GAS-COOLED REACTOR
ADVANCED REACTOR TECHNOLOGIES PROGRAM

July 16, 2024

Fuel Performance Modeling Status Update and Potential Model Improvements

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ART TRISO Fuel Performance Modeling Technical Lead - INL

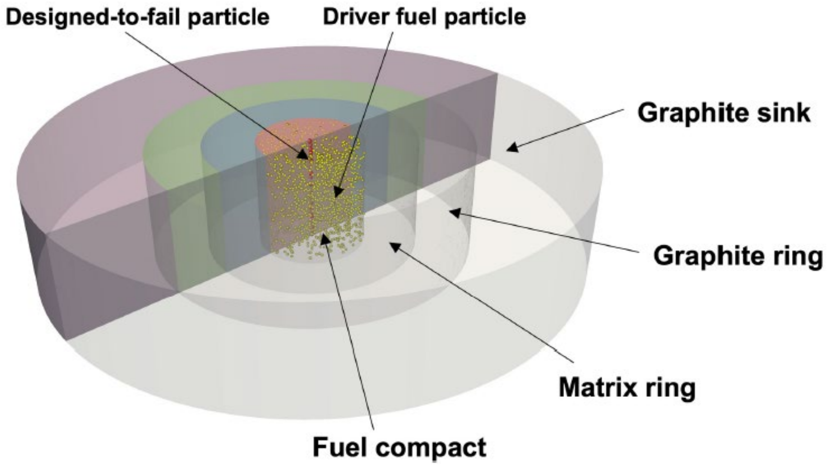
DOE ART GCR Review Meeting

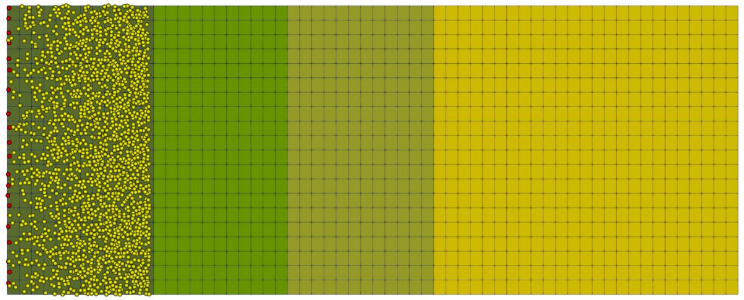
Hybrid Meeting at INL

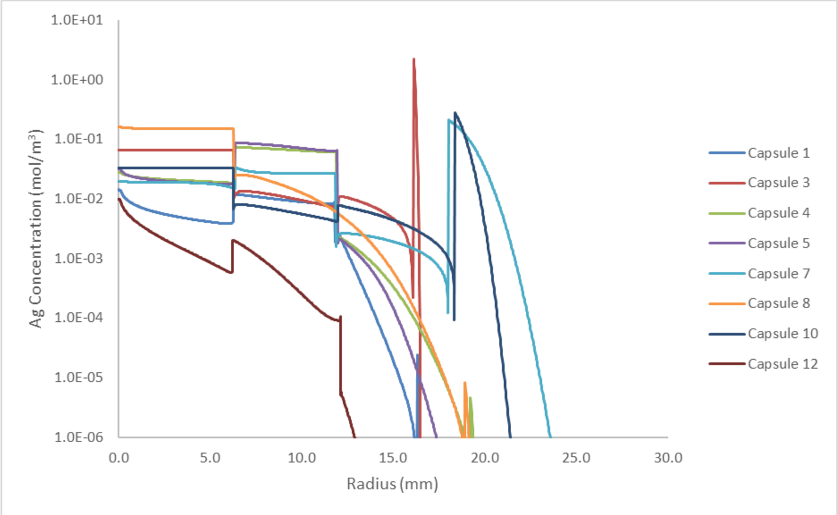
July 16–18, 2024

Outline

- Introduction
- Overview of TRISO fuel performance modeling
- TRISO fuel performance modeling codes PARFUME/BISON
- AGR experiment support
- Identified modeling improvements
- BISON smeared cracking model
- BISON fission product source term
- AGR-3/4 reirradiation heating test
- Summary

