INL/CON-23-75557-Revision-0

Development and application of sorption mass transfer models for fission product transport in TRISO fuel systems using BISON

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Changing the World's Energy Future

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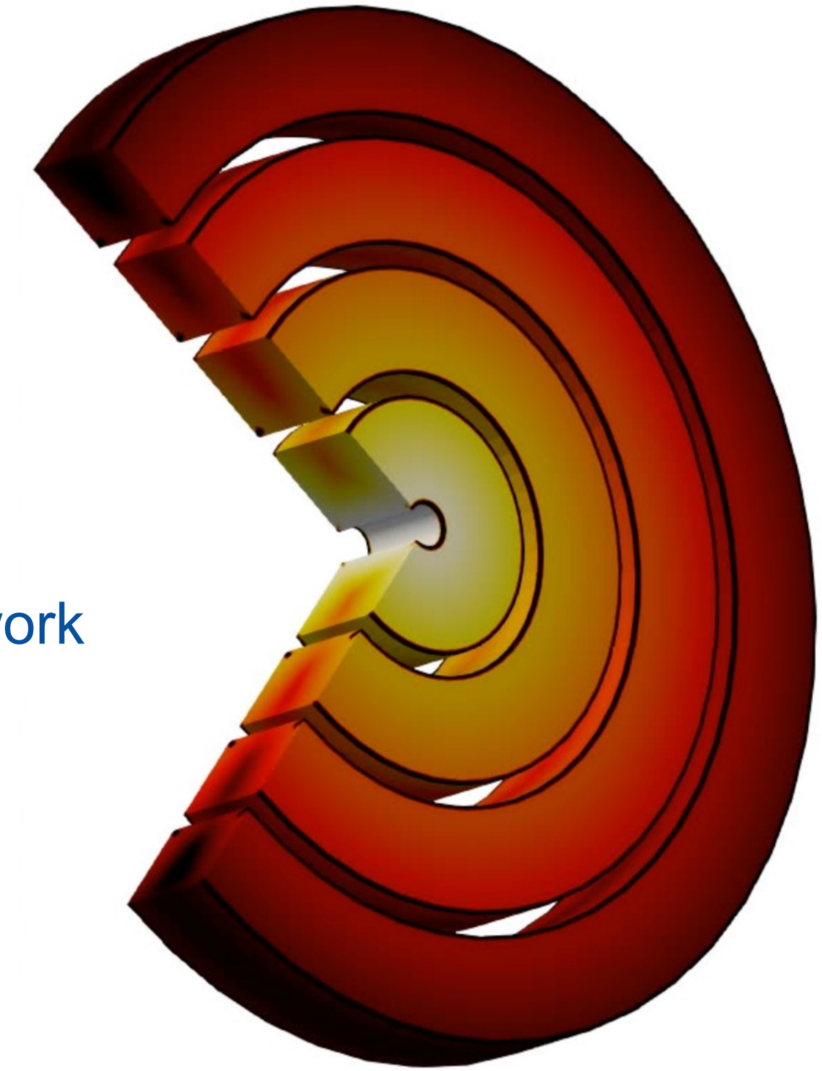
Development and application of improved fission product transport models for TRISO fuel systems analysis in BISON

Outline

- Background
  - TRISO particle anatomy
  - Fission product transport
  - BISON
- Implicit sorption
  - Model development
  - Applications
  - Particle scale validation
- Explicit sorption
  - Model development
  - Applications
- Ongoing and future work
  - Source terms
  - Local effects
  - Integral validation



J. Hirschhorn, A. Riet, unpublished work.

The goals for modeling TRISO fuel performance

- NRC provides guidance for nuclear power plants in 10 CFR Part 50 (primarily for monolithic LWR technology)

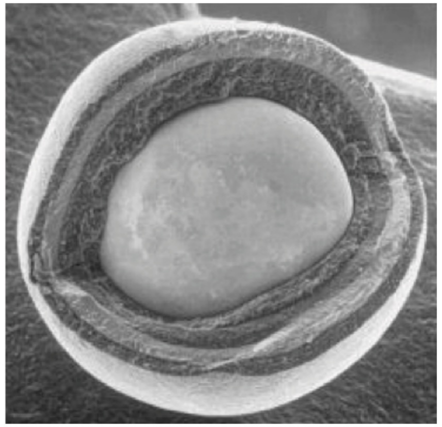
- Additional guidance for SMRs and non-LWRs is given in NUREG-0800, NUREG-2246, and other topical reports

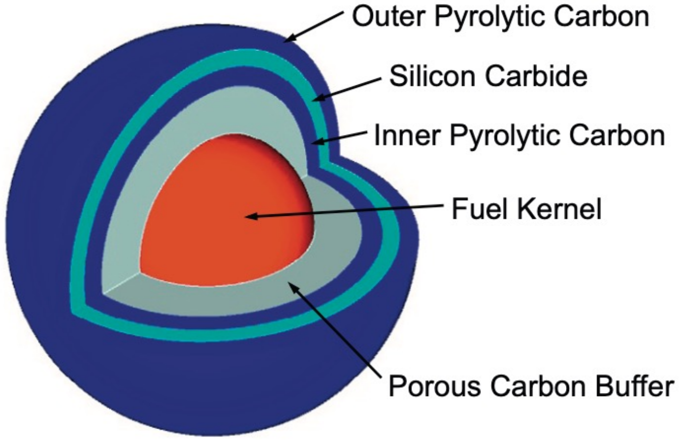
Specification	General Purpose(s)
Functional requirements	Maintain geometry, cooling, containment, and reloading capabilities
Operational requirements	Dictate power level, duty cycle, and requirements for performance during normal and off-normal operation (qualitative)
Fuel design criteria	Establish reactor- and fuel-specific specifications to ensure the above are met (quantitative)

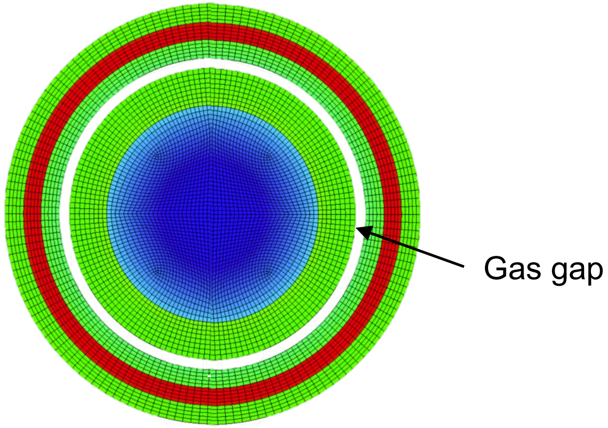
- General underlying goals include
  - Providing reactivity control
  - Maintaining cooling
  - Providing for fuel handling and storage
  - Enforcing quality standards
  - <u>Containing radioactive nuclides</u>
  - Recordkeeping

- Both intact and failed particles release fission products (FPs)

- We need to calculate
  - <u>How much radioactivity is released</u> from each
  - The probability of particle failure







