

NEAMS fuels modeling for fast reactors: FY24 accomplishments and outlook for FY25

Presenters: Christopher (Topher) Matthews, Jacob Hirschhorn, and Yinbin Miao



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Nitride Fuels Modeling Overview

Presenter: Christopher (Topher) Matthews

Contributors: Anton Schneider, P.C. Simon, Michael Cooper,



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Uranium Nitride: Recent Accomplishments

- Developed first-of-a-kind mechanistic model for UN fission gas release and swelling
 - Revived dislocation model in BISON
 - Adapted lower-length scale UN parameters
- Quantitatively capturing swelling behavior in UN
- Expanded assessment data base and high burnup extension forthcoming in FY25

Uranium nitride capable BISON ready for external users







Contents lists available at [ScienceDirect](https://www.sciencedirect.com)

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

Mechanistic nuclear fuel performance modeling of uranium nitride

Jason T. Rizk^{a, }, Michael W.D. Cooper^a, Pierre-Clément A. Simon^{b, }, Anton J. Schneider^a,
David A. Andersson^a, Stephen R. Novascone^{b, }, Christopher Matthews^{a, },*

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^b Computational Mechanics and Materials Department, Idaho National Laboratory, Idaho Falls, ID 83415, USA



Continuing work focused on 1) chemistry dependence, 2) porosity dependence, and 3) application to TRISO

Lower Length Scale (DFT & EP)

- Defect stability and kinetics
 - U_i, V_U
 - N_i, V_N
 - $\{2U_i\}$
 - $\{Xe:2V_U\}$
 - etc.

• Defect stability & mobility

Meso-Scale (Centipede)

- Free Energy Cluster Dynamics (FECD)
 - Defect concentrations (irradiation-enhanced)
 - Self-diffusivity
 - Gas atom diffusivity
 - Defect clusters
 - Perfect interstitial dislocation loops
- Sensitivity to temperature, chemistry, and irradiation

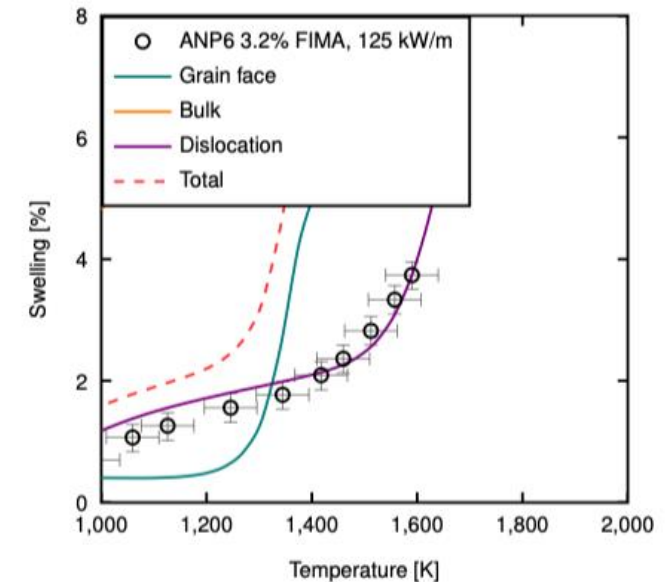
CALPHAD
calculations

• Sink strength

Engineering-Scale (BISON)

- SIFGRS: Fission Gas Model
 - Fission gas concentration
 - Bubble formation and growth
 - Collection along dislocations and grain boundaries
 - Fission gas release
 - Swelling

~3% FIMA



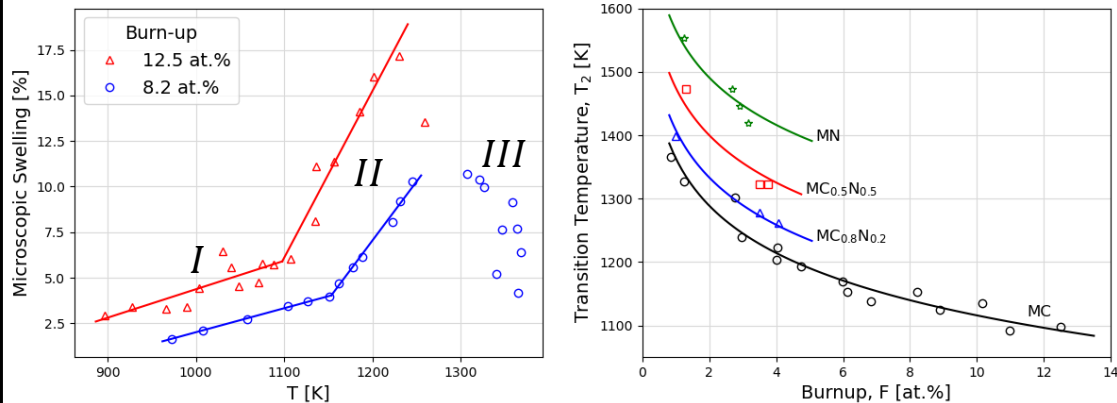
energy

UN Modeling Approach: Capture breakaway swelling first

Mechanistic modeling allowed for
mechanism not to be picked a priori

Experimental observation: “Breakaway Swelling”

- Sudden change in the rate that microscopic swelling increases with temperature once a threshold temperature is reached (Region *I* → *II*)
- Greater burn-up causes lower transition temperatures



Microscopic swelling in MC

The transition temperature (*I* → *II*) for breakaway swelling in MCN fuel

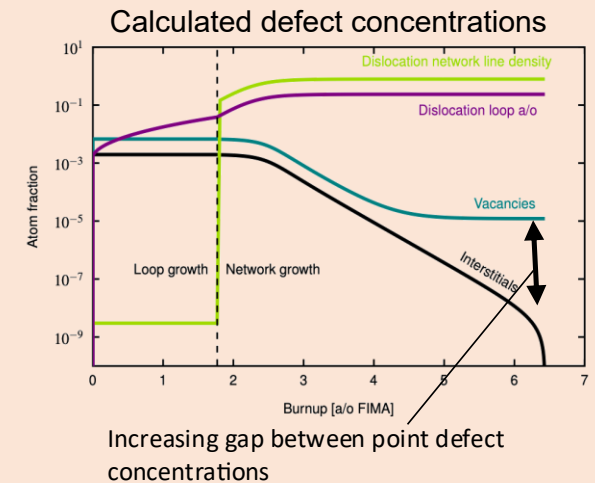
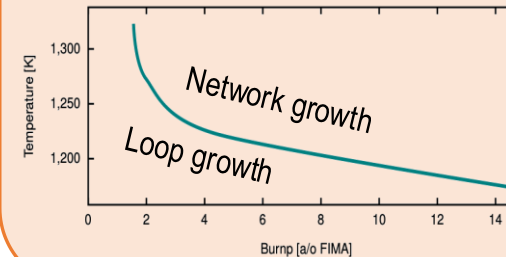
- Region *II* associated with both larger intra- and inter-granular bubbles
- Third region (*III*) of decreased swelling after a greater threshold temperature
 - Large interconnected grain boundary bubbles
 - Release of gas from grain interior into porosity

**Need to understand this phenomenon for
mechanistic fuel performance model**

Mechanism(s) responsible for the transition?

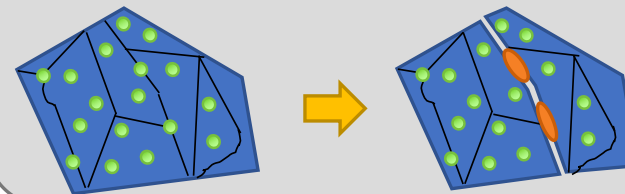
Extended defects consume point defects?

- The dislocation network more efficiently traps interstitials
- Vacancies trap at bubbles instead of annihilating through recombination

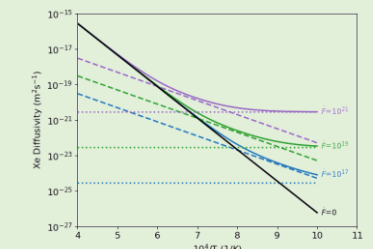


Recrystallization?

- The accumulation of extended defects makes it energetically favorable to form new grain boundaries
- Grain boundaries trap gas atoms and grow larger bubbles



Diffusion mechanism transition?



