INL/MIS-25-84688-Revision-0

# NEAMS fuels modeling for HTGRs: FY24 accomplishments and outlook for FY25

April 2025



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**Jacob Aaron Hirschhorn**

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**Idaho National Laboratory**
**Idaho Falls, Idaho 83415**

**http://www.inl.gov**

**Prepared for the**
**U.S. Department of Energy**
**Under DOE Idaho Operations Office**
**Contract DE-AC07-05ID14517**

# NEAMS fuels modeling for HTGRs: FY24 accomplishments and outlook for FY25

Presenter: Jacob Hirschhorn

Contributors (alphabetically): Larry Aagesen, Chaitanya Bhave, Somayajulu Dhulipala, Jacob Hirschhorn, Wen Jiang, Stephen Novascone, Antonio Recuero, Pierre-Clément Simon, Ryan Sweet, and Mathew Swisher

# Outline

- NEAMS TRISO modeling background and overview
- Overview of FY24 activities
- FY24 activities detail
- FY24 engagement and broader impacts
- FY25 outlook

# NEAMS TRISO modeling background and overview

| 2012 | 2013 | 2014 | 2015 | 2016 | 2017 | 2018 | 2019 | 2020 | 2021 | 2022 | 2023 | 2024 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Stage 1 | | | | | | Stage 2 | | | | Stage 3 | | |
| • Developed and implemented baseline TRISO modeling capabilities in BISON | | | | | | • Improved internal mesh generation and Monte Carlo capabilities for TRISO simulations<br>• Implemented PARFUME models in BISON<br>• Began incorporating LLS-informed models for select TRISO properties/behaviors<br>• Performed baseline BISON verification and validation (AGR-1, AGR-2, and IAEA CRP-6) | | | | • Implemented fast integration and variance reduction methods for TRISO failure probability<br>• Increased focus on LLS-informed model development, including for layer diffusivities and Pd penetration<br>• Implemented various improvements to matrix property, particle debonding, and gap mass transport models<br>• Expanded BISON validation cases to AGR-3/4<br>• Developed and implemented advanced uncertainty quantification methods to help identify high-priority improvements | | |

## Looking ahead

- Expand BISON TRISO validation database to AGR-5/6/7, transient experiments, etc.
- Incorporate advanced behavioral models to enable failure probability calculations under realistic conditions
- Enhance and expand models for compact matrix performance

Based on works by W. Jiang.

# Overview of FY24 activities

## Engineering scale

- INL/RPT-24-80567: Complete development of critical capabilities for TRISO fission product source term calculations and quantify mechanisms for Pd penetration of SiC

- INL/RPT-24-78711: Mortar-based cohesive zone model with application to TRISO particle debonding

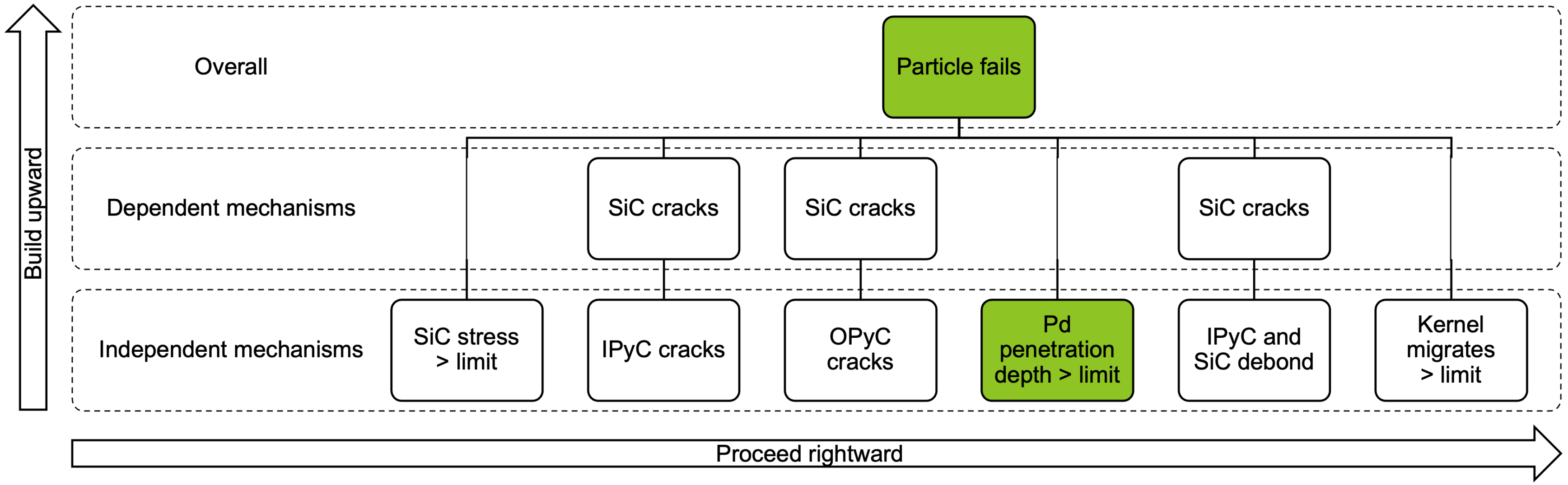
- INL/RPT-24-79964: Bayesian analysis of TRISO fuel: quantifying model inadequacy, incorporating lower-length-scale effects, and developing parallel active learning capabilities