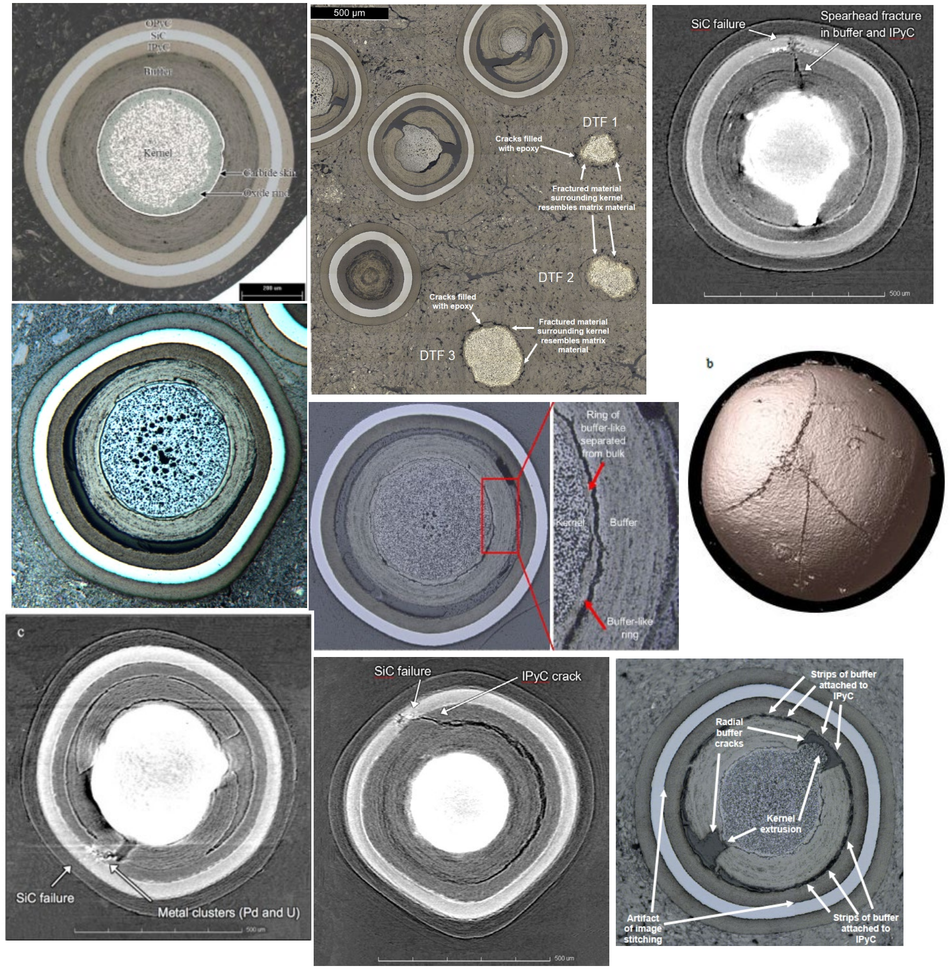






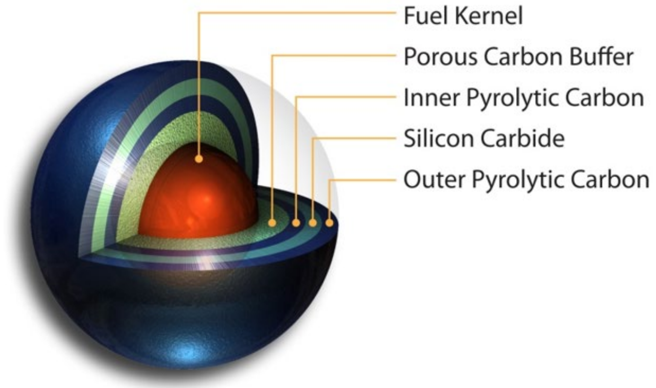
Introduction

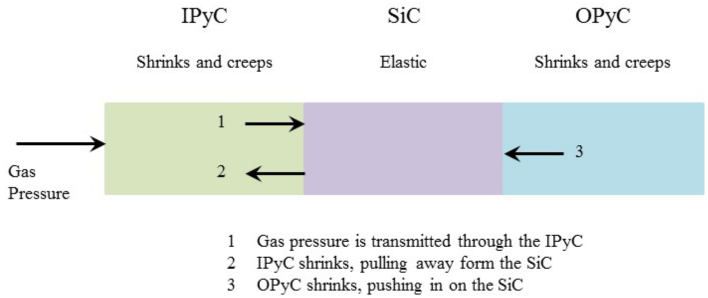
- Why fuel performance modeling?
  - Addresses:
    - Fuel particle failure
      - Structural
      - Thermal
      - Chemical
    - Fission product transport
      - Fuel-compact matrix
      - Fuel-element graphite
  - Assists in the:
    - Fuel design and fabrication
    - Optimization
    - Experiment design
    - Fuel behavior
- Objective:
  - Enhance the understanding of fuel behavior and fission product transport
  - Improve the fuel performance and fission product models
  - Develop advanced models using new methods
  - Provide validated tools to industry

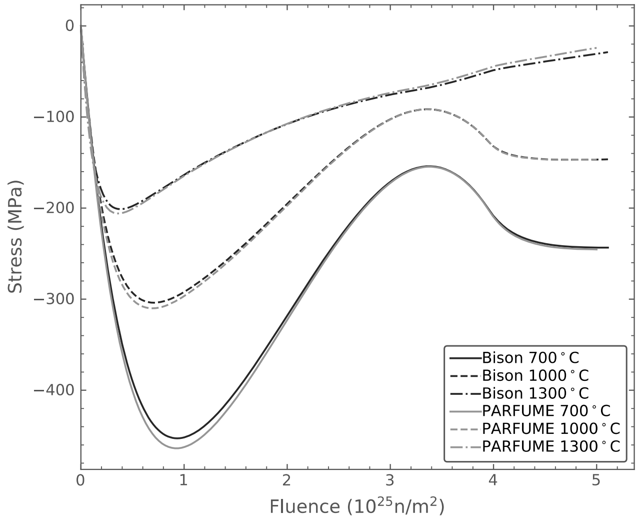


TRISO Fuel Performance Modeling

- Basic fuel particle behavior
  - Several physical phenomena influence the behavior of the particles including fission gas production and irradiation effects
- Applications of fuel performance modeling
  - Optimize particle design
  - Plan irradiation experiments
  - Identify tolerances of specifications
  - Estimate reactor fuel performance
- Existing TRISO fuel performance codes
  - PARFUME: Spherical symmetry to reduce the particle response to a 1D model and uses closed-form analytical solution for the stress-strain-displacement relationship.
  - BISON: uses finite element method to solve the basic thermo-mechanics and mass diffusion equations. This avoids the simplifications necessary for a closed form solution.







PARFUME – PARticle FUel ModEl

- Fuel Performance Code PARFUME
  - An integrated mechanistic code that evaluates the thermal, mechanical, and physico-chemical behavior of TRISO fuel particles
  - Capable of evaluating fuel particle failure under both irradiation and accident conditions
  - Tracks the probability of fuel particle failure given the particle-to-particle statistical variations in physical dimensions and material properties.