Modeling plan:

- Start with UO_2
- Adapt for UN

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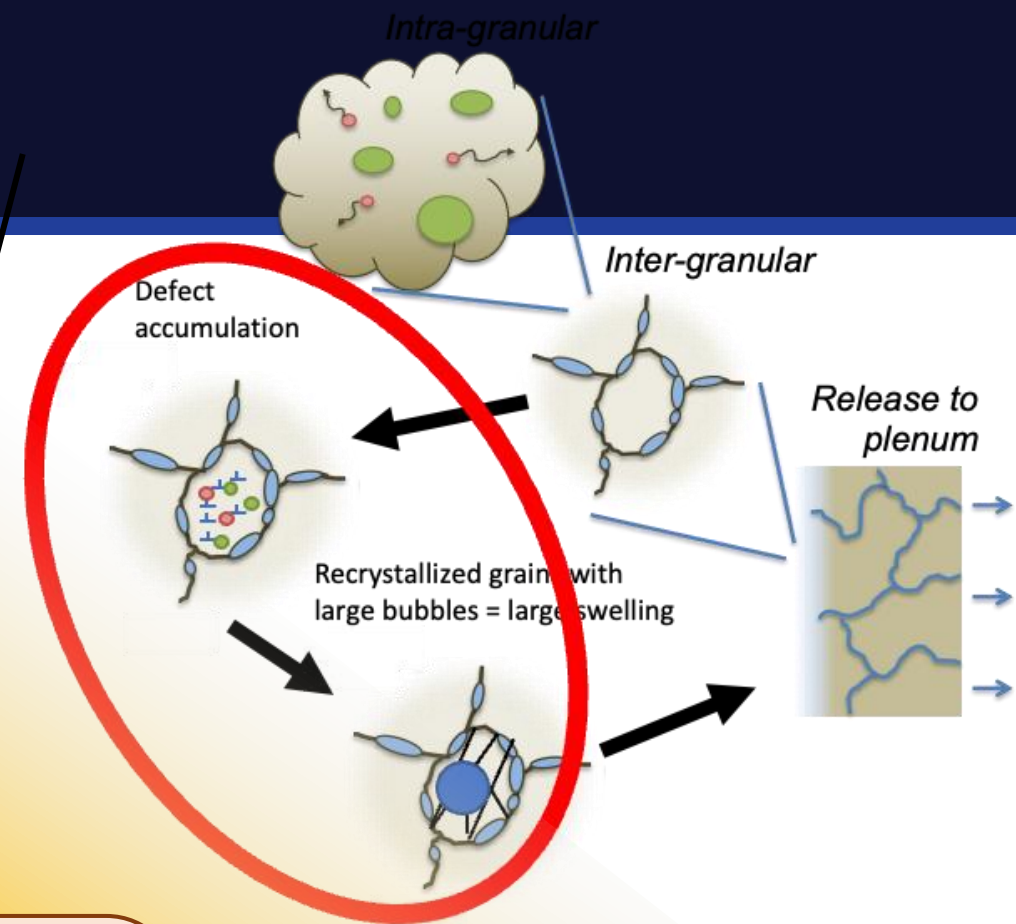
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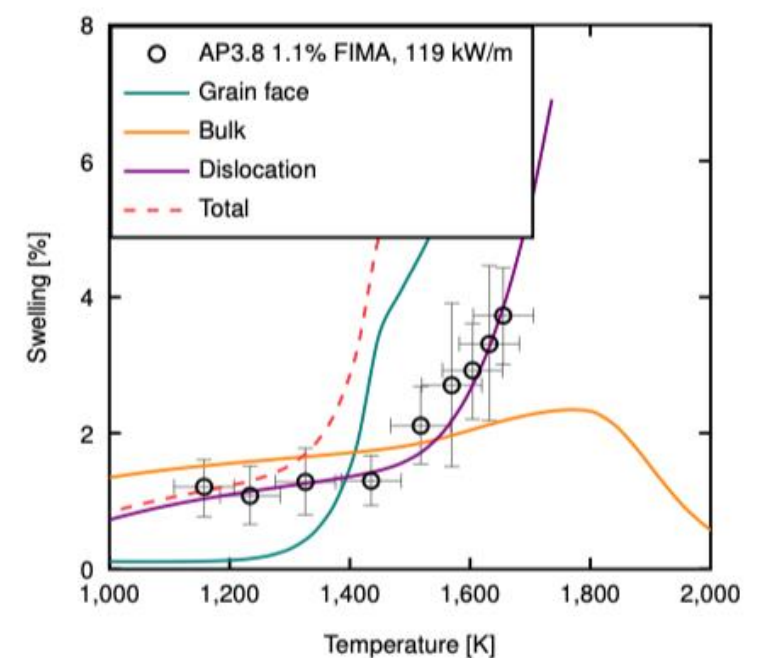
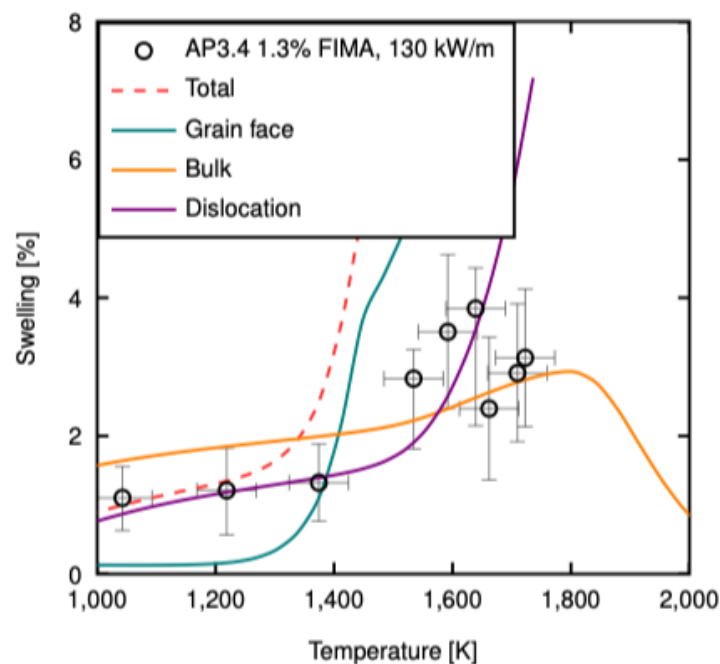
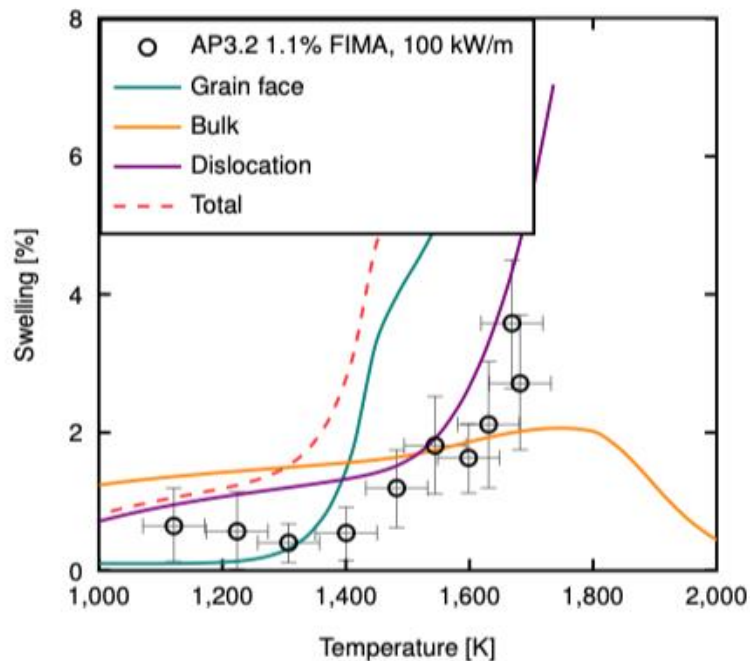
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Mechanistic Model Results

- Quantitative Comparison to data with (almost) no calibration
- Upturn corresponds to self-diffusivity
- Constant dislocation density

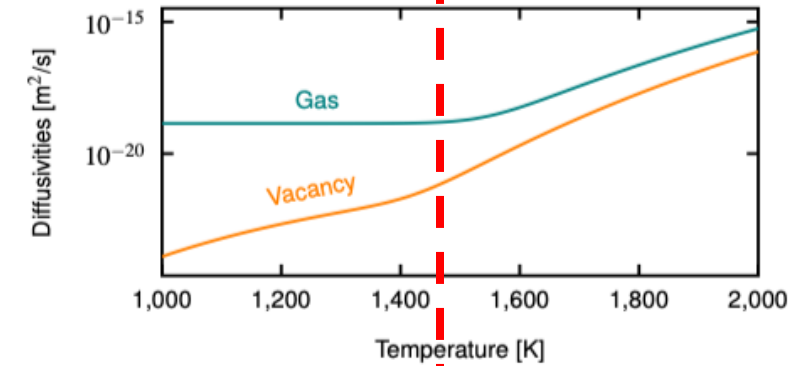
~1% FIMA



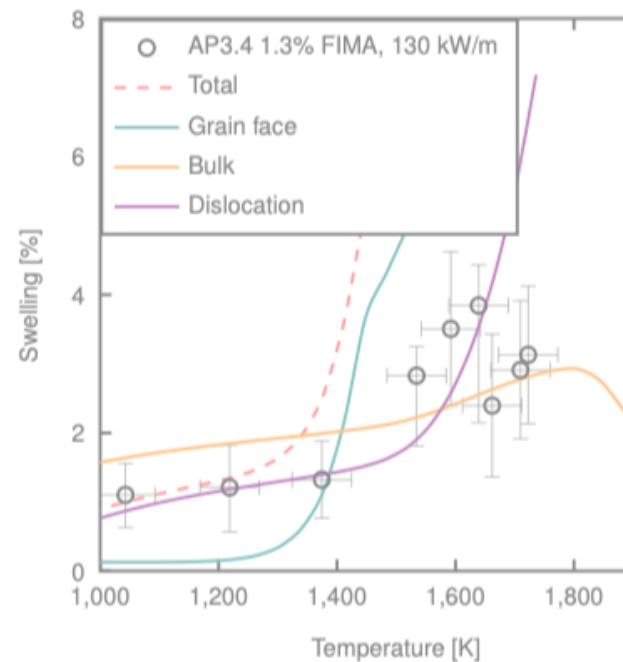
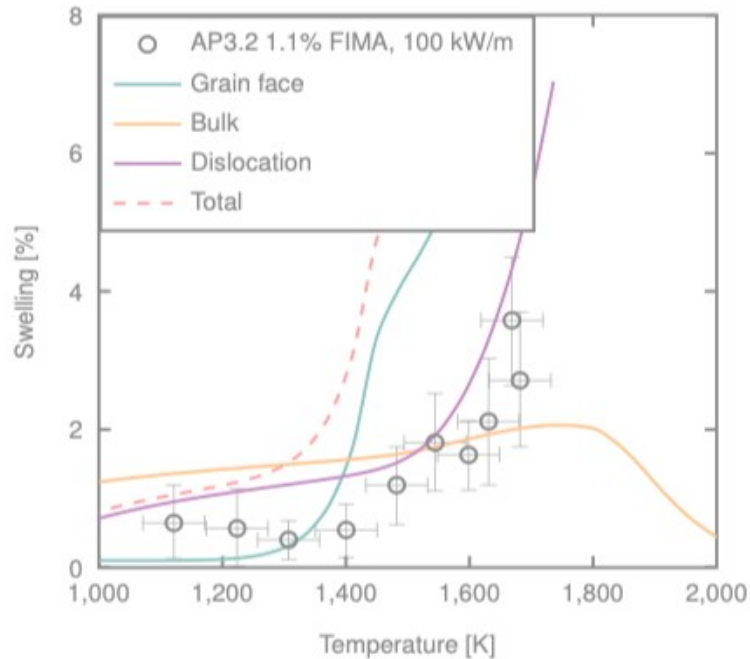
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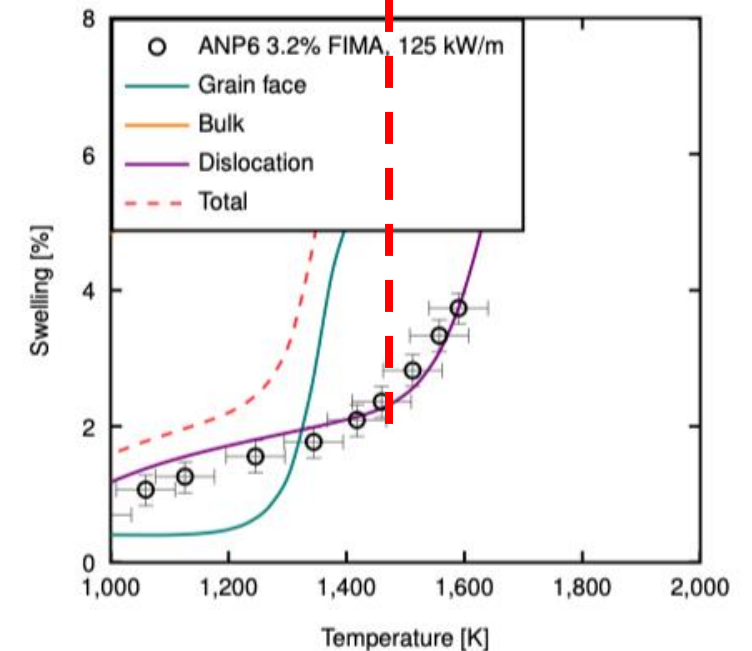
Diffusivities



~1% FIMA



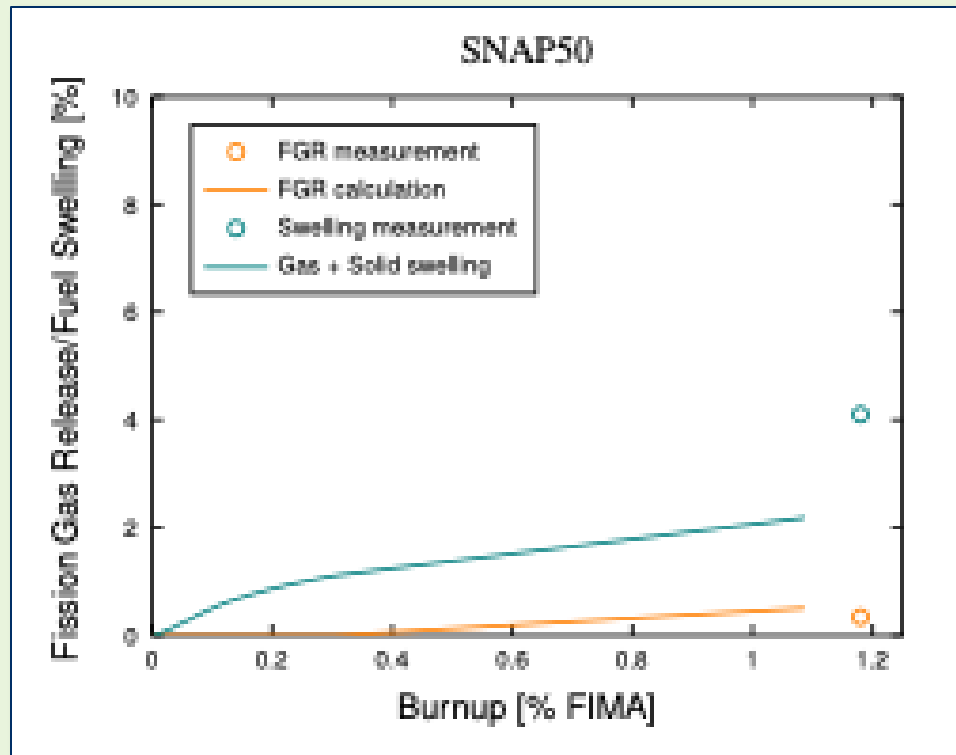
~3% FIMA



Integral experiments: Combined assessments with same parameters

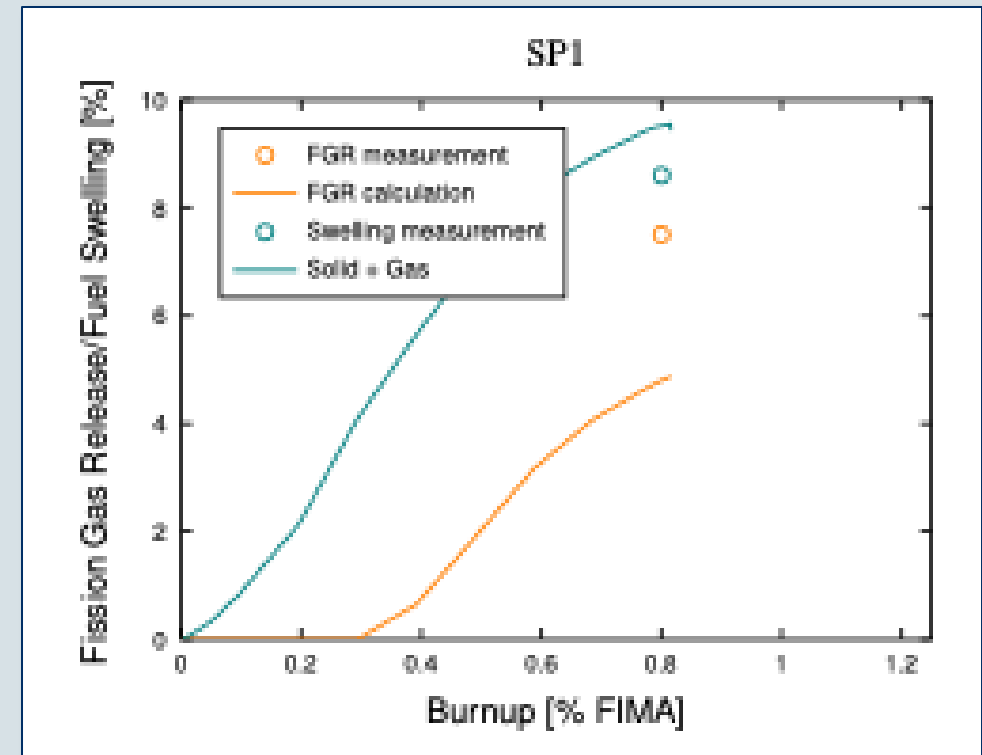
SNAP50-57-672 (MTR)

- Model with best historical data
- Temperatures [K]: 1430, 1500 (avg, max)
- Fsnrates [fsn/m³/s]: 1-1.5x10¹⁹ (avg, max)



SP1 (EBR-II)

- Model with best historical data
- Temperatures [K]: 1800, 2050 (avg, max)
- Fsnrates [fsn/m³/s]: 3-3.3x10¹⁹ (avg, max)



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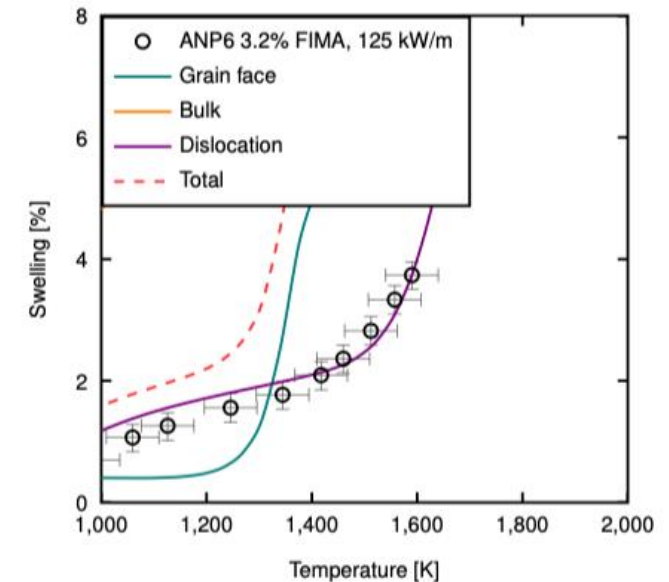
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energy

Metallic Fuels Capabilities Overview

Presenter: Christopher (Topher) Matthews

Contributors: Michael Cooper, Anton Schneider, P.C. Simon, Jacob Hirschhorn, Larry Aagesen, Yinbin Miao, Latif Yacout



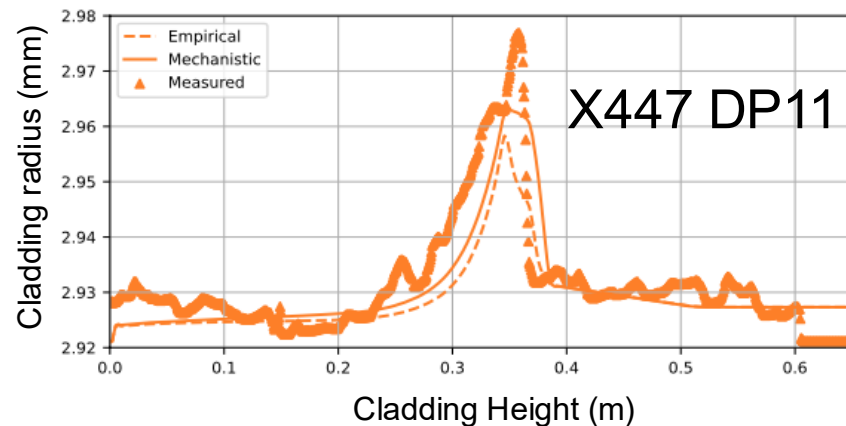
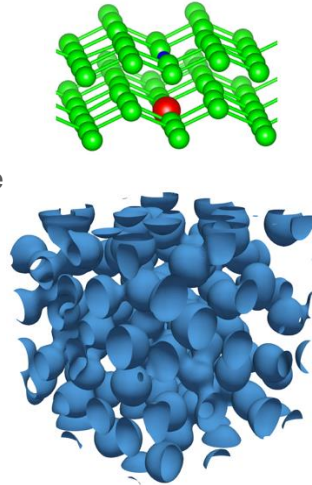
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Metallic fuel Highlights (1/2)

FCCI

- FY24: Developed mechanistic model for FCCI in U-Zr fuel
- Performed multi-scale calculations to determine effective lanthanide diffusivity
- BISON model for lanthanide production, transport, wastage layer growth
- Predictions agree well with X447, MFF-3
- Readily extensible to new fuel designs (annular, lined cladding)
- FY24: model for liquefaction risk on fuel side due to Fe diffusion from cladding to fuel



Baseline capabilities

- Metallic fuel baseline capabilities established
- Developed new correlations, models, physics
- VTB example forthcoming

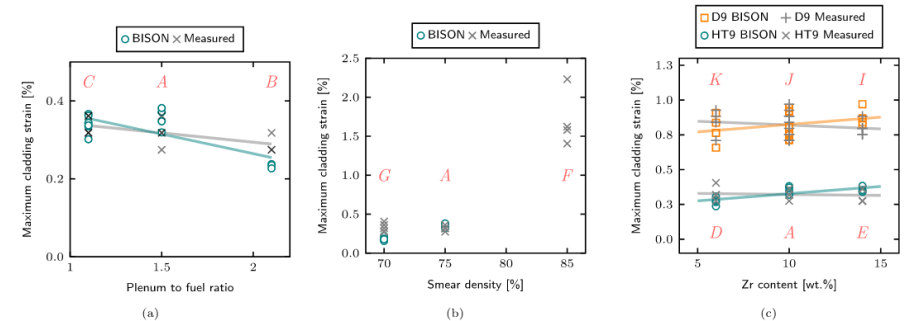
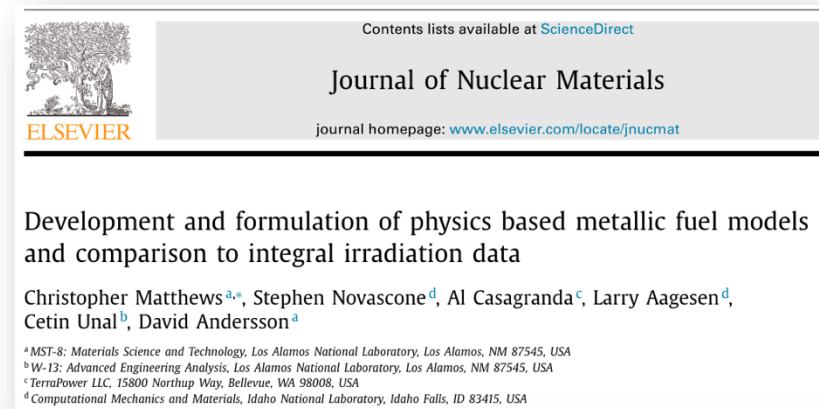


Fig. 9. Comparison between BISON results and EBR-II experimental data of cladding strain vs. a) plenum to fuel ratio with HT9 cladding, b) smear density with HT9 cladding, c) zirconium content [wt. %] with HT9 cladding, and d) zirconium content [wt. %] with D9 cladding.

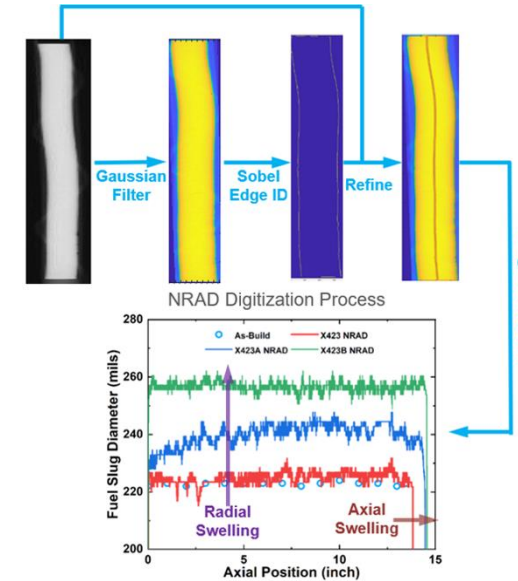
Metallic fuel Highlights (2/2)

FIPD/OPTD Powered Metal Fuel Assessments

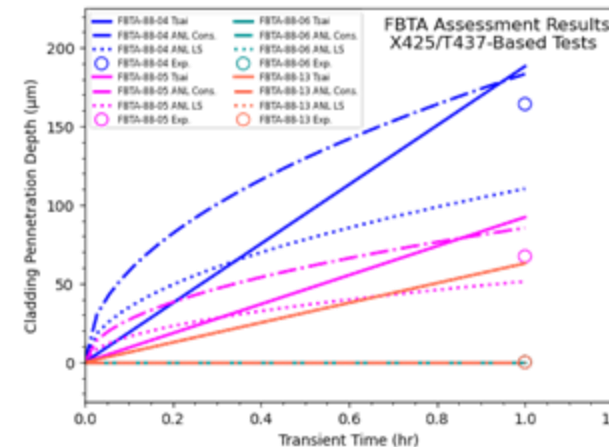
- **FIPD-BISON/OPTD-BISON Integration**
 - Data repository as a BISON submodule
- **Steady-State EBR-II Irradiation**
 - Established X423 Assessment
 - Focus: low-burnup fuel swelling
 - Powerful tools for swelling model V&V
 - Enhanced the Existing X447 Assessment
 - Focus: FCCI/cladding degradation
 - Advanced models adopted for improved predictions
- **Out-of-Pile Tests on EBR-II Irradiated Pins**
 - FBTA Assessment Case
 - 4 tests based on one fuel pin (X425/T418)
 - Improved empirical eutectic penetration correlations
 - WPF Assessment Case
 - 1 test (FM-1) based on one whole X425/T437 pin
 - Run till cladding breach at high temperature

FY2023 Publications

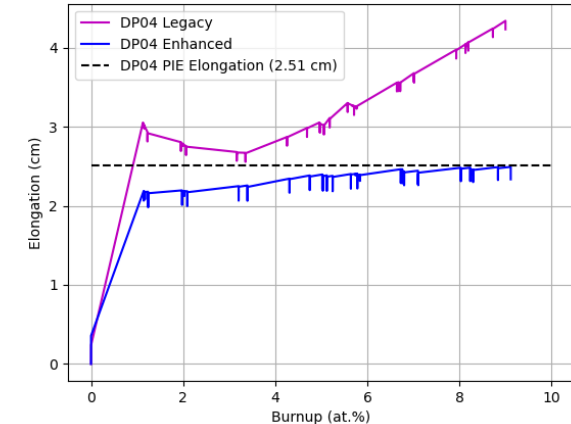
- [1] Miao, Yinbin, et al. "BISON-FIPD integration enhanced low-burnup SFR metallic fuel swelling model evaluation framework." Nuclear Engineering & Design 414 (2023): 112611.
- [2] Shu, Shipeng, et al. "Improved correlations of the fuel/cladding liquid penetration rate with the out-of-pile transient database." Nuclear Engineering & Design 417 (2024): 112819.
- [3] Technical Report ANL-NEAMS-23/6
- [4] Technical Report ANL-NEAMS-23/7



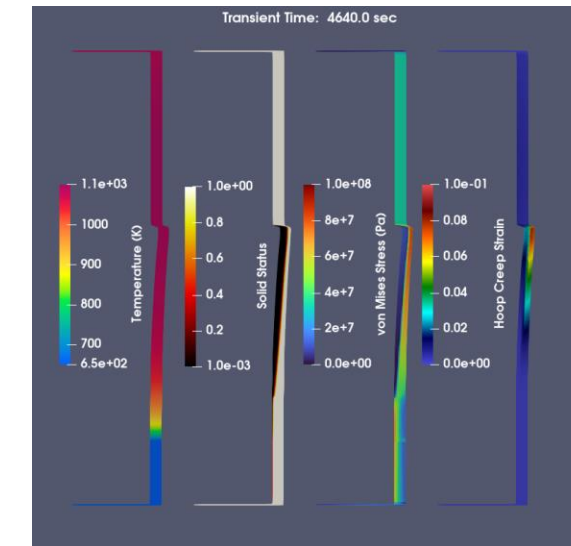
Use of NRAD data for swelling model assessment (X423)



Cladding eutectic penetration kinetics (FBTA)



Improved fuel axial growth prediction (X447 enhancement)



Transient cladding penetration & deformation (WPF FM-1)

BISON Metallic Fuel Model Validation

Historical Database Implementation with FIPD & OPTD

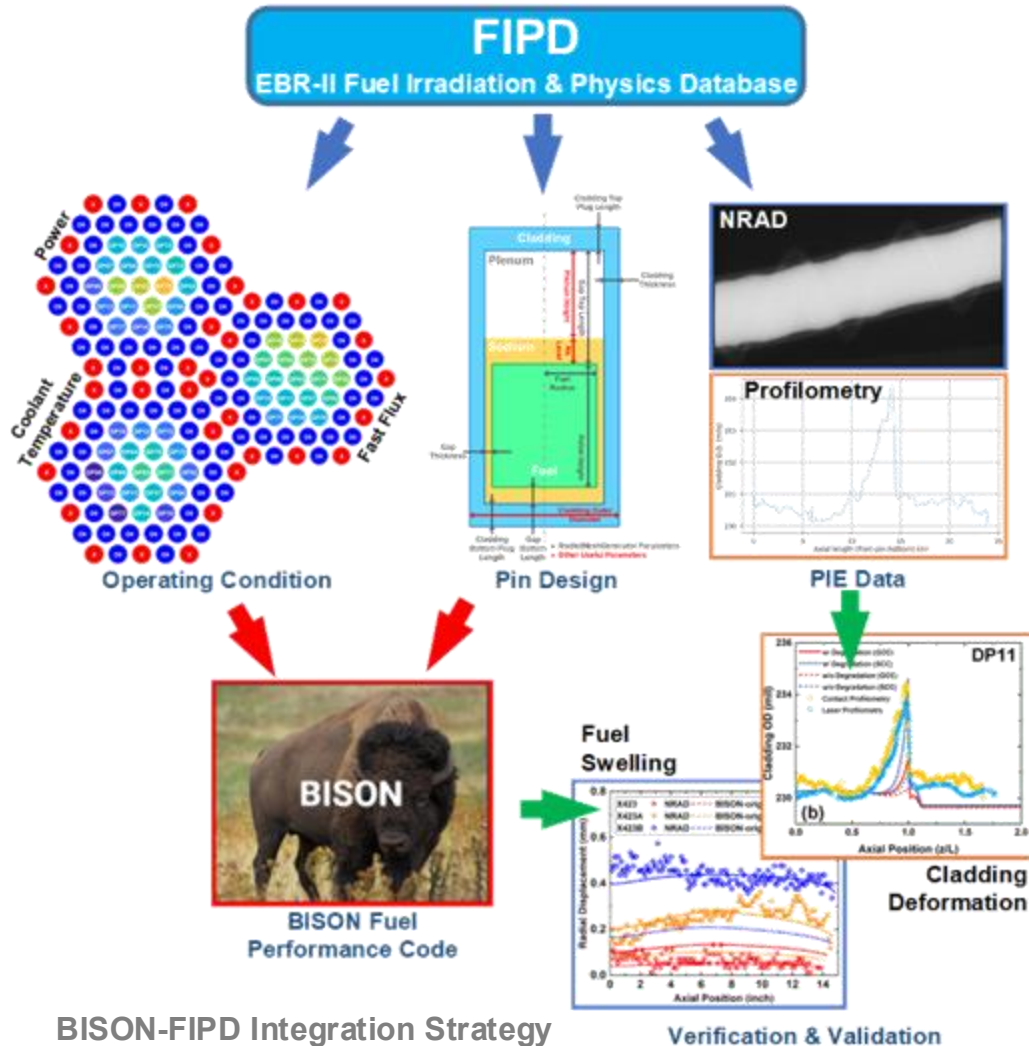
Yinbin Miao, Aaron Oaks, Shipeng Shu, Abdellatif Yacout

Argonne National Laboratory

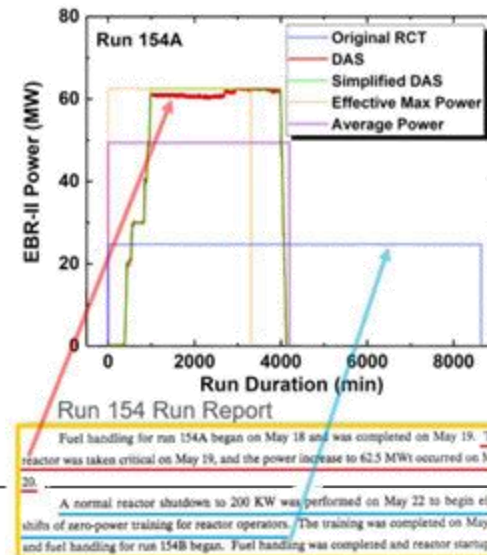
May 29, 2025

NEAMS Annual Review: Fast Reactor (Virtual)

BISON-FIPD Integration



- **V&V BISON's Metal Fuel Capabilities** by Leveraging Legacy EBR-II Database w/ QA
 - **FIPD[†]**: steady-state in-pile irradiation experiments
 - Model implementation
 - Implement legacy descriptive fuel correlations.
 - Complement/validate adv. mechanistic models
 - BISON-FIPD integration tools to facilitate data usage
 - **BISON-FIPD Integration Powered Assessment Cases**

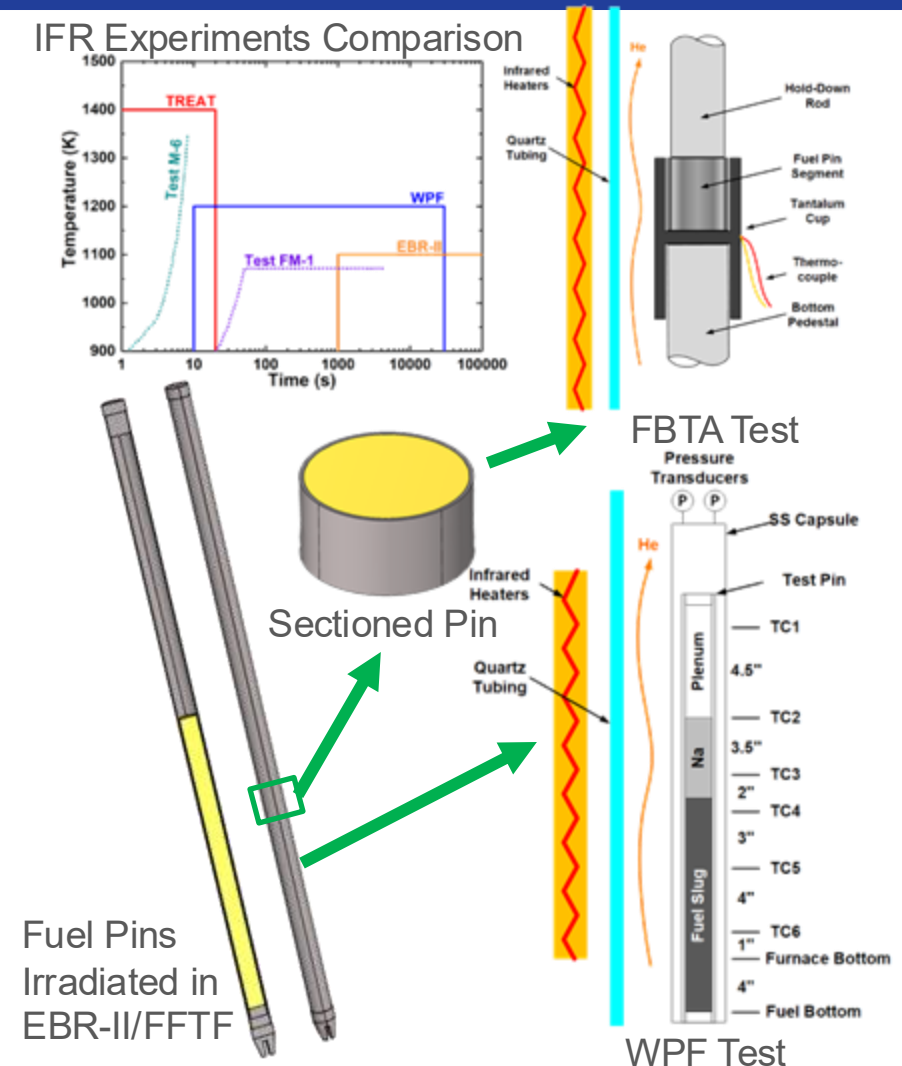
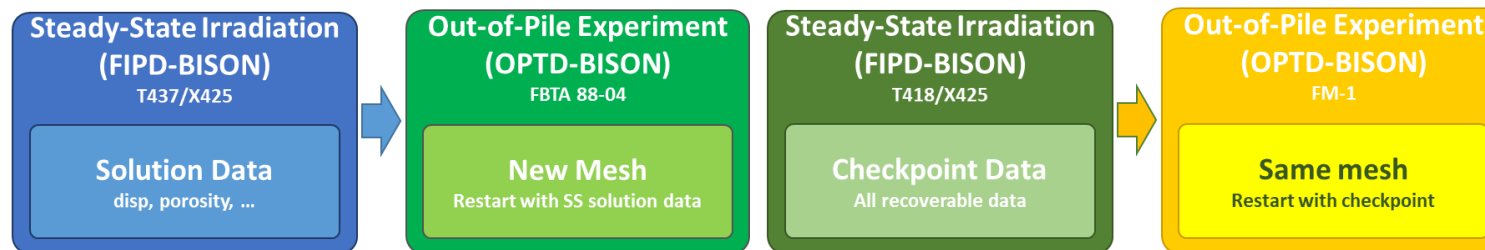


FIPD QA Being Performed Following NRC Approved QAPP

[†]FIPD (Metallic Fuels Irradiation & Physics Database) is supported by US DOE-NE's Advanced Reactor Technologies (ART) Fast Reactor Program (FRP) and NE-4 Advanced Fuels Campaign (AFC).

BISON-OPTD Integration

- Assessment Using OPTD[†] Database
 - Out-of-pile Transient Experiments
 - Fill gap between TREAT (M-series) & EBR-II tests
 - Models can be used by them in the future
 - FBTA and WPF (FM-series)
 - Use BISON-FIPD for steady-state
 - Initial conditions for out-of-pile transient cases
 - Use BISON-OPTD for transient
 - Implement models to cover all essential physics
 - Create assessment case for V&V
 - 4 FBTA tests & WPF-1



[†]OPTD (Out-of-Pile Transient Database) is supported by US DOE-NE's Advanced Reactor Technologies (ART) Fast Reactor Program (FRP).

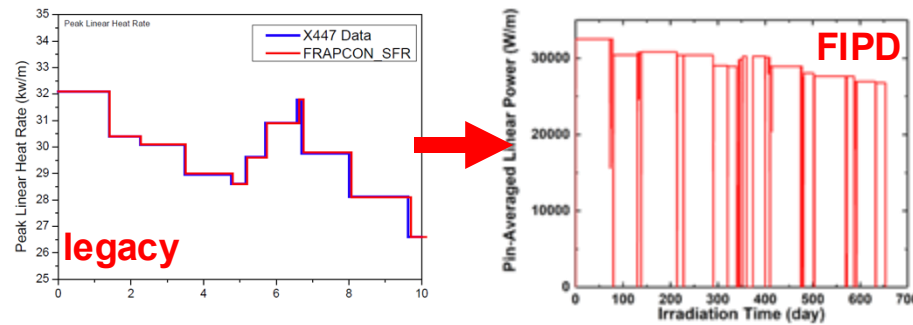
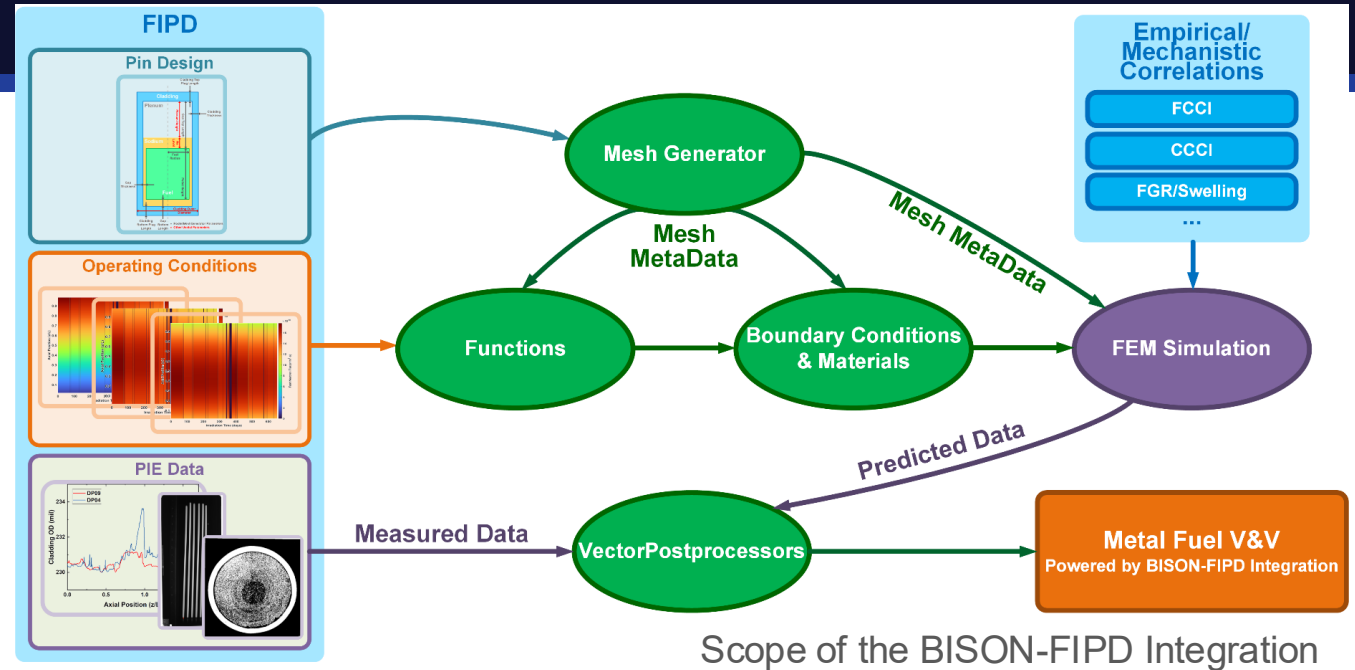
Databases Integration Framework

- FIPD Integration Objects in BISON

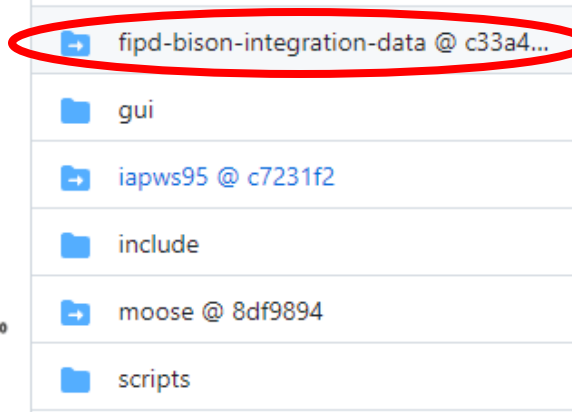
- Mesh Generation
- Irradiation Conditions
- PIE Comparisons

- Data Integration

- Data Submodule of BISON
 - FIPD
 - Pin design parameters
 - Operating conditions
 - NRAD/profilometry,...
 - OPTD
 - Pin information
 - Furnace test conditions
 - Penetration/liquefaction



Detailed Operating Conditions from FIPD



Data Submodule in BISON

Overview: Databases Powered Validation Platforms

- Assessment cases powered by FIPD/OPTD integration
 - Steady State / Normal Operation
 - (EBR-II) X447 → High temperature fuel-cladding compatibility (FCCI) – **FY24 Enhancements**
 - (EBR-II) X423 → Low burnup fuel swelling behavior / “Fat” fuel slugs
 - (EBR-II) X425 → High burnup cladding behavior (FCMI)
 - (EBR-II) X441 → enhance existing important X441 assessment case
 - (EBR-II) X501 → TRU-loaded fuel
 - Potential (Phenix) METAPHIX-Series
 - Out-of-Pile/Furnace Transient
 - (FBTA) 124 Tests → cladding-fuel interface liquefaction in irradiated fuel
 - (WPF) FM-1 → short-term cladding failure at over temperature
 - More FM-Series tests with a focus on long-term demonstration tests
- Prior FYs
- **FY24 Achievements**
- **FY25 Ongoing**
- **Planned**



X447 Assessment Case

[1] Y Miao et al., *Nucl. Eng. Des.*, 385 (2021) 111531

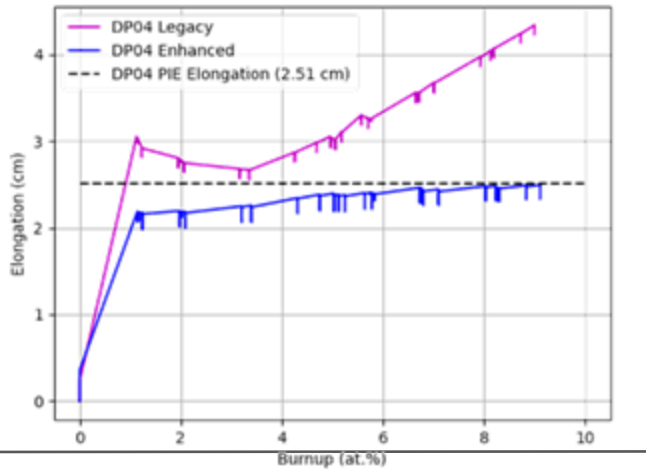
[2] https://mooseframework.inl.gov/bison/metallic_fuel/EBR2/X447/doc/X447.html

[3] https://mooseframework.inl.gov/virtual_test_bed/sfr/eb2_x447_dp11/index.html

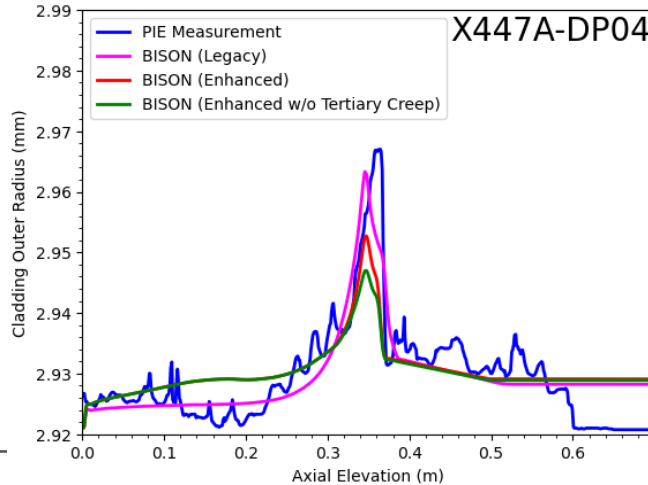
[4] L Aagesen et al., INL/RPT-24-81050 (2024)

Cladding Degradation Model Evaluation

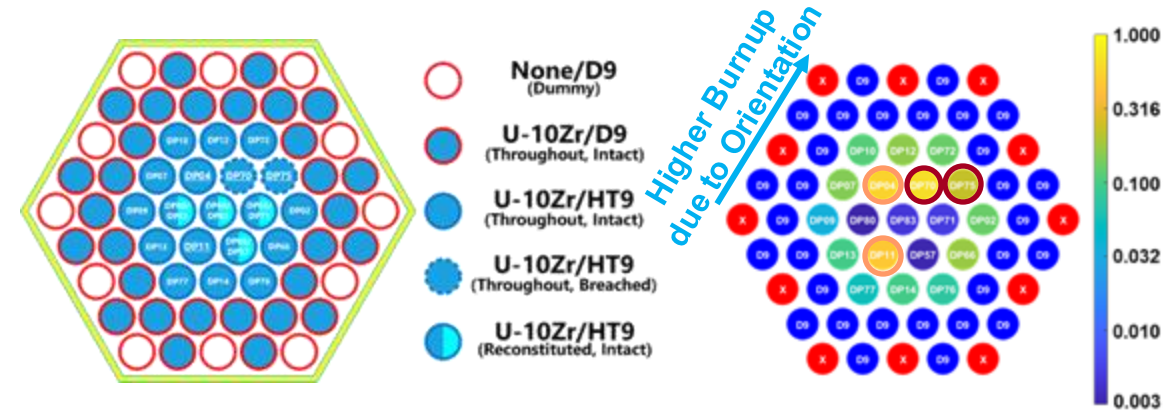
- Integral Fast Reactor Program X447 Experiment
 - U-10Zr/HT9:** 15 pins to 10 at.%; 8 pins to 5 at.%
 - Hi-Temp (>600°C) FCCI found to limit the fuel operating envelope
 - 2 of 15 U-10Zr/HT9 pins irradiated to ~10% BU failed
- Up-to-date modeling approaches including Mortar and AD
- Demonstration of BISON-FIPD Integration
 - More consistent prediction using FIPD-based data
- VTB Demonstration Example (DP11)



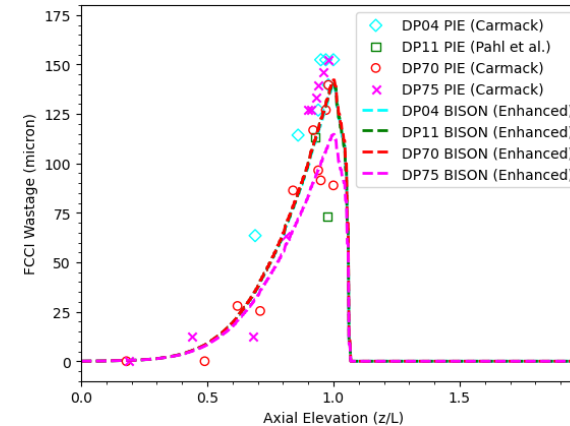
Predicted fuel elongation compared with PIE (DP04).



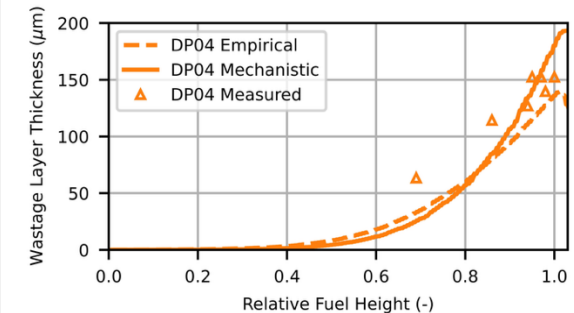
Predicted cladding deformation compared with PIE (DP04).



X447/A Subassembly and CDF predicted for HT9 pins [1]



FCCI Wastage: BISON vs. PIE

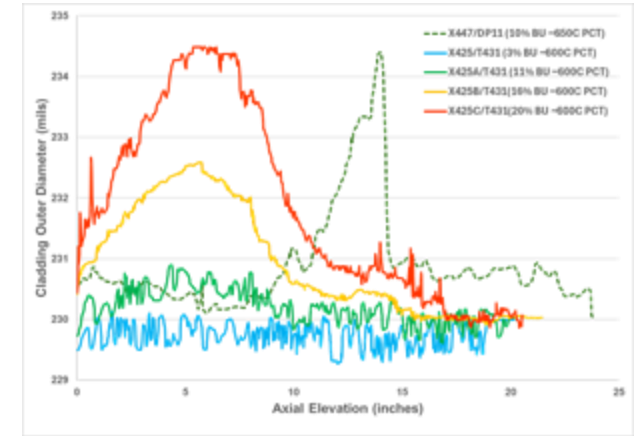


Mechanistic FCCI model validation using the assessment case [4]

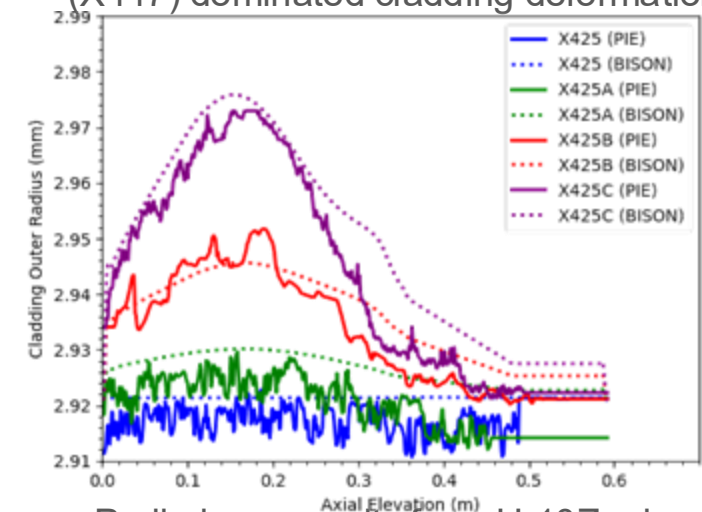


X425 Assessment Case (FY25 Ongoing)

- High-Burnup Behavior (FCMI) Assessment
 - Integral Fast Reactor Program X425 Experiment
 - **U-10Zr-xPu fuel** + HT9 Cladding
 - 17 U-10Zr pins; 11 U-8Pu-10Zr pins; 2 U-19Pu-10Zr pins
 - Reach ~20 at.% burnup
 - Three reconstitution for PIEs
 - Profilometry at ~3 at.%, 10 at.%, 16 at.% and 20 at.% burnup
 - Two main focuses
 - FCMI and cladding deformation
 - Mortar contact model/friction coefficient
 - Fuel hot pressing/cladding creep models (MFH/surrogate models)
 - Fuel axial growth
 - Anisotropy: Pu dependence and difference for “fat” slugs (X423 and X430)
 - Mortar contact model/friction coefficient



Comparison b/t FCMI (X425) and FCCI (X447) dominated cladding deformation



Preliminary results for a U-10Zr pin



TRU Irradiation Experiments (Planned)

[1] M.K. Meyer et al., *J. Nucl. Mater.*, 392 (2008) 176
 [2] L. Capriotti et al., *J. Nucl. Mater.*, 539 (2020) 152279
 [3] H. Ohta et al., *Nucl. Technol.*, 190 (2015) 36

- TRU-Involved Experiments

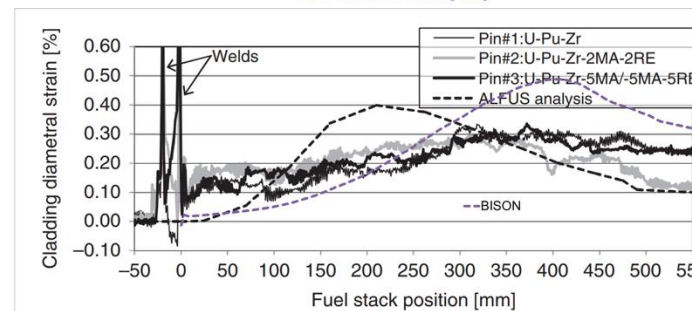
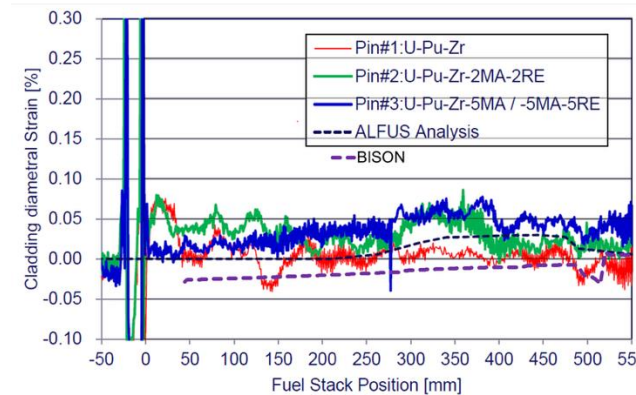
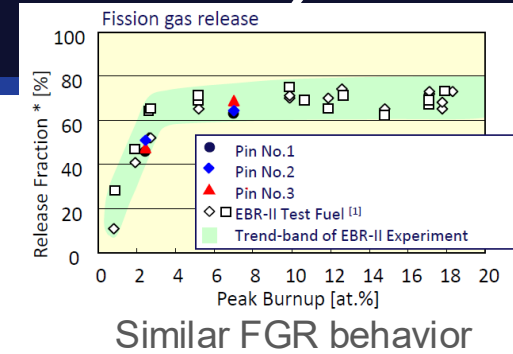
- IFR Experiment X501

- 2 irradiated pins
 - U-20.2Pu-9.1Zr-1.2Am-1.3Np
 - ~7 at.% burnup

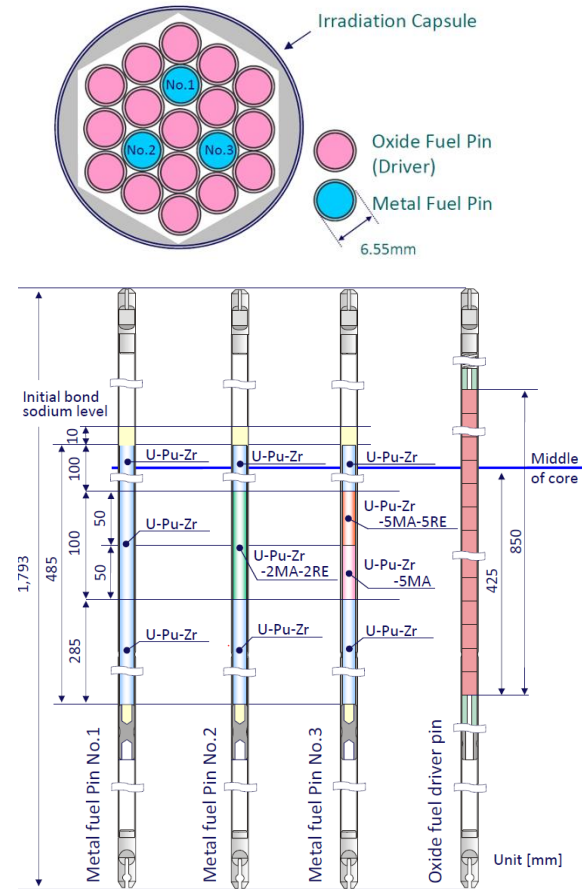
- FIPD-BISON integration

- METAPHIX-Series Experiments

- 3 irradiated pins per capsule
 - U-19Pu-10Zr
 - U-19Pu-10Zr-2MA-2RE/5MA-5RE/5MA
 - 3 capsules → 2.5, 7, and 10 at. % burnup
- BISON simulations (IAEA benchmark)
 - METAPHIX-1 and METAPHIX-2



METAPHIX Cladding Deformation (ALFUS data, courtesy of T. Ogata)



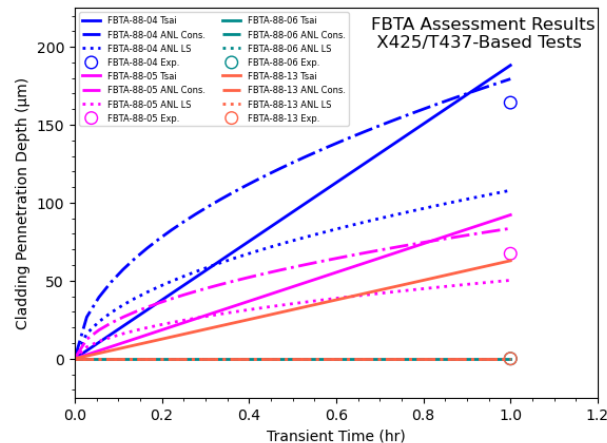