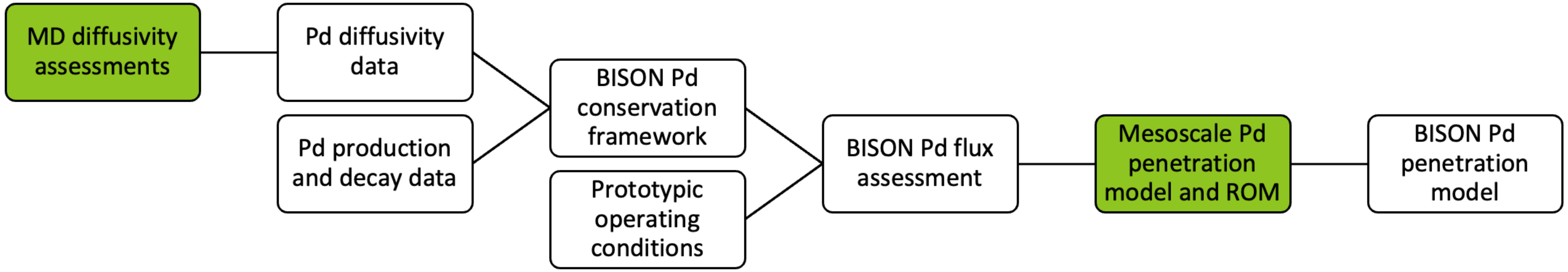
## Lower-length scale

- INL/RPT-24-80441: Lower length scale model for palladium attack of silicon carbide in TRISO fuel

# Pd and transport assessment (INL/RPT-24-80567)

- Pd fission products can migrate to and react with the SiC, degrading
  - Structural integrity
  - Fission product retention
- Empirical models
  - Correlate to temperature
  - Were fit to data with considerable scatter
- A mechanistic multiscale modeling framework is being developed