Early particle fuel performance codes were 1-D and considered only pressure vessel failure

- Various irradiation experiments had greater levels of failure than could be predicted by pressure vessel failure alone
- PIE results from NP-MHTGR and other experiments have revealed that other multi-dimensional effects may have contributed to the observed fuel failures
- To investigate these failure mechanisms, INL started development of an integrated mechanistic fuel performance modeling code called PARFUME

By 2000, the main components of PARFUME consisted of

- Closed form stress solution for a three-layer particle
- Monte Carlo sampling of particle attributes
- Failure probabilities calculated with Weibull distributions in coating layer strengths

By 2005, major code enhancements were in place which included

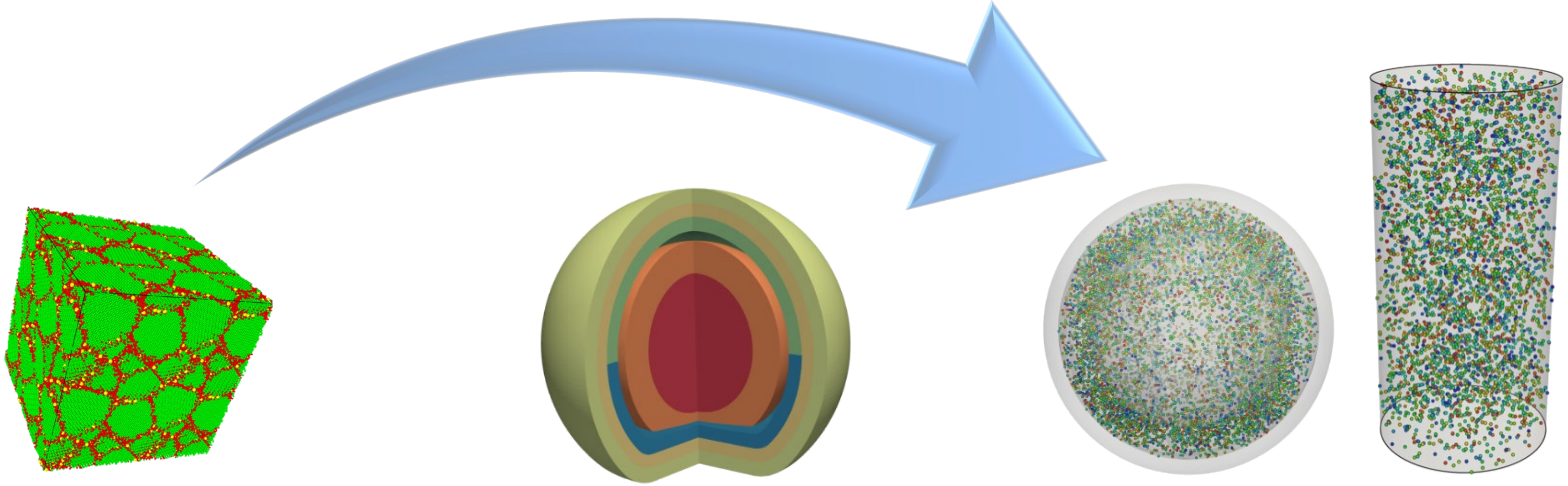
- Particle sampling performed by a multiple integration technique allowing for very small failure probabilities to be calculated
- Kernel migration and Pd penetration failure mechanisms considered
- Consistent set of material properties

By 2007, safety test conditions could be modeled within PARFUME where

- Particle layer failures are synchronized with fission product diffusion
- Correlations from TMAP (Tritium Migration Analysis Program) are used to calculate fission product diffusion

BISON

- Overarching objective to deliver an integrated set of predictive computational tools for nuclear fuel performance analysis and design.
- One of its major goals is to have a great amount of flexibility in how it is used, including in the types of fuel it can analyze, the geometry of the fuel being modeled, the modeling approach employed, and the dimensionality and size of the models.
- Fuel forms that can be modeled include standard light water reactor fuel, emerging light water reactor fuels, tri-structural isotropic fuel particles, and metallic fuels.



Lower-length scale modeling

- **Fission gas release model:** Xe, Kr diffusivity in UCO
- **Fission product diffusivity:** Silver diffusion in SiC, Pd Penetration

TRISO particle

- **Thermal-mechanical modeling**
  - **Failure analysis:** asphericity, IPyC cracking and debonding
- **Fission product diffusion through layers**

Pebble and Compact modeling

- **Failure probability calculation**: Monte Carlo and Fast Integration Approach
- **Fission product diffusion through matrix**
- **Particle-Matrix interaction**

BISON

2021 R&D 100 WINNER

➢ Wen Jiang – NC State, INL

2012 | 2013 | 2014 | - - - 2017 | 2018 | 2019 | 2020 | 2021 | 2022 | 2023 | 2024

Stage 1 | **Stage 2** | **Stage 3**

- 2012: First major BISON paper was published. Paper focused on LWR fuel but also had a TRISO example[1].
- 2013: The BISON team decided to add a baseline TRISO capability, including thermal, mass diffusion, and mechanical models. A first BISON TRISO paper was published.[2]
- 2017: Very little interest from potential stakeholders. No interest → no funding → no development.
- 2018: Added an internal 1D TRISO mesh generation capability [6]
- 2019: Developed MOOSE's Monte Carlo massive sampling capability (100 millions) [4]
- 2019: Started to model 2D failure modes [4]
- 2020: Implemented all PARFUME models in BISON [4]
- 2020: Developed Monte Carlo failure probability calculation [4]
- Incorporate fission product diffusivity in UCO Kernel from lower length scale modeling [5]
- 2021: V&V: AGR-1, IAEA CRP benchmark problems [6] AGR-2 [8]
- Effective thermal conductivity for TRISO and matrix [7]
- Develop fast integration approach [9] and variance deduction method [11] to compute failure probability
- Develop capability to model debonding
- Determine fission product diffusivity in SiC from lower length modeling [10]
- Implement Graphite thermal-mechanical properties
- Improve fission product diffusivity in SiC from LLS
- Particle and matrix coupling
- V&V on fission product release a diffusivity calibration and optimization [12,13]
- investigate Pd penetration
- Mass transfer model