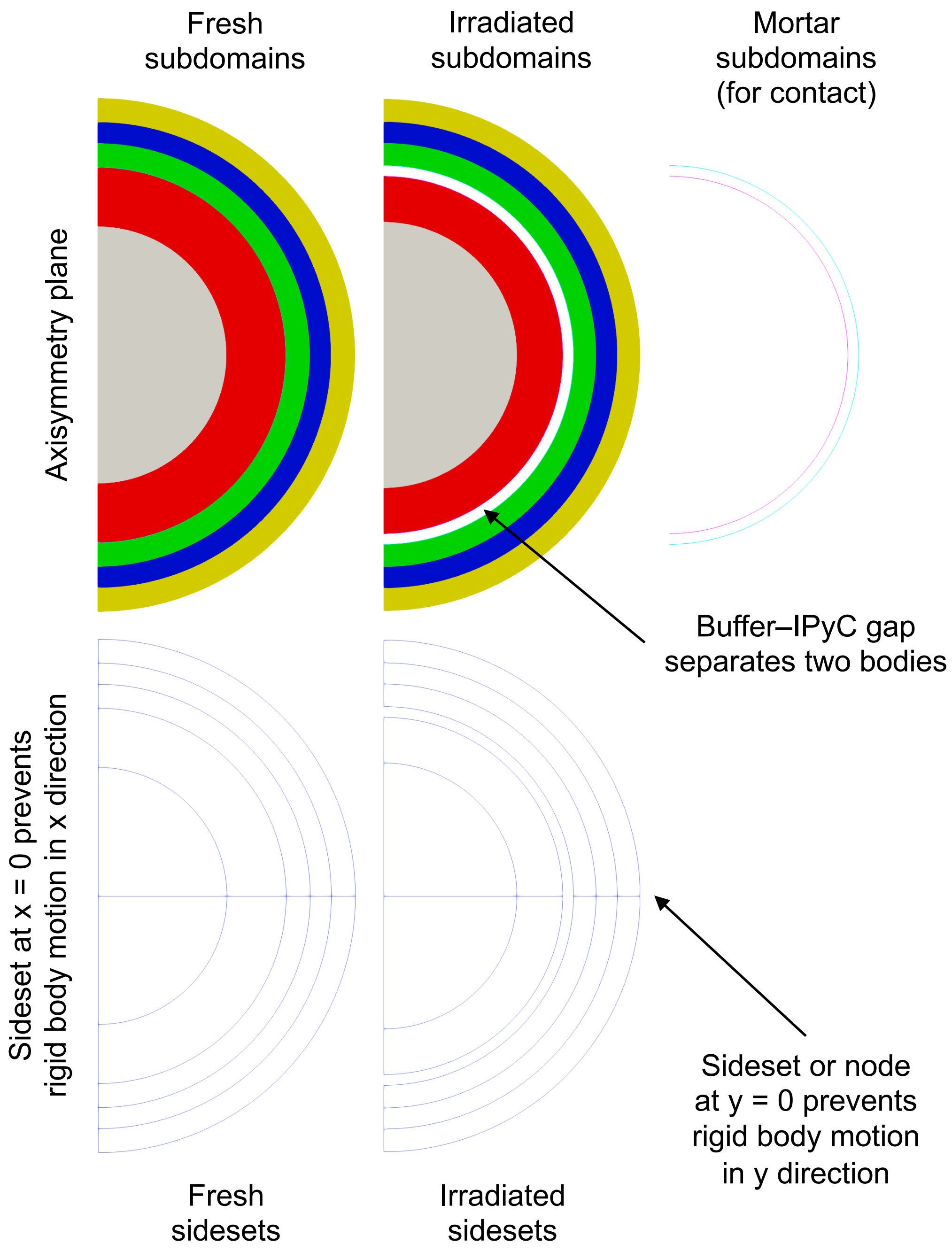
TRISO particle anatomy

- TRISO fuel forms consist of multi-layer, encapsulated fuel particles arranged within graphite, SiC, or other carbonaceous matrices into pebbles or compacts

Layer	Material	General Purpose(s)
Fuel kernel	UCO or UO_2	Produces heat (and fission products)
Buffer	Low density carbon	• Accommodates mechanical deformation of neighboring layers • Decouples the nuclear component from the containment component • Provides free volume to accommodate fission gas release
Inner pyrolytic carbon (IPyC)	High density carbon	• Supports the silicon carbide • Contributes to retention of non-metallic FPs
Silicon carbide (SiC)	SiC	• Acts as primary pressure vessel • Contributes to retention of metallic FPs
Outer pyrolytic carbon (OPyC)	High density carbon	• Similar to the IPyC • Protects the SiC during the overcoating and compaction

J. Hales, et al., Journal of Nuclear Materials 443 (2013) 531-543.

The particles themselves serve as the first barrier to FP release



- FPs of interest typically include isotopes of Cs, Sr, Ag, Kr, Xe, I, Pd

- We model FP production, transport, decay, and release
  - Intra-layer and compact matrix diffusion are modeled as effective Fickian diffusion
  - At the compact scale, particle source terms are weighted by failure probabilities

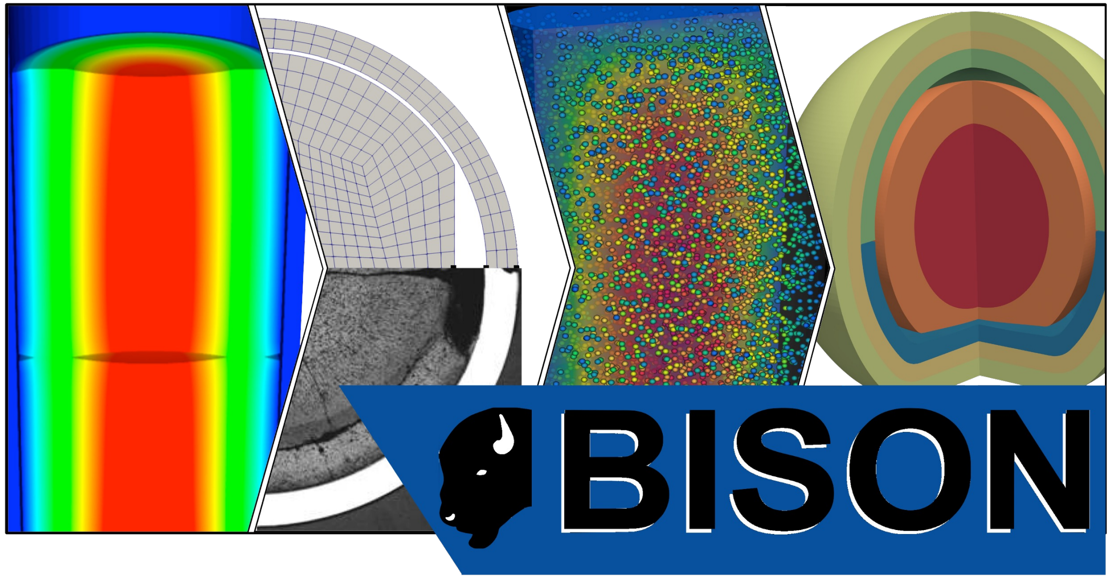
- The gas gap that forms at the buffer–IPyC interface during operation requires additional considerations
  - Thermal contact
  - Mechanical contact
  - Sorption mass transfer

What is BISON?

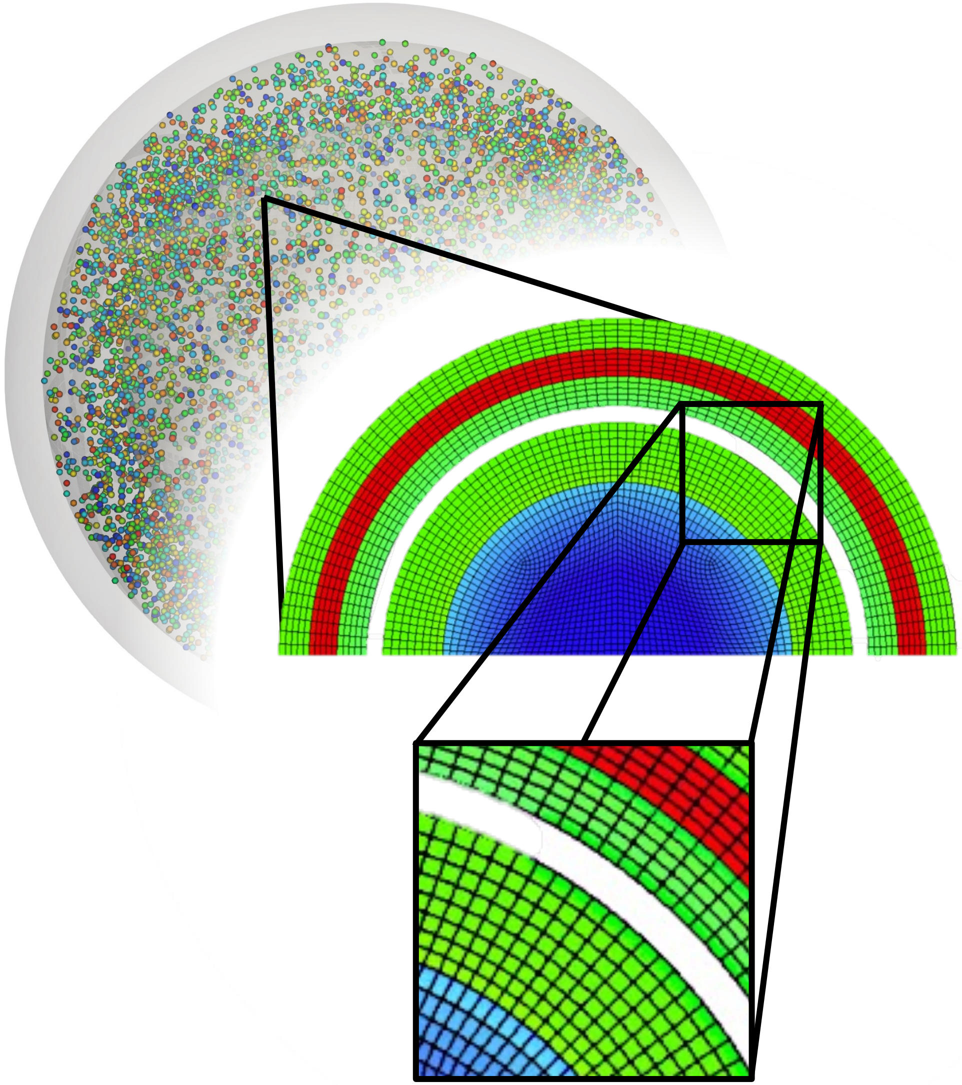
- BISON is a finite element-based nuclear fuel performance code
- Its development is currently funded by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program and a variety of other sources
- BISON is based on the MOOSE Framework
- BISON
  - Is free to use, but US Export Controlled
  - Attracts diverse users and developers
  - Is used for engineering and research
  - Inherently considers multiphysics
  - Can couple to multiscale codes
  - Scales well from laptops to clusters
  - Features a flexible, modular design
  - Is under continuous development
- User, Developer, and Customer- or application-specific trainings are available
  - Email or call me!