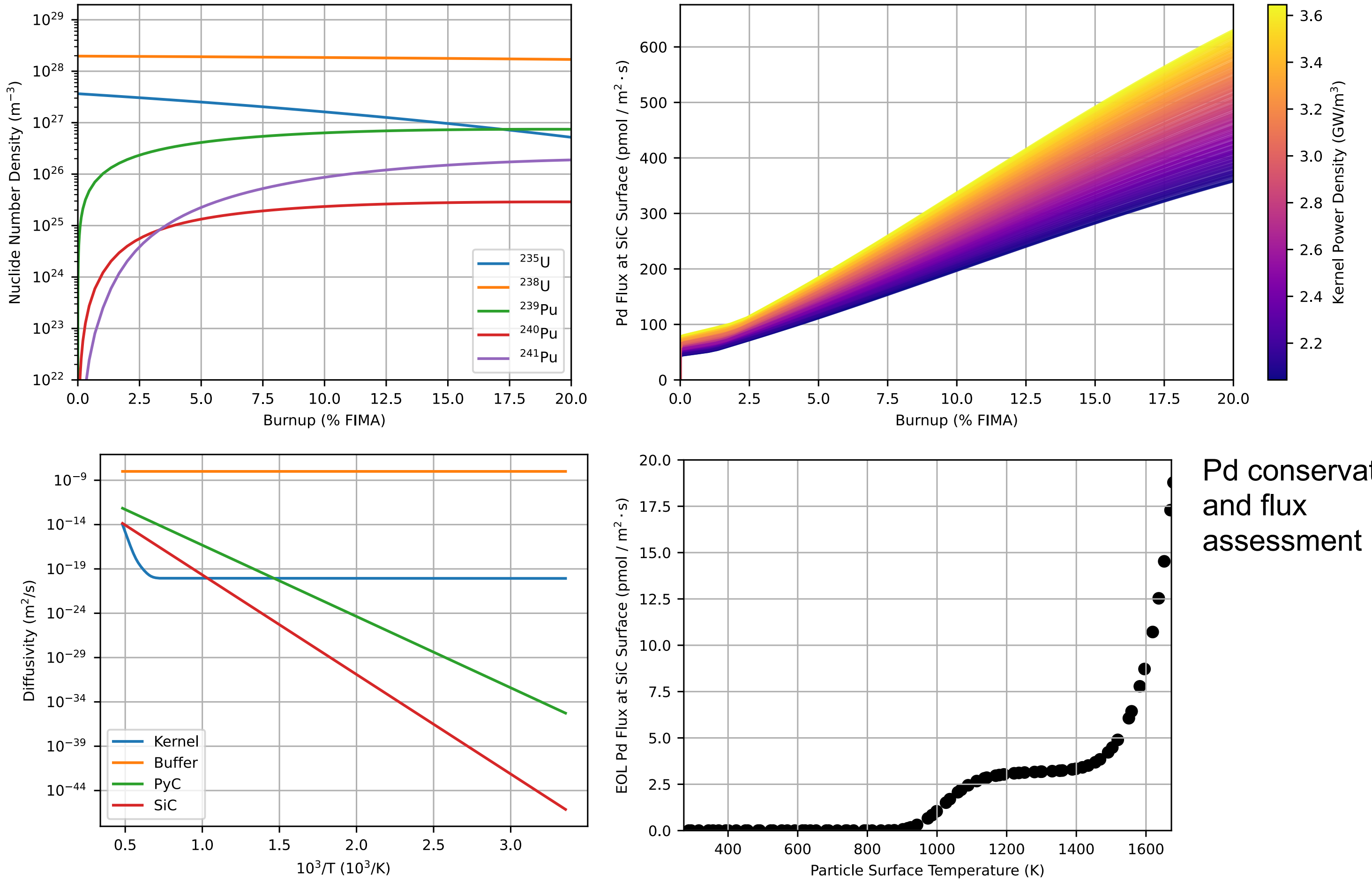



J. Hirschhorn, et al. INL/RPT-24-80567.

# Pd and transport assessment (INL/RPT-24-80567)

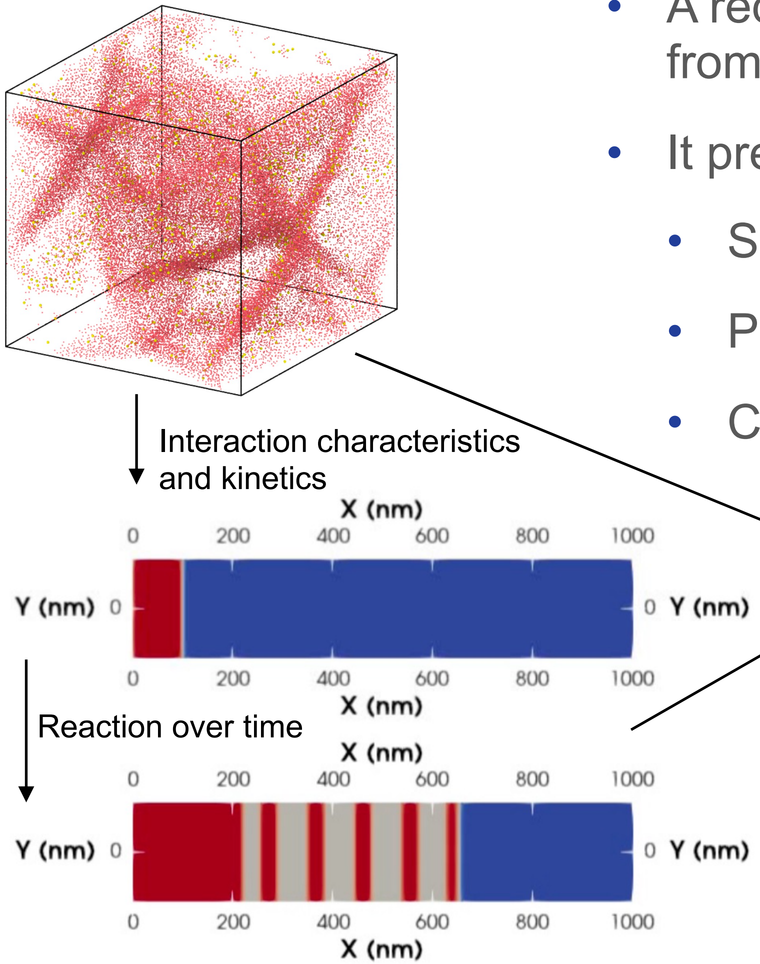
- Developed a fuel burnout- and breeding-dependent Pd source term
- Developed a Pd conservation framework using diffusivities from LANL and the literature to model Pd transport, production, and loss
- Assessed Pd fluxes at the SiC surface for a range of particle designs and operating conditions
- The results were used to inform lower-length scale model development




Pd conservation and flux assessment

# *Mechanistic LLS-informed Pd modeling (INL/RPT-24-80441)*

- Molecular dynamics analyses of polycrystalline SiC were conducted to assess
  - Potential energies associated with Pd in various microstructural positions
  - Corresponding diffusivities
- A phase-field model was developed to predict formation of Pd silicides using the
  - Pd flux assessed at the engineering scale
  - Properties assessed at the atomistic scale