[1] R.L. Williamson et al, Multidimensional multiphysics simulation of nuclear fuel behavior, JNM, 2012
[2] J.D. Hales et al, Multidimensional multiphysics simulation of TRISO particle fuel, JNM, 2013
[3] R.L. Williamson, et al, Bison: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms, NT, 2020
[4] W. Jiang et al, TRISO particle fuel performance and failure analysis with BISON, JNM, 548, 152795, 2021
[5] X.Y. Liu et al, Atomistic and cluster dynamics modeling of fission gas (Xe) diffusivity in TRISO fuel kernels, JNM, 561, 153539, 2022
[6] J.D. Hales et al, Modeling fission product diffusion in TRISO fuel particles with BISON, JNM, 548, 152840, 2021
[7] A. Toptan et al, FEA-aided investigation of the effective thermal conductivity in a medium with embedded spheres, NED, 381, 2021
[8] J. D. Hales, et al, Numerical Evaluation of AGR-2 Fission Product Release, JNM, 558, 153325, 2022
[9] W Jiang, et al, Efficient High-Fidelity TRISO Statistical Failure Analysis using Bison: Applications to AGR-2 Irradiation Testing, JNM, 153585, 2022.
[10] P.-C. A. Simon et al., Mechanistic calculation of the effective silver diffusion coefficient in polycrystalline silicon carbide: application to silver release in AGR-1 TRISO particles, JNM, 153669, 2022
[11] S.L.N. Dhulipala et al, Accelerated Statistical Failure Analysis of Multifidelity TRISO Fuel Models, JNM, 153604, 2022
[12] A Toptan et, al, Verification of MOOSE/Bison's heat conduction solver using combined spatiotemporal convergence analysis, JVVUQ, 2002
[13] A Toptan et al, Verification of Bison fission product species conservation under TRISO reactor conditions, JNM, 154105, 2023

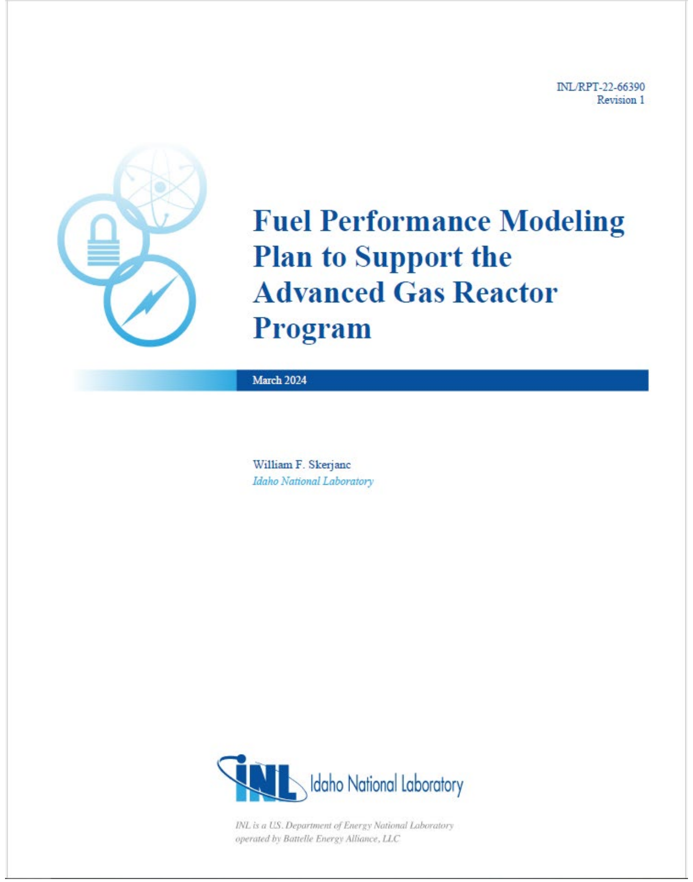
Fuel Performance Modeling to Support AGR Experiments

AGR-1	AGR-2	AGR-3/4	AGR-5/6/7
• Pre-irradiation prediction (**EDF-5741**) • Fission product release comparison to in-pile PIE (**INL/EXT-14-31975**) • Fission product release comparison to safety test PIE (**INL/EXT-14-31976**)	• Pre-irradiation prediction (**ECAR-1020**) • Safety test predictions (**INL/EXT-14-33082**) • Fission product release comparison to in-pile and safety test PIE (**INL/EXT-20-59448**) • Comparison between PARFUME and Bison (**INL/EXT-20-59890**)	• Pre-irradiation prediction (**INL/EXT-16-38280**) • Irradiation as-run predictions (**INL/EXT-21-65160 BISON**) • In-pile irradiation PIE comparison (**INL/RPT-22-69003**) • Fission product transport model [ongoing] (**INL/RPT-22-69040, INL/RPT-23-74853**) • Heating test PIE comparisons of as-irradiated compacts to model predictions (**INL/RPT-23-74505**) • Heating test PIE comparisons to re-irradiated compacts to model predictions (**FY-24**)	• Pre-irradiation prediction (**INL/EXT-17-43189**) • Fuel performance basis for fuel specification (**ECAR-2341**) • Irradiation as-run predictions (**INL/EXT-21-64576**) • Safety test predictions (**FY-25**) • Fission product release comparison to in-pile PIE (**FY26**) • Fission product release comparison to safety test PIE (**FY-27**)

Ref.: Skerjanc, W.F., “Fuel Performance Modeling Plan to Support the Advanced Gas Reactor Program,” Idaho National Laboratory, INL/RPT-22-66390 Rev. 1, 2023.