NEAMS
Nuclear Energy Advanced Modeling and Simulation

2021 R&D 100 WINNER



Governing transport equations

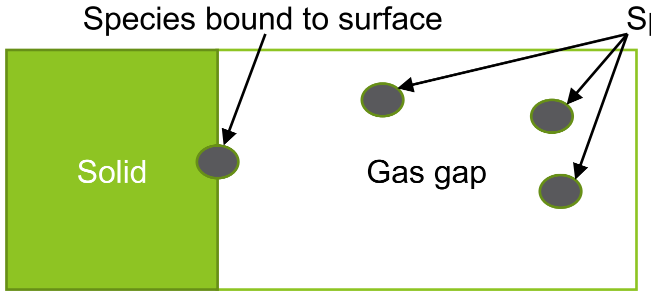


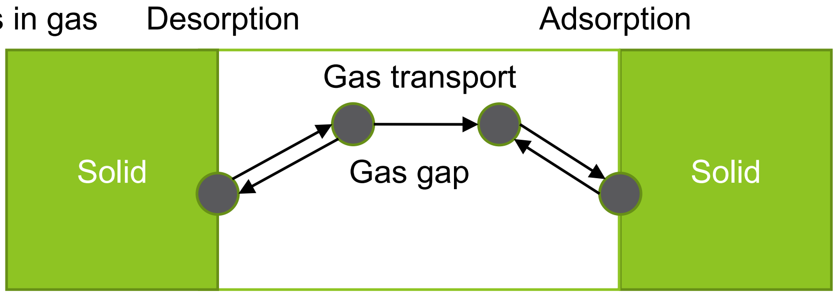
- Effective Fickian diffusion with production and decay

$$\frac{\partial c}{\partial t} = \nabla \cdot D \nabla c_s + \dot{P} - \lambda c$$

where c_s is the FP concentration,
D is the diffusivity,
$\dot{P}$ is the production rate density,
and λ is the decay constant

Implicit sorption mass transfer through unmeshed gas gaps





- Assume
  - Partial pressure is homogeneous in the gap (equal at both surfaces)
  - Mass transfer across the unmeshed gap is instantaneous (implicit sorption assumption)
  - *Engineering scale properties represent surface conditions (i.e., density)*

- FP partial pressures at each surface are described by sorption isotherm data

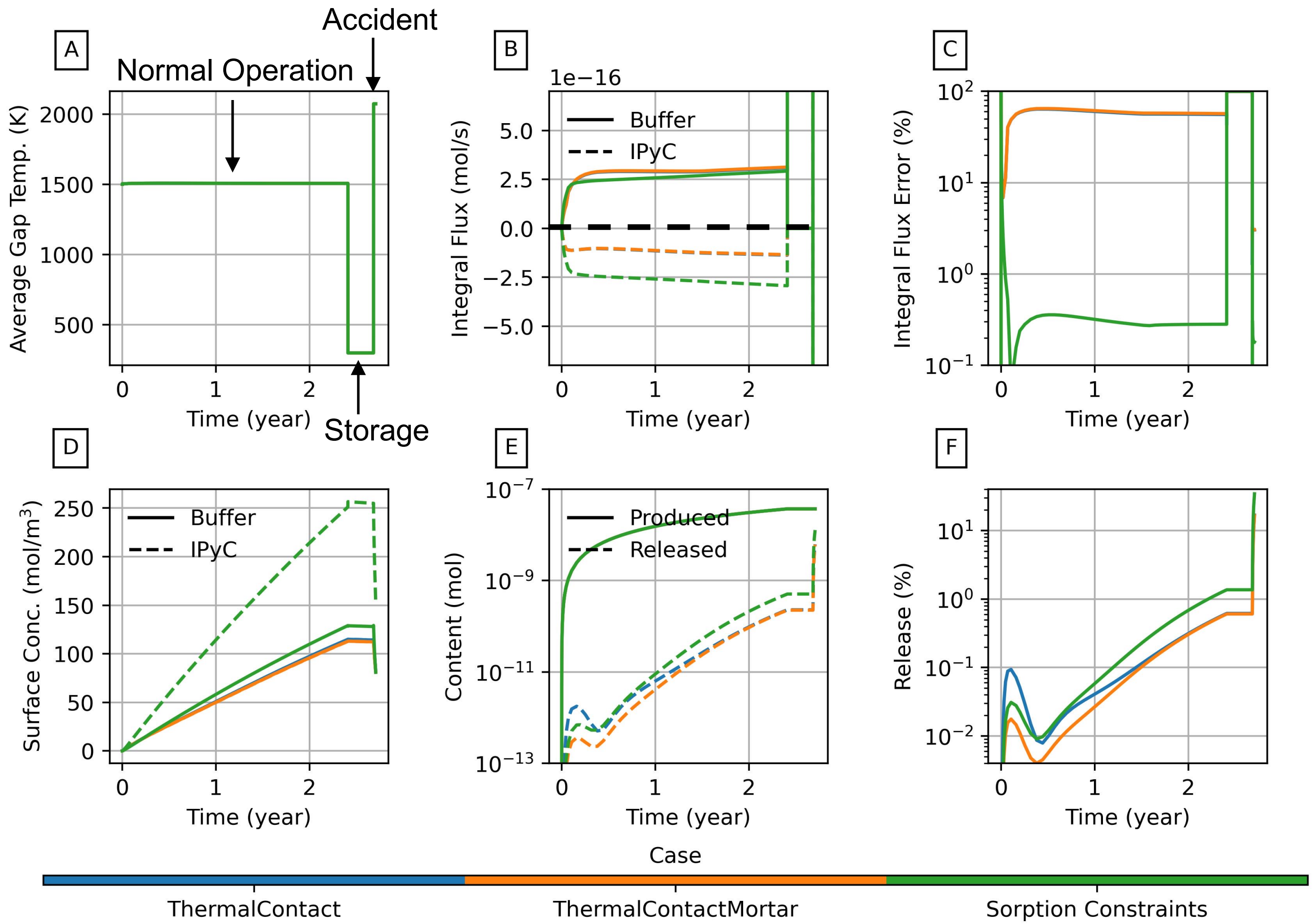
$$P = \exp\left[\left(A + \frac{B}{T}\right) + \left(D - 1 + \frac{E}{T}\right)(d_1 - d_2 T)\right] c_s + \exp\left(A + \frac{B}{T}\right) c_s^{\left(D + \frac{E}{T}\right)}$$

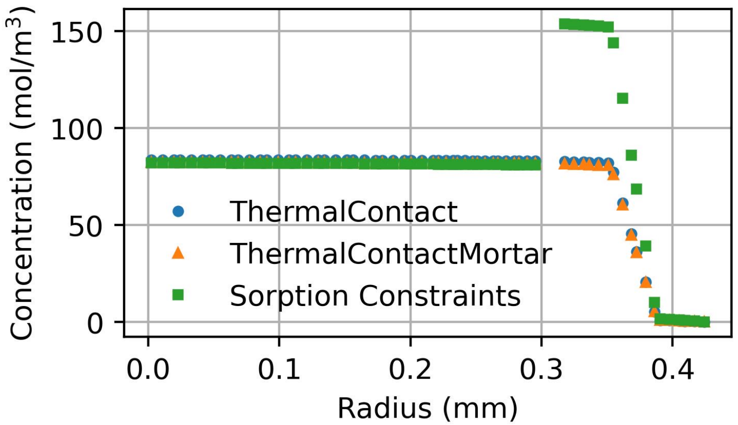
(Henrian) (Freundlich)

- Integral flux preservation is given by $\int_{\Omega_1} \boldsymbol{J_1} \cdot \boldsymbol{n_1} d\Omega_1 + \int_{\Omega_2} \boldsymbol{J_2} \cdot \boldsymbol{n_2} d\Omega_2 = 0$

Parameter	Description
P	Partial pressure
c_s	Concentration
T	Temperature
A	Sorption constants
B	
D	
E	
d_1	
d_2	
J	Mass flux
n	Outward unit normal
Ω	Surface area