Simulation results demonstrate that interaction microstructure (lamellar versus precipitates) depends on the spatial heterogeneity of the applied mass flux

- A reduced order model (ROM) was developed from the phase-field model for use in BISON
- It predicts Pd penetration as a function of
  - SiC grain structure
  - Pd and SiC reactant kinetics
  - Change in Pd flux with penetration depth

$$P_{Pd}(t) = \sqrt[3]{\frac{18V_m f r_{SiC}^2}{\pi}\int_{t=0}^{t} J_{Pd}(t)dt + r_{SiC}^3} - r_{SiC},$$

Incorporates the thermodynamics of Pd silicide formation to describe the depth of interaction region as a function of mass flux

$$f = \frac{m_i D_{Pd}^{GB}}{2d_{GB}D_{Pd}^{GB} + (m_i - 2d_{GB})D_{Pd}^{bulk}}.$$

Accounts for microstructural and geometric effects

C. Bhave, et al. INL/RPT-24-80441.

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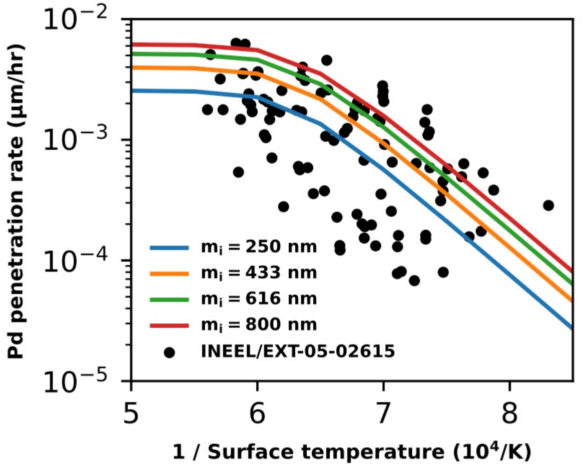
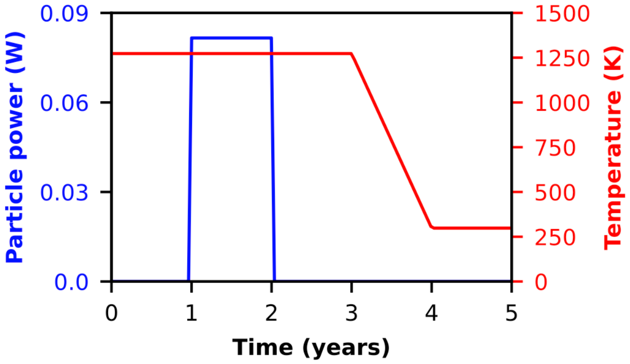
# Mechanistic LLS-informed Pd modeling (INL/RPT-24-80441)