INL AGR-BISON TRISO Fuel Performance Modeling Workshop

- Workshop held at INL with AGR program staff and the BISON development team
- Objective:
  - Identify modeling gaps
  - Prioritize AGR experimental data to be incorporated in models
- NEAMS BISON 5-year plan
  - **Improve failure predictions**
  - Large moisture ingress events
  - **Improve fission product transport**
  - Extend capabilities to UN fuel
  - Material models for graphite pebbles and compacts
  - **V&V particle fuel simulation capabilities**
- AGR-3/4 experiment
  - Fission product sorption isotherm models
  - Kernel/layer diffusivities
  - Vapor phase transport
  - Incorporation of AGR-3/4 PIE data


INL/RPT-22-66390
Revision 1

Fuel Performance Modeling Plan to Support the Advanced Gas Reactor Program

March 2024

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INL Idaho National Laboratory

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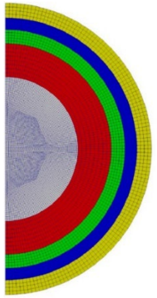
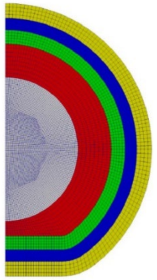
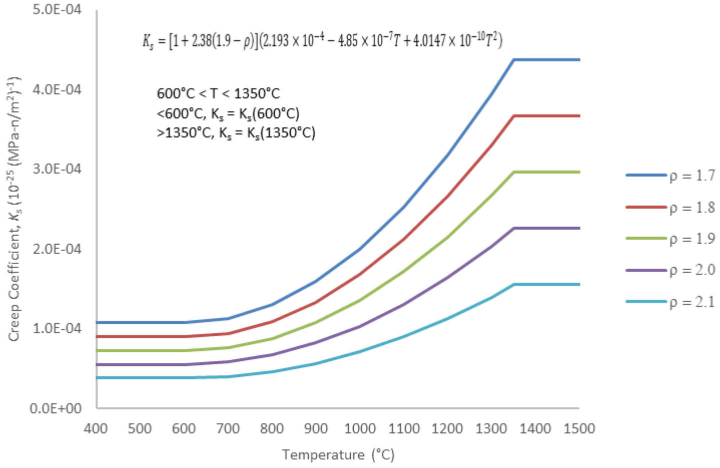
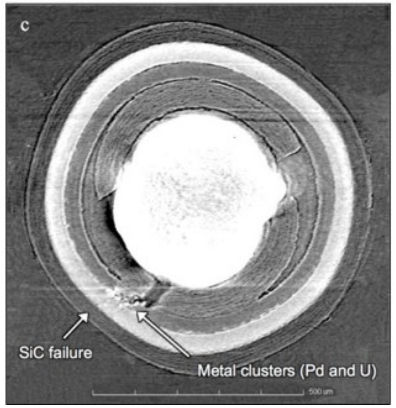
Modeling Improvements

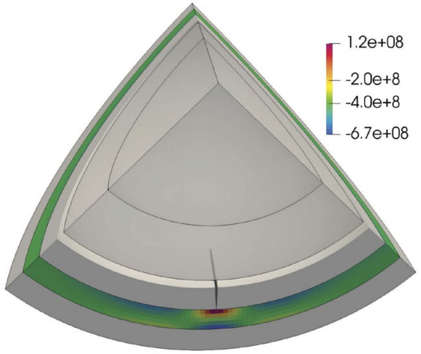
Modeling Improvements	Data Availability	Impact to Model
PyC creep rate	Low	High
IPyC failure prediction validation	Medium	High
Thermomechanical buffer layer modeling	High	Medium
SiC-OPyC separation and OPyC-matrix interaction	Medium	Low
Particle faceting	Medium	Low
Localized Pd attack with IPyC failure	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