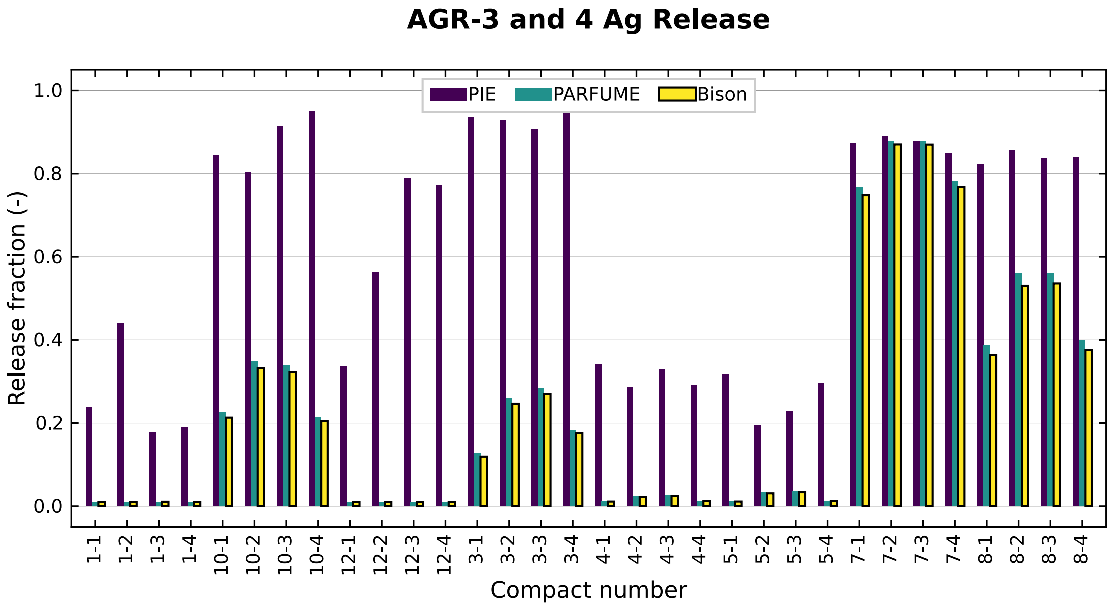
Implicit sorption demonstration: accident simulation with Cs



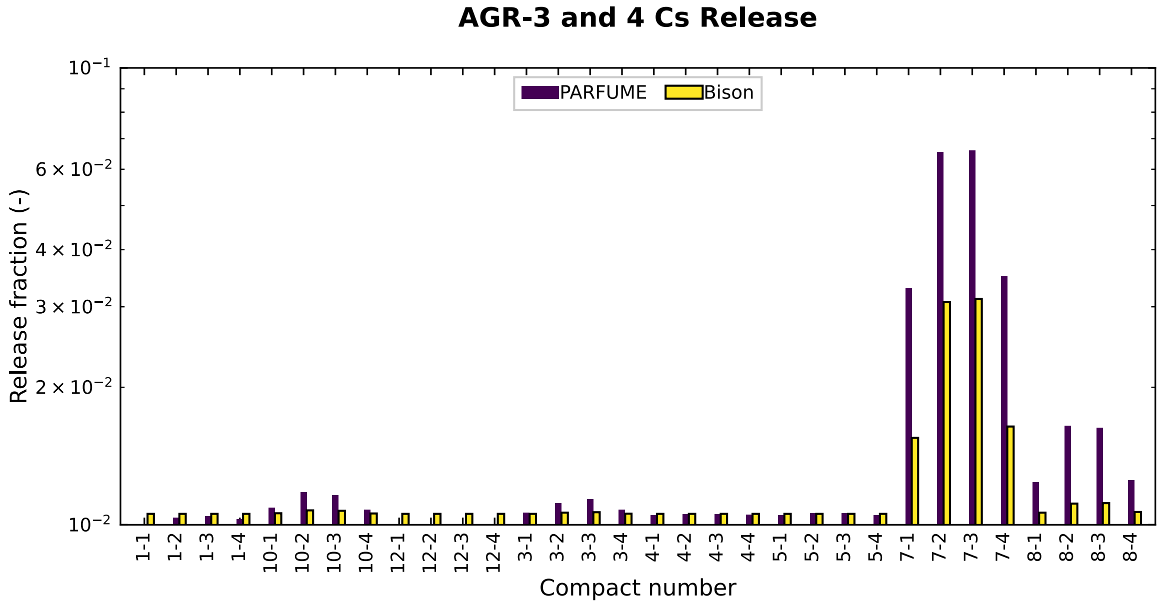


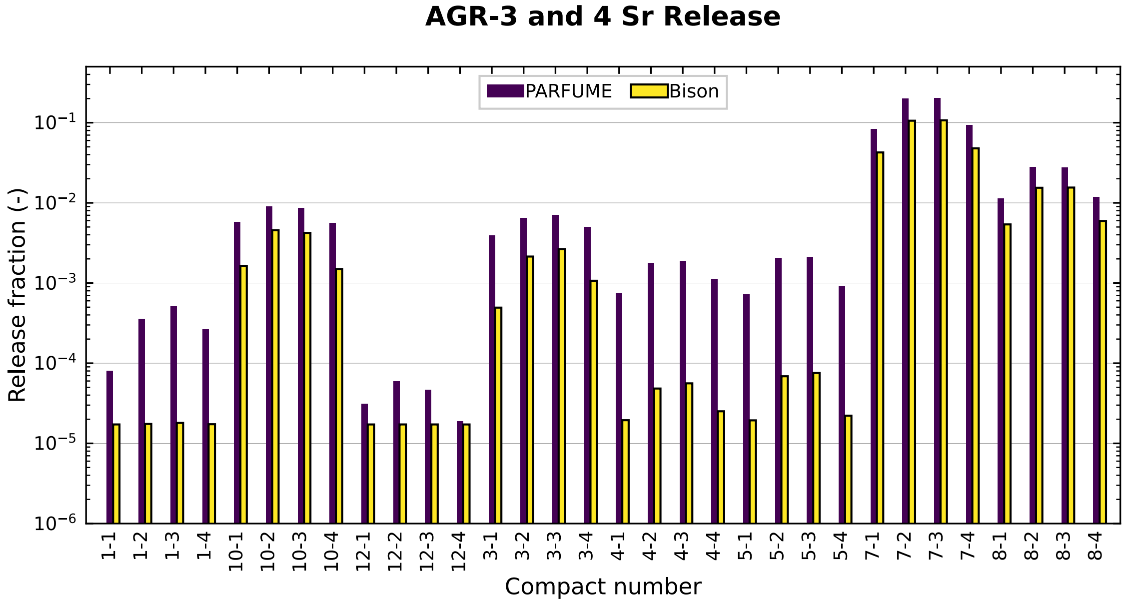
J. Hirschhorn, et al., Improved Fuel Particle and Compact Matrix Fission Product Release Prediction with Improved Mass Transfer Model (2023).

Overview of the AGR-3/4 assessment: FP release



- Simulations were conducted without sorption to model fission product release
- Predictions compare similarly to those of PARFUME
- There exists room for improvement