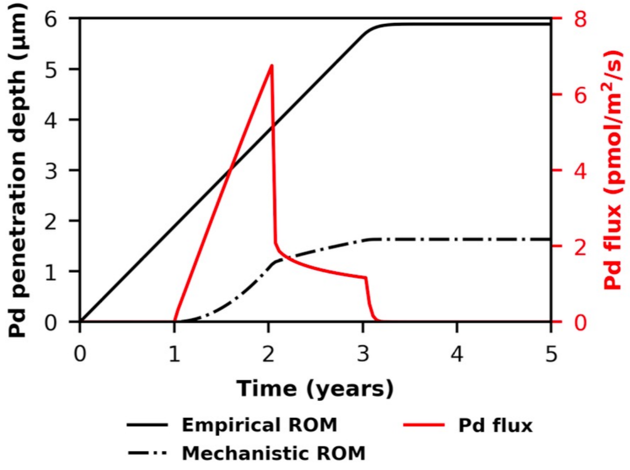
- Preliminary demonstration and validation exercises exhibit the expected behaviors
  - The ROM predicts reasonable Pd penetration rates and suggests possible explanations for the data scatter
  - The ROM offers improves performance over the empirical correlation for time-varying operating conditions due to its sensitivity to Pd inventory and mass flux
- FY25 work will focus on
  - Investigating the impacts of Ag on Pd–SiC thermodynamics and kinetics
  - Refining the phase-field model and the associated BISON ROM
  - Validating the models to legacy data and quantifying uncertainties