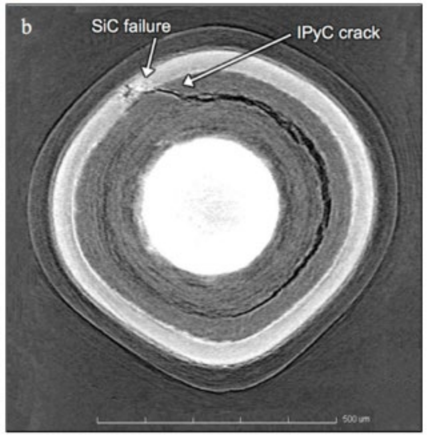


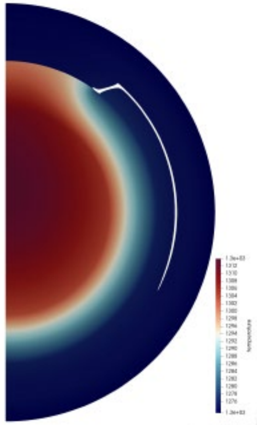










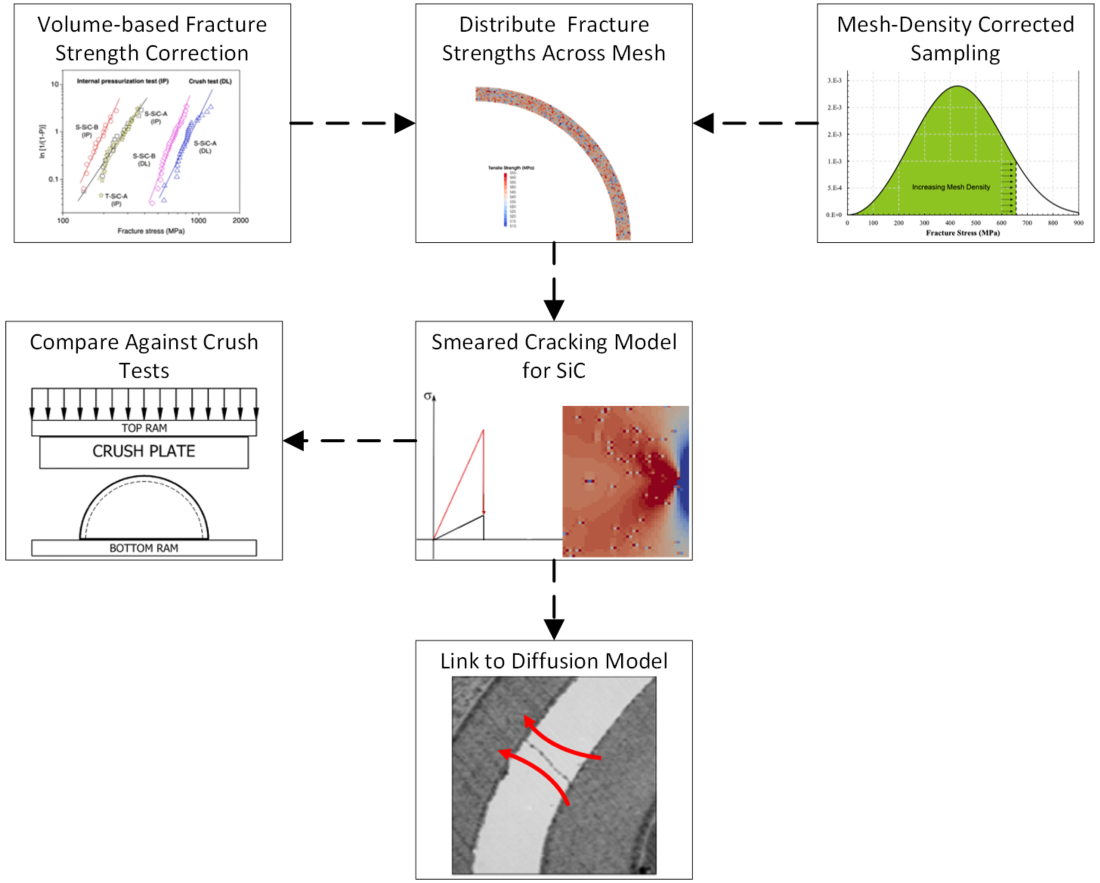


Ref.: Skerjanc, W.F., "Fuel Performance Modeling Plan to Support the Advanced Gas Reactor Program," Idaho National Laboratory, INL/RPT-22-66390 Rev. 1, 2023.

Evaluation of Fission Product Diffusion through Fractured SiC

➢ Ryan Sweet – INL

- Current diffusion models consider bulk diffusion across TRISO layers which affect FP migration calculations.
  - Enable statistical fracture of SiC layer (and eventually PyC layers)
  - Surface diffusion through cracked SiC effectively “short circuits” through layer diffusion path
  - Independent of crack width, but needs to reliably identify fracture and crack penetration
  - Analogous process underway to simulate statistical debonding process

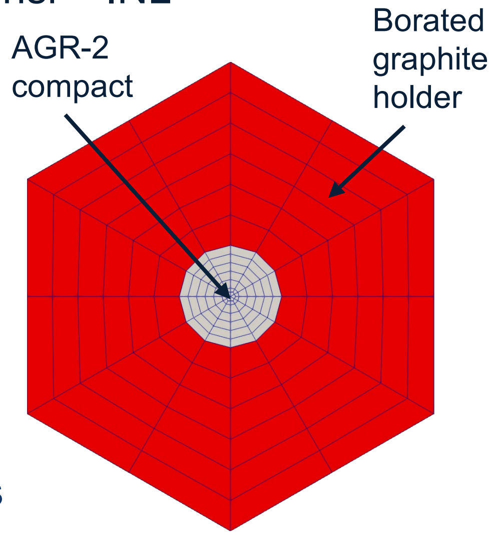


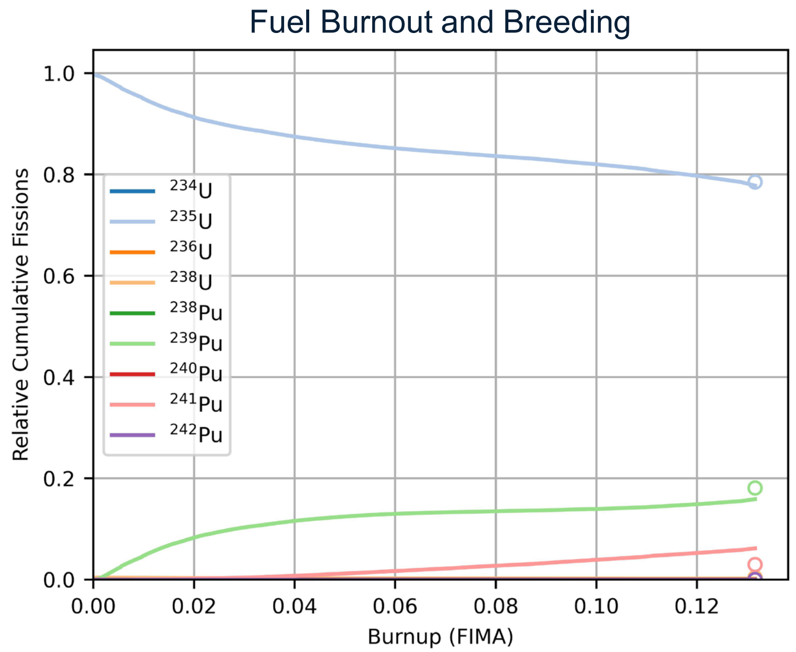
Hong, Seong-Gu, et al. "Evaluation of the fracture strength for silicon carbide layers in the tri-isotropic-coated fuel particle." Journal of the American Ceramic Society 90.1 (2007): 184-191.
Davis, Brian C., et al. "Fracture strength and principal stress fields during crush testing of the SiC layer in TRISO-coated fuel particles." Journal of Nuclear Materials 477 (2016): 263-272.