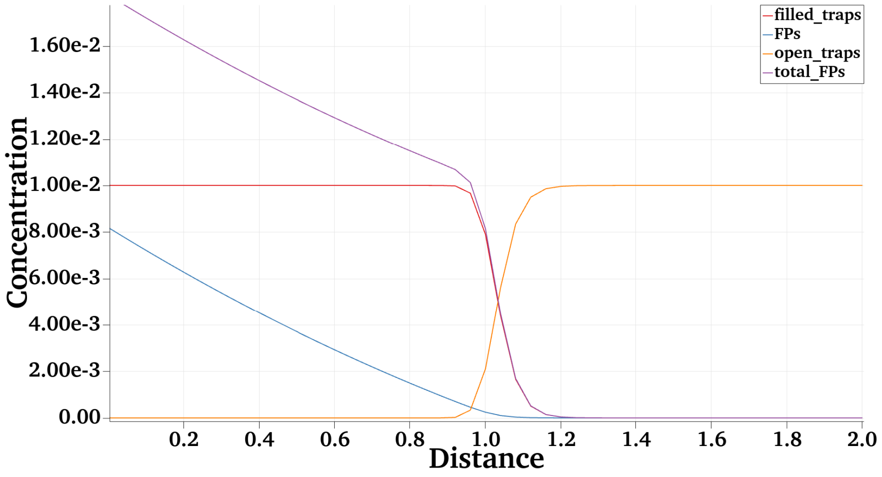


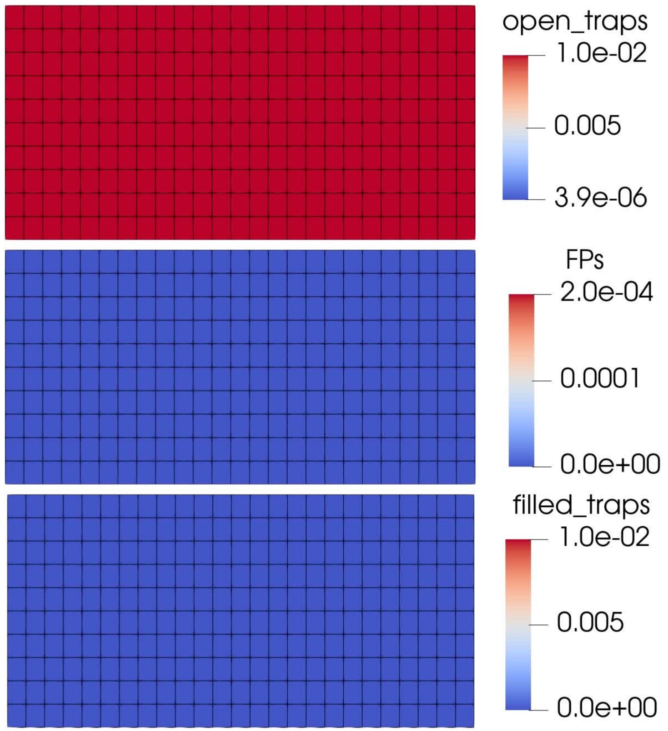


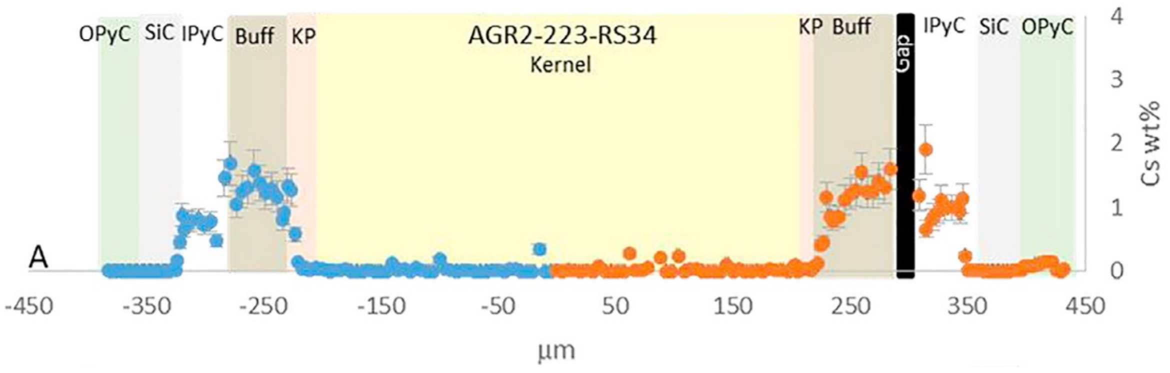
J. Hirschhorn, A. Toptan, et al., INL/RPT-23-73972, 2023.

FP trapping in porous and non-porous layers may also influence FP transport and post-irradiation inventory

- Active area of research and development
- Pores and vacancies can trap FPs, influencing transport and post-irradiation inventory
- In addition to sorption, may be needed to enable <u>particle scale validation</u>

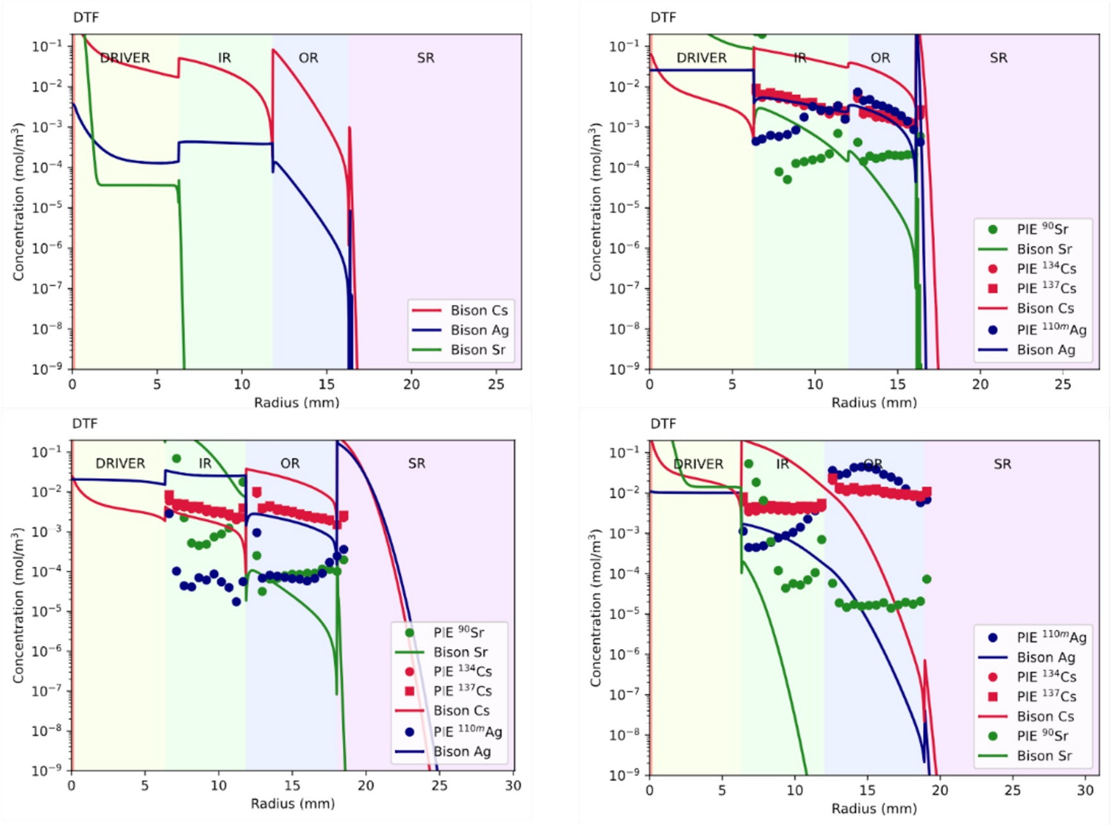




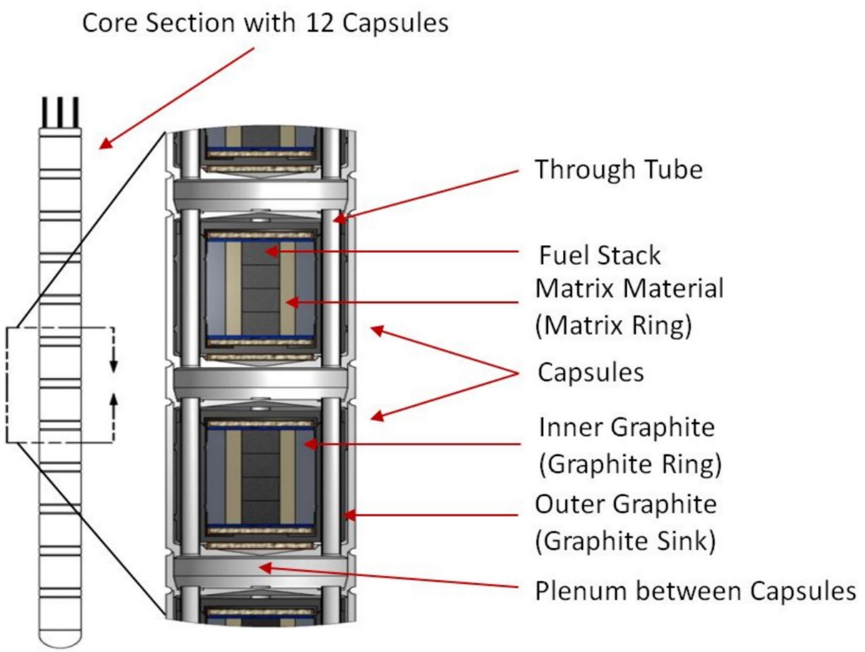


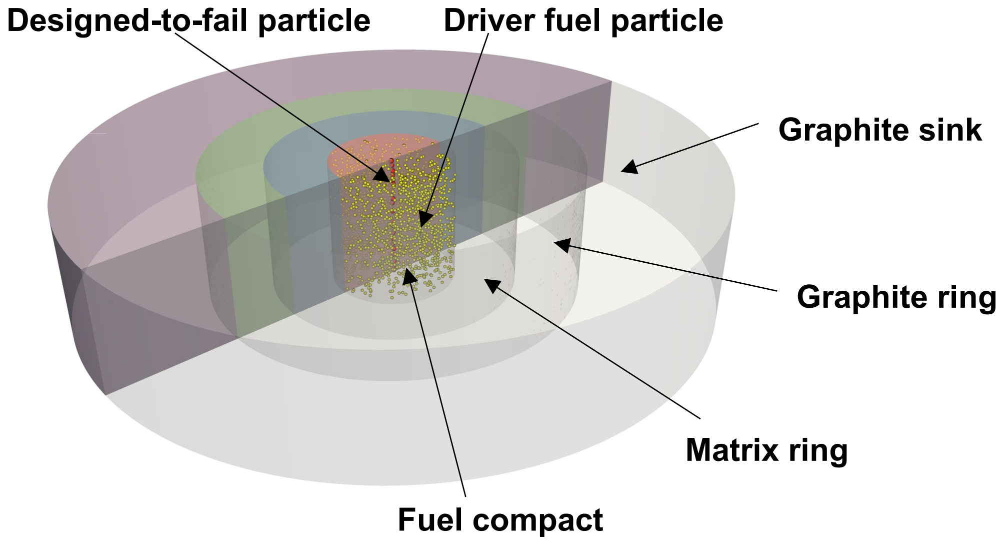
Ryan Sweet. Unpublished work.
K. Wright, et al., Journal of Nuclear Materials 559 (2022) 153468.

