation rate and the resulting accumulated inventory is an important input in the development of the fission product transport model. Ensuring the correct inventory will instill greater confidence in the transport model. The typical application of the fuel performance codes however, is to calculate the fractional release of a particular element/isotope. Since the release is relatively proportional to the accumulated inventory, the predicted release fraction is not influenced by the total fission product inventory.

Release-to-Birth Ratios

Data Availability – High

R/B data from AGR-1, 2, and 3/4 have already been collected and analyzed. Based on this data, an empirical model has already been developed. There is also potential to modify the current PARFUME (German) mechanistic model to reflect the AGR data.

Impact to Model – Medium

A new AGR based R/B model (either empirical or mechanistic) will provide the users with an additional option to calculate the R/B ratio of short-lived fission product isotopes built on the current AGR UCO fuel design.

Table A1. Data availability and impact to the models for identified modeling improvements.

Modeling Improvements	**Data Availability**	**Impact to Model**
PyC creep rate	Low	High
IPyC failure prediction validation	Medium	High
Thermomechanical buffer layer modeling	High	Medium
SiC-OPyC separation and OPyC-matrix interaction	Medium	Low
Particle faceting	Medium	Low
Localized Pd attack with IPyC failure	Medium	Low/High
Kernel migration in UCO fuel	Medium	Low
Fission product transport model	High	High
Fission product generation	High	Medium
Release-to-birth ratio	High	Medium