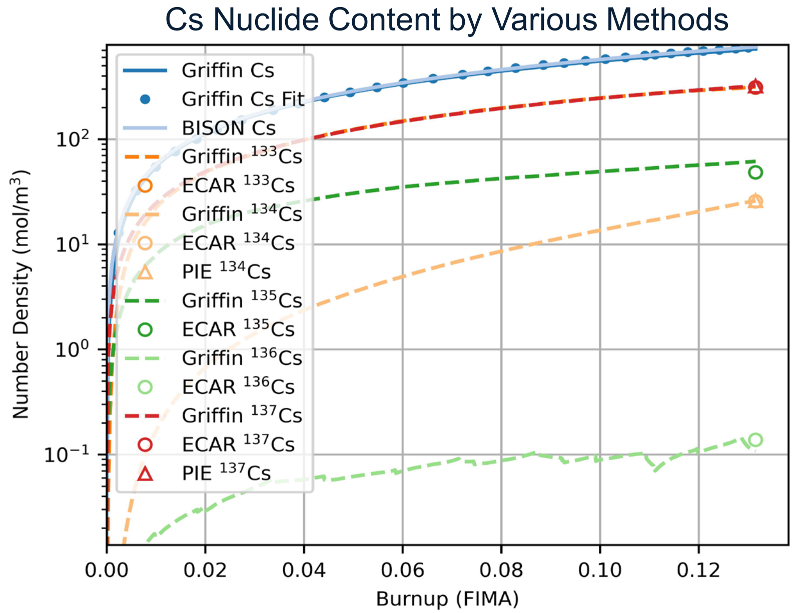
Nuclide-specific fission product source term development

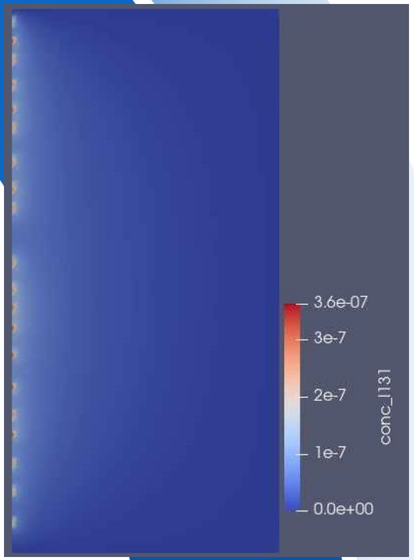
➢ Jacob Hirschhorn and Javier Ortensi – INL

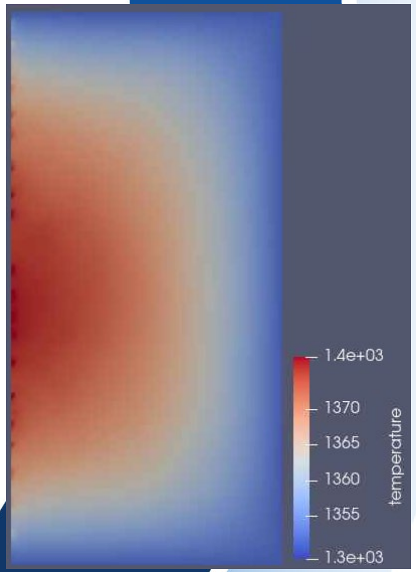
- Developed representative cross sections for AGR-2 as functions of burnup and temperature
- Modeled decay and transmutation of 1690 nuclides during AGR-2 irradiation in Griffin
- Validated predictions against EOL MCNP/ORIGEN calculations and PIE measurements for key nuclides
- Ongoing work
  - Validate predictions against time-resolved MCNP/ORIGEN calculations for additional nuclides
  - Use predictions to develop simplified burnup-dependent fission yields for use in BISON
  - Apply the models to interpret AGR-3/4 re-irradiations
- Future work: assess additional AGR experiments and refine models to develop generalized nuclide-specific source terms for use in BISON