Overview of the AGR-3/4 assessment: implicit ring modeling



- Implicit sorption mass transfer capabilities were applied across radial gas gaps between concentric rings
- Gap thicknesses were not modeled, but the thicknesses of the rings were conserved





J. Hirschhorn, A. Toptan, et al., INL/RPT-23-73972, 2023.
B. Collin, INL/EXT-15-35550, 2015.
Adapted from works by Wen Jiang, et al.

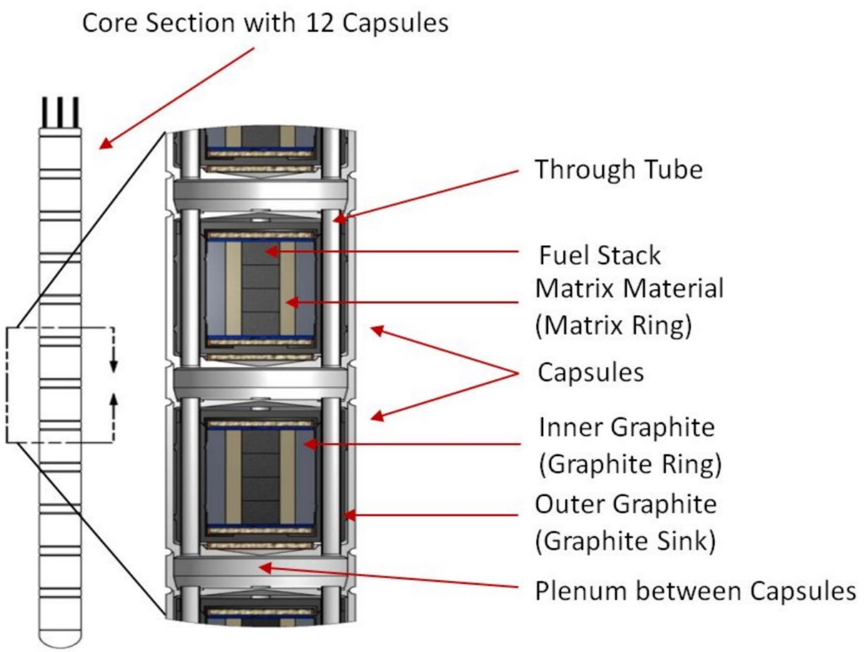
Explicit sorption mass transfer through meshed gas gaps

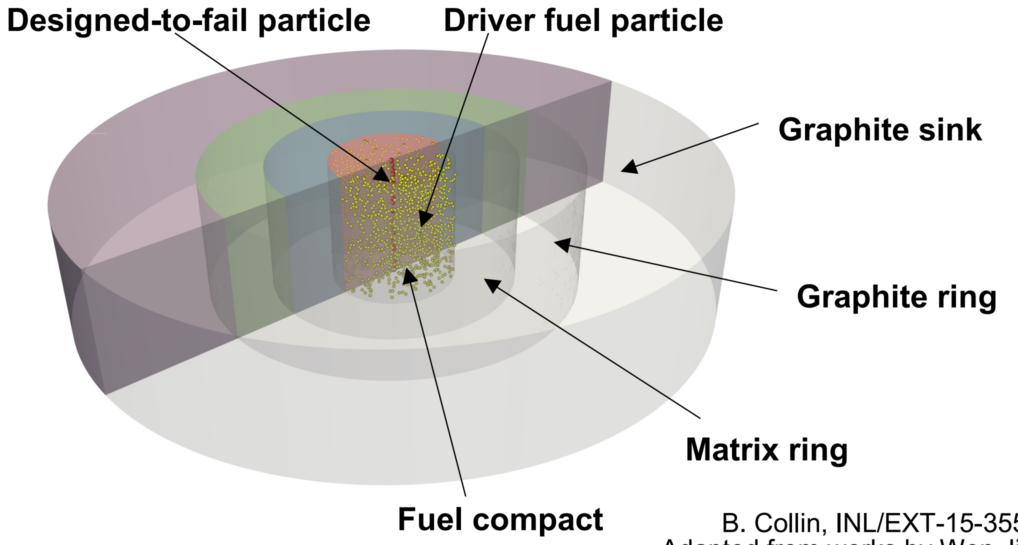
- Needed when
  - There is the potential for long range FP transport through gas gaps
  - A gas gap separates more than two bodies
- FP concentration in the gas (c_g) is solved for using an ideal gas assumption

$$c_g = \frac{P(c_s, T)}{RT}$$

where R is the ideal gas constant

- Example: graphite rings in AGR-3/4
  - Irradiate UCO fuel to provide a known source of fission products for transport through the rings
  - Determine fission product diffusivities in and sorptivities in particle, compact, and matrix materials





B. Collin, INL/EXT-15-35550, 2015.
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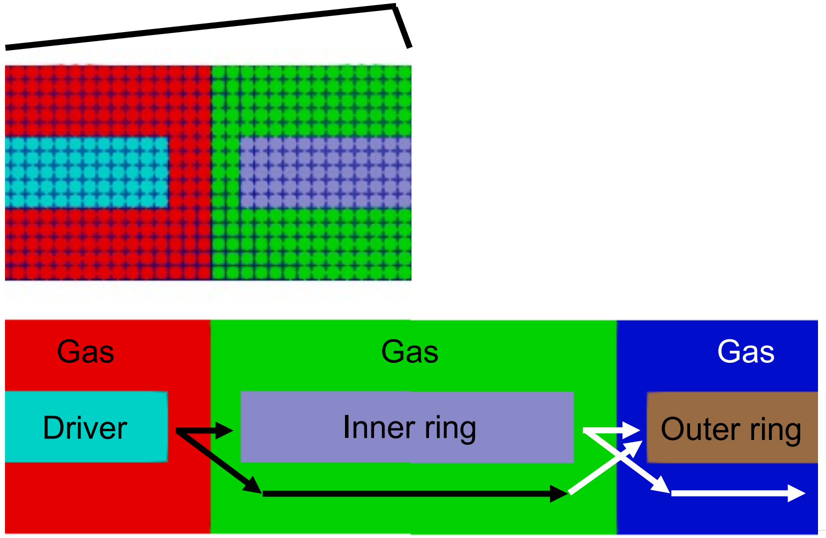
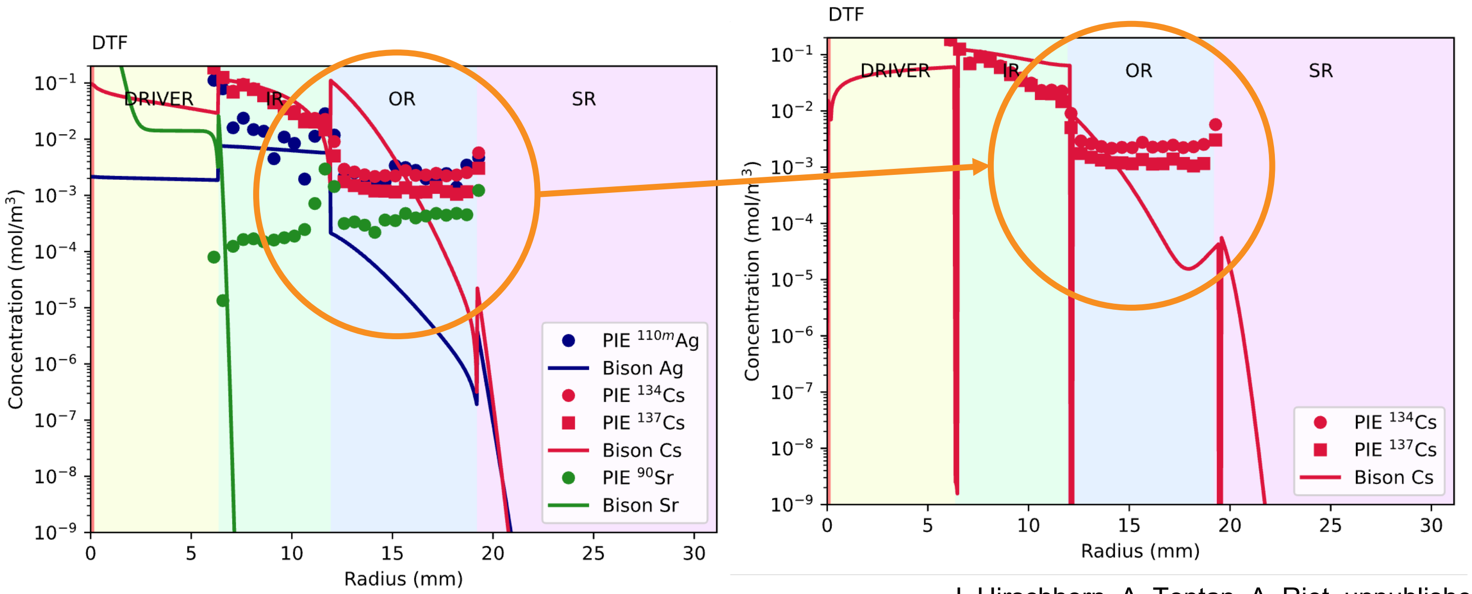
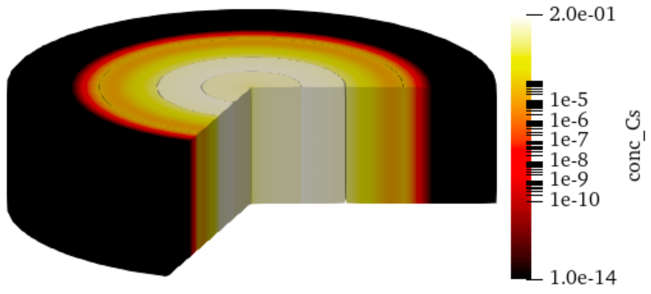
Ongoing work: AGR-3/4 with explicit ring modeling



- FPs were expected to diffuse through concentric rings in series
- The presence of interconnected gas gaps between rings may have put them in parallel (“short circuit” hypothesis)

- Explicit sorption mass transfer being applied within gas gaps
- Better represent trends observed in the radial FP scans
- Expected to facilitate diffusivity and sorptivity calibration



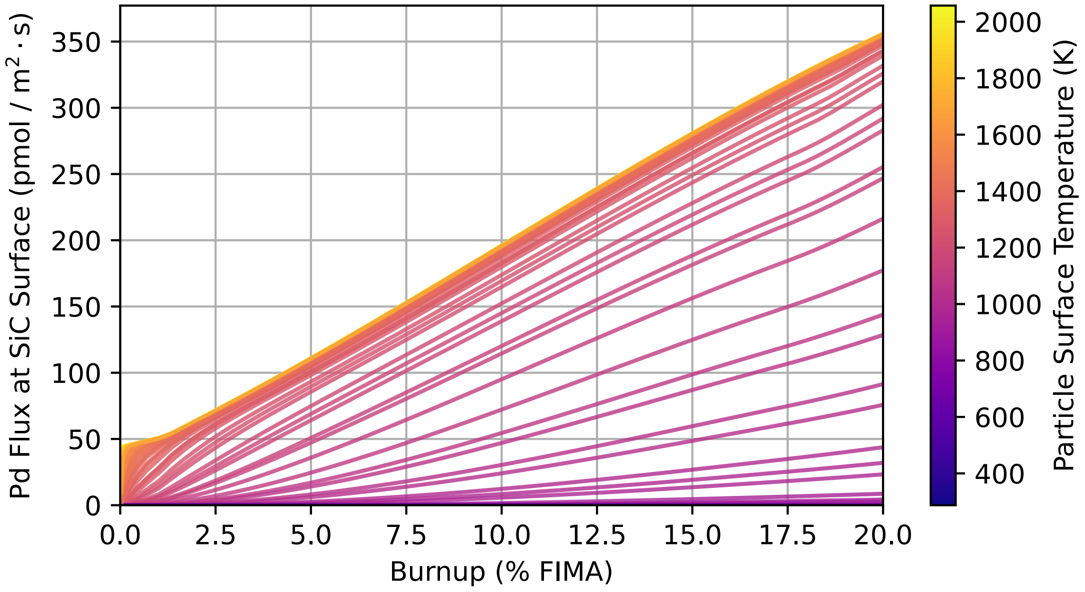


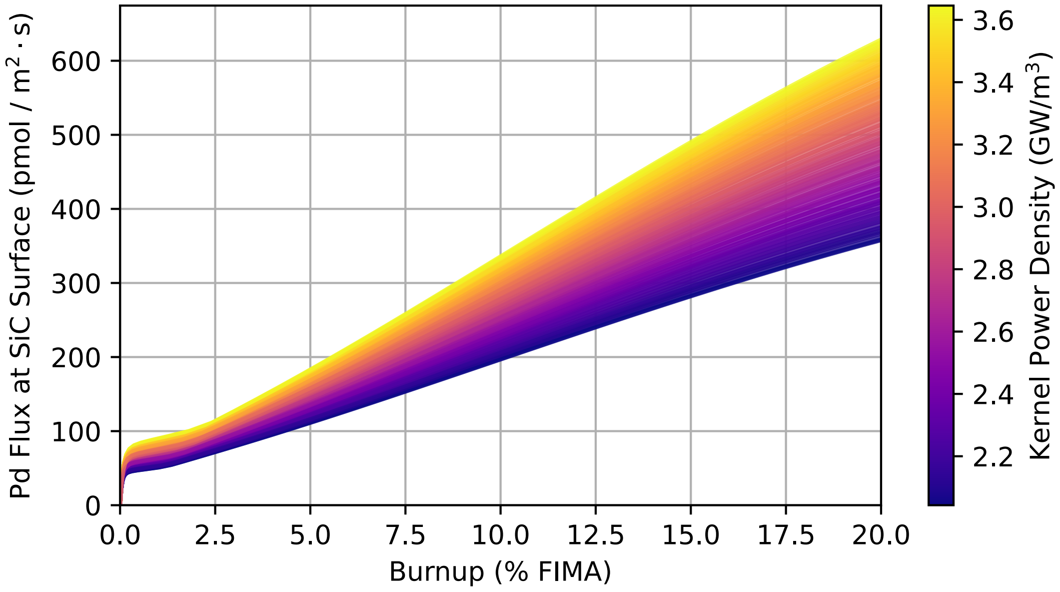
J. Hirschhorn, A. Toptan, A. Riet, unpublished work.

Improved burnout- and breeding-dependent source terms

- Chemical interaction between Pd FPs and SiC can contribute to particle failure
- Reactions depend on the Pd flux, and therefore Pd production and transport
- Pd production depends strongly on fuel burnout and breeding
- Improved production models are being developed to capture these effects

Nuclide	Fractional Pd Yield
^{235}U	0.0158
^{238}U	0.0874
^{239}Pu	0.1581
^{241}Pu	0.2451

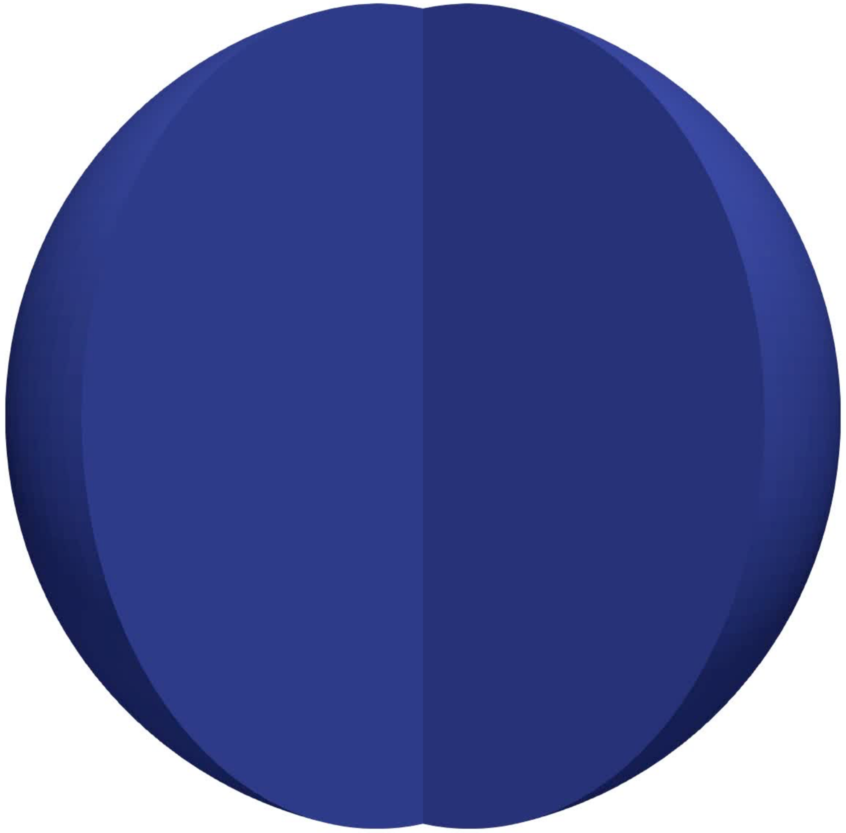




J. Hirschhorn, R. Sweet, unpublished work.

Implicit sorption + damage for localized FP flux effects

- Mechanical deformation and failure affects FP transport (both in degree and character)
- Post-irradiation examination has observed coupled and highly localized failure and thermochemical behaviors
- Improved multiphysics analysis techniques are being developed to study and predict non-uniform FP transport in the presence of
  - Particle layer cracking
  - Partial and full layer debonding



Other ongoing and future work

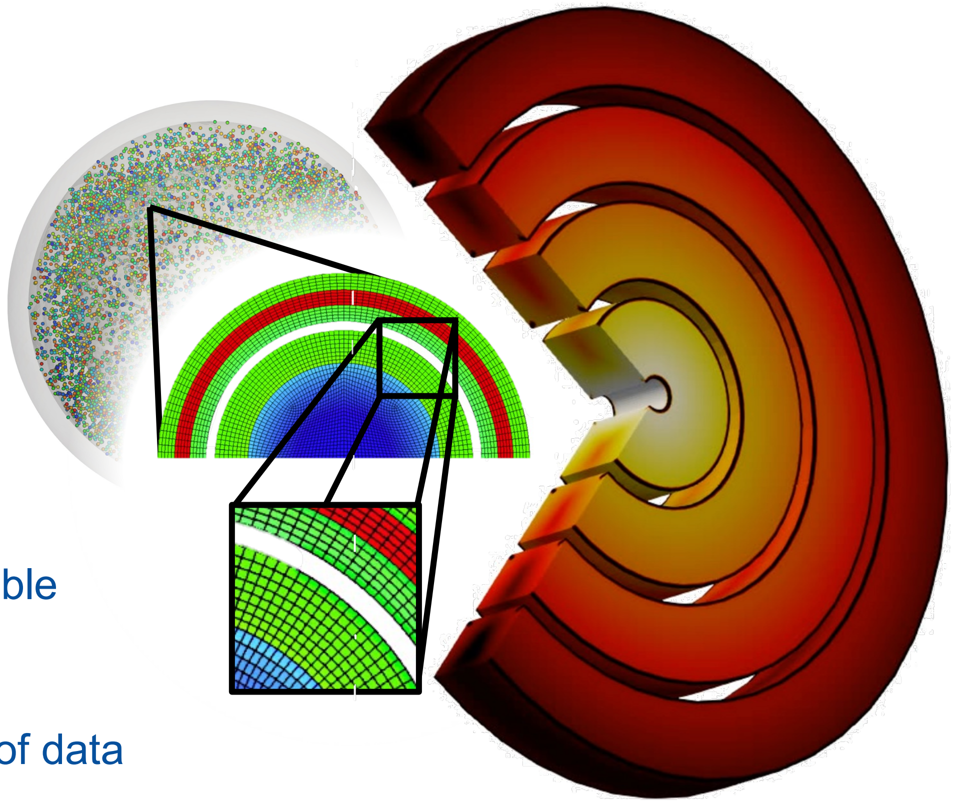
- Existing AGR assessments are continuously updated as data and modeling capabilities become available
  - Experimental data
  - Material property data
  - Behavioral models

- Additional assessments are being targeted in collaboration with AGR
  - AGR-5/6/7: reference-design particles during normal and off-normal

- Particle (versus integral compact) scale validation
  - Enable separate versus integral effects validation
  - Compare sorption and trapping (in porous and non-porous layers) simulations to particle scans

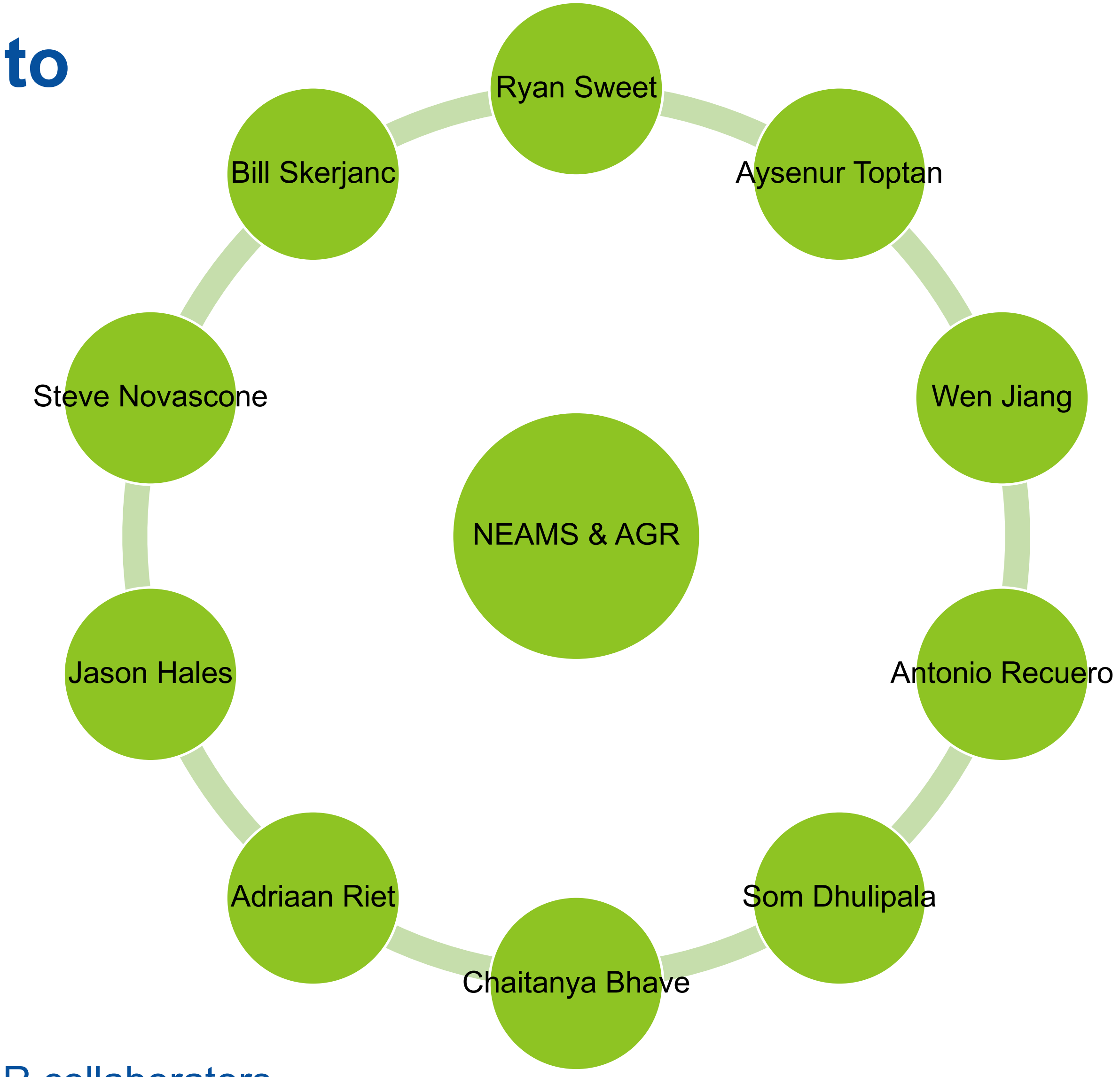
Summary

FP production and transport → Failure behaviors and FP release → Source terms, qualification, and licensing



- Numerous capabilities are being developed to supplement existing BISON TRISO fuel performance models
  - Implicit sorption and trapping models, which will also enable particle-scale validation
  - Explicit sorption models, which will enable interpretation of data from AGR-3/4
  - Improved burnout- and breeding-dependent FP source terms
  - Multiphysics failure analysis techniques, which can be applied to capture more realistic localized thermochemical effects

Many thanks to



- Other NEAMS and AGR collaborators
- Many others from industry and throughout the lab complex

Idaho National Laboratory

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