Comparison to legacy experimental data



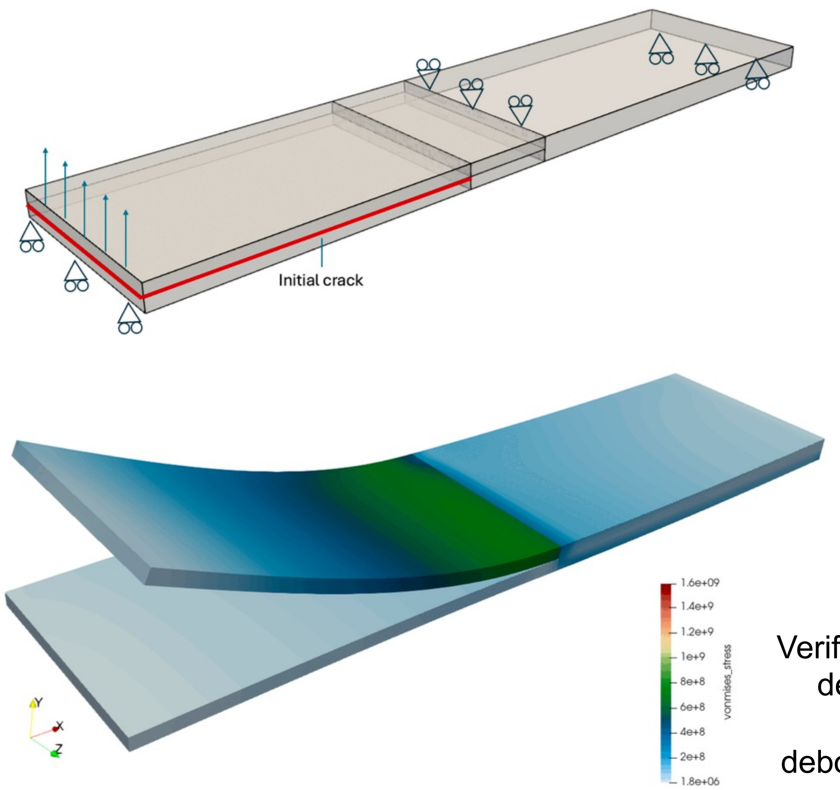



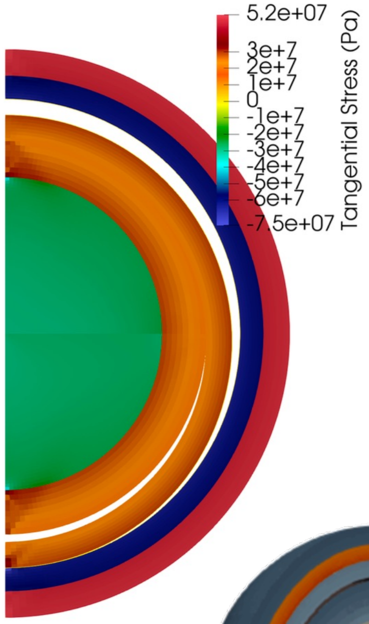

Realistic dependencies on particle Pd inventory and temperature



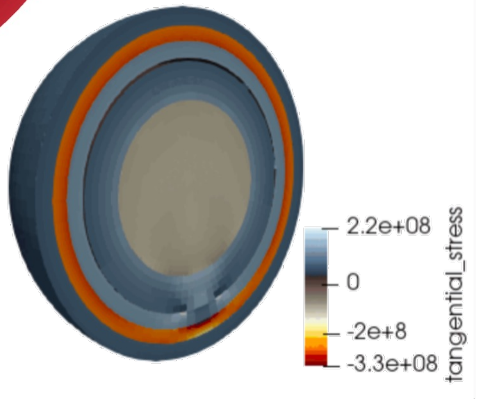
# *Mortar cohesive zone debonding modeling (INL/RPT-24-78711)*

- A preliminary mortar formulation for cohesive zone modeling was developed, implemented, and demonstrated
- The model improves the robustness and accuracy of TRISO debonding calculations, enabling more realistic simulations of
  - Asymmetric particle temperature distributions due to partial debonding
  - Fission product transport
  - Cascading multiphysics failure behaviors



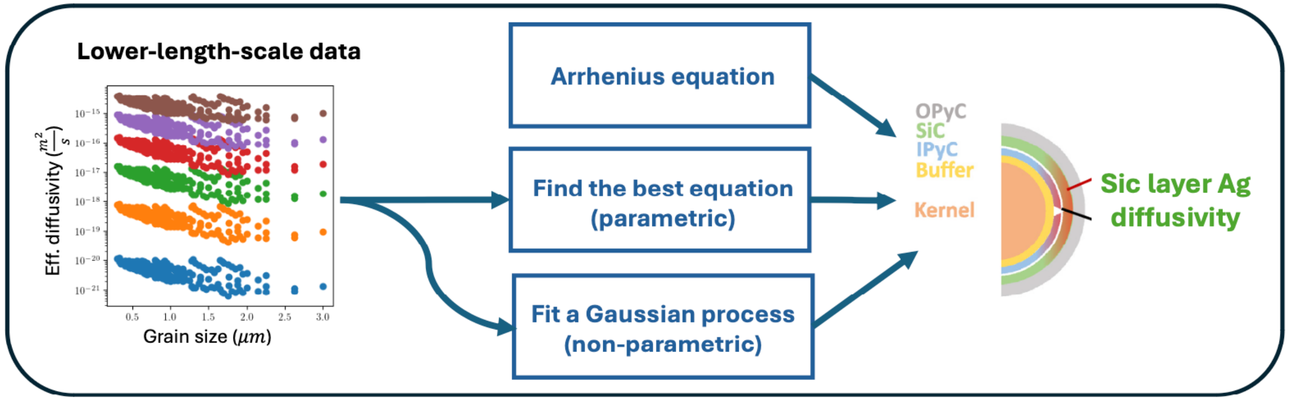




Verification exercises demonstrate more realistic partial debonding behaviors



# *Bayesian analysis of model inadequacy (INL/RPT-24-79964)*

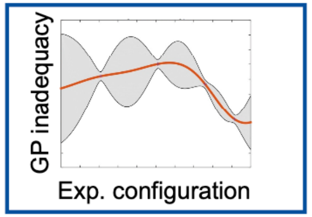
- Parametric and non-parametric methods for incorporating LLS-informed TRISO models into BISON were assessed against empirical Ag diffusivities
- A new Bayesian framework was developed, implemented, and applied to AGR-1. AGR-2. and AGR-3/4 data and assessments, allowing quantification of uncertainties associated with
    - Model inadequacy (including physics and operating conditions)
    - Model parameters
    - Experimental noise



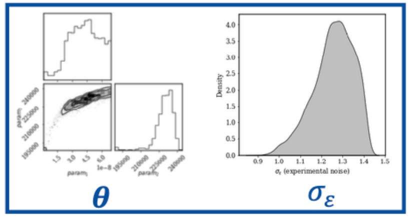

**Module 1**
Best estimate of the model parameters $\boldsymbol{\theta}$

Standard Bayesian calibration
or
Deterministic optimization

**Module 2**
GP inadequacy term hyper-parameters $\boldsymbol{\gamma}_{\delta}$

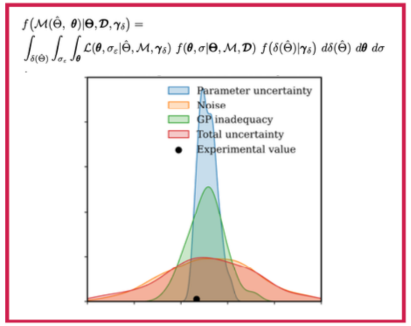



**Module 3**
Inverse UQ of $\{\boldsymbol{\theta}, \sigma_{\varepsilon}\}$




Bootstrapping the experimental data into two batches for fitting the GP inadequacy term and performing inverse UQ. Associated sensitivity analyses.

**Module 4**
Posterior predictive distribution




Uncertainty contributions can be applied to identify high-priority improvements

S. Dhulipala, et al. INL/RPT-24-79964.

# FY24 engagement and broader impacts

DOE programs

- Advanced Reactor Technologies
  - Supported development of multi-scale simulations for TRISO transient fuel performance and experiment design/interpretation
- Advanced Gas Reactor
  - Supported development of preliminary nuclide-specific fission product source terms with Griffin
  - Supported development of multi-scale simulations for AGR-3/4 re-irradiation experiments

Industry and academia

- Delivered BISON trainings
  - For general audiences in a university setting
  - Directly to industry partners
- Participated in various direct industry collaborations
  - Provided continuing routine and on-demand support
  - Literature review and BISON upkeep
  - VTB upkeep
- FY24 journal articles to date: 1 published, 2 in preparation/review

# Overview of FY25 activities

Engineering scale

- Implement user-friendly mortar debonding models for TRISO coating layers using Advanced Gas Reactor Program material property data and apply uncertainty quantification to begin to assess model adequacy and data needs
- Update and refine TRISO assessment input files to better represent recent developments and to be consistent for TRISO simulations
- Develop assessments for particle fuel transient experiments and separate effects tests
- Begin to assess thermal, mass, and particle-particle stress interactions at the compact scale to provide guidance for follow-on work focused on matrix performance

Lower-length scale

- Investigate high-temperature Pd-Ag-SiC interaction mechanisms using molecular dynamics and incorporate them into the Pd penetration phase-field model
- Complete expansion of the existing multiscale low-temperature Pd penetration model to account for high temperatures and Ag interactions, validate models against experimental data, and quantify uncertainties associated with its predictions

# FY26 and beyond

- Near-term NEAMS Fuels TRISO priorities
  - **Demonstrate the ability to model observed failure behaviors** by validating Pd penetration models to AGR and separate effects data and incorporating them into failure probability calculations
  - **Bolster the existing BISON validation database** by developing and extending assessments for steady-state, transient, and separate effects experiments
  - **Support qualification, licensing, and further development** through broad and systematic application of uncertainty quantification
  - **Increase prediction accuracy** by investing in material property and behavioral model development for pyrolytic carbon, SiC, and UCO
- We are here for you, and we need your feedback
- Questions and comments: Jacob.Hirschhorn@inl.gov

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