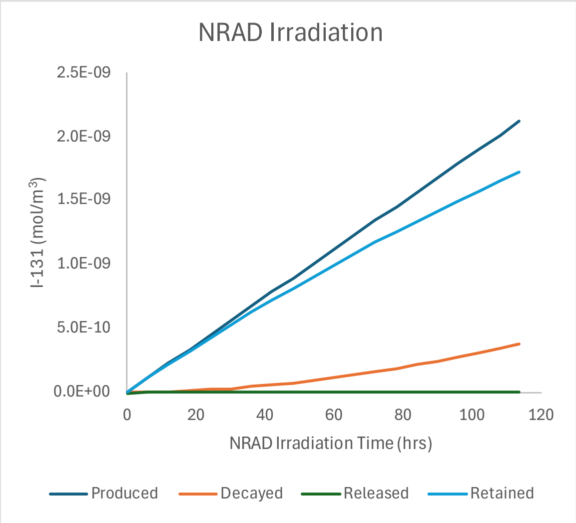


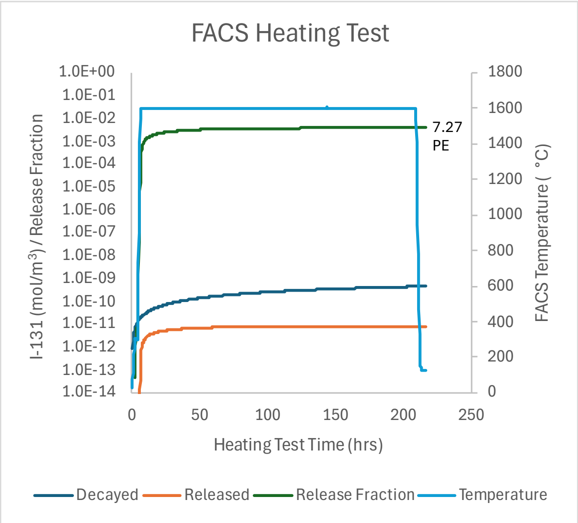


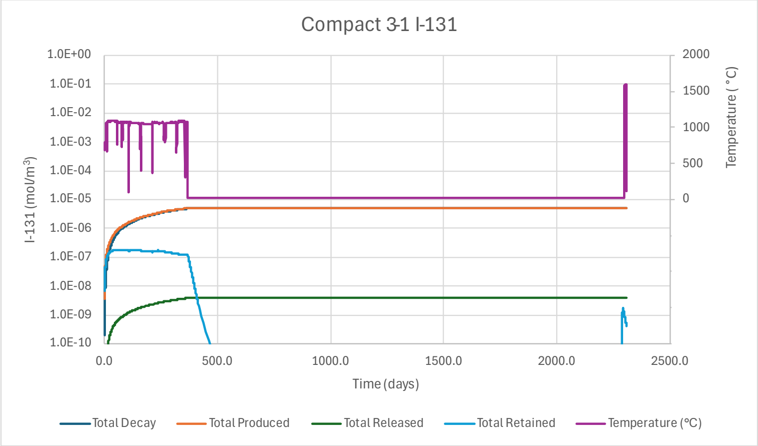
AGR-3/4 Compact Reirradiation Heating Tests

- Model AGR-3/4 compacts from ATR irradiation to FACS heating test

ATR Irradiation	Storage	NRAD Irradiation	Storage	FACS Heating Test
369.1 days	~1900 days	~120 hours	~5 days	~210 hours

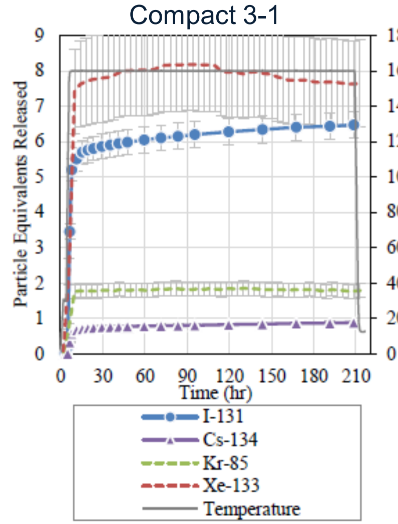






- Compare predicted release to measured experimental data from FACS furnace heating tests

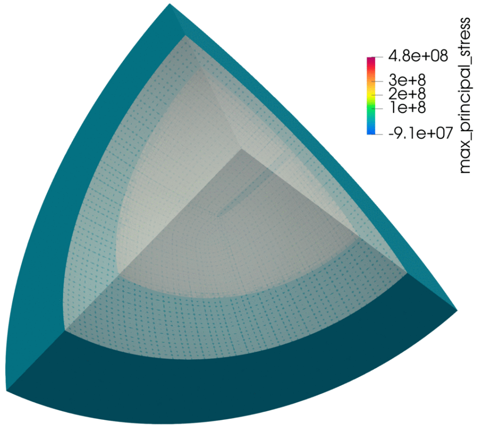
- Predict release of short-lived fission products I-131 (8.02 days) and Xe-133 (5.24 days)
- Use nuclide specific FP source term development for FP accounting (generation, decay, release, retained)
- Diffusivities obtained from IAEA-TECDOC-978
  - I-131 & Kr-85 uses Xe 133 diffusivities

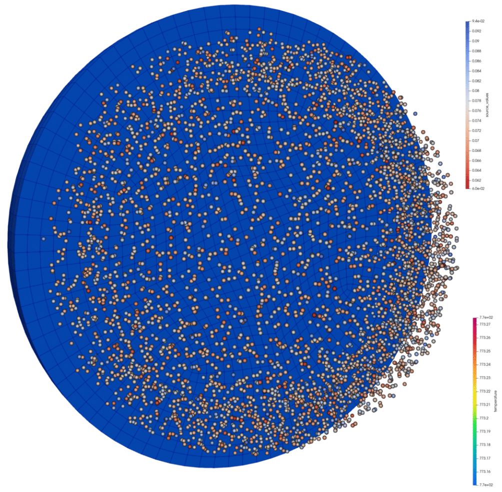


J.D. Stempien, et al, Reirradiated and Heating Testing of AGR-3/4 TRISO Fuels, Proceedings of HTR 2021, HTR-2021-3004

Summary

- Continued support of AGR experiments and PIE activities
- New TRISO fuel performance models and methods continue to be developed
  - These models require advanced simulation capabilities available in BISON
  - Continued collaboration with NEAMS to identify and leverage capabilities for stakeholders
- Potential modeling improvements have been identified and prioritized based on AGR data availability





GAS-COOLED REACTOR

ADVANCED REACTOR TECHNOLOGIES PROGRAM

Thank You

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NEAMS BISON TRISO Development:
- Jacob Hirschhorn (INL)
- Ryan Sweet (INL)
- Wen Jiang (NC State, INL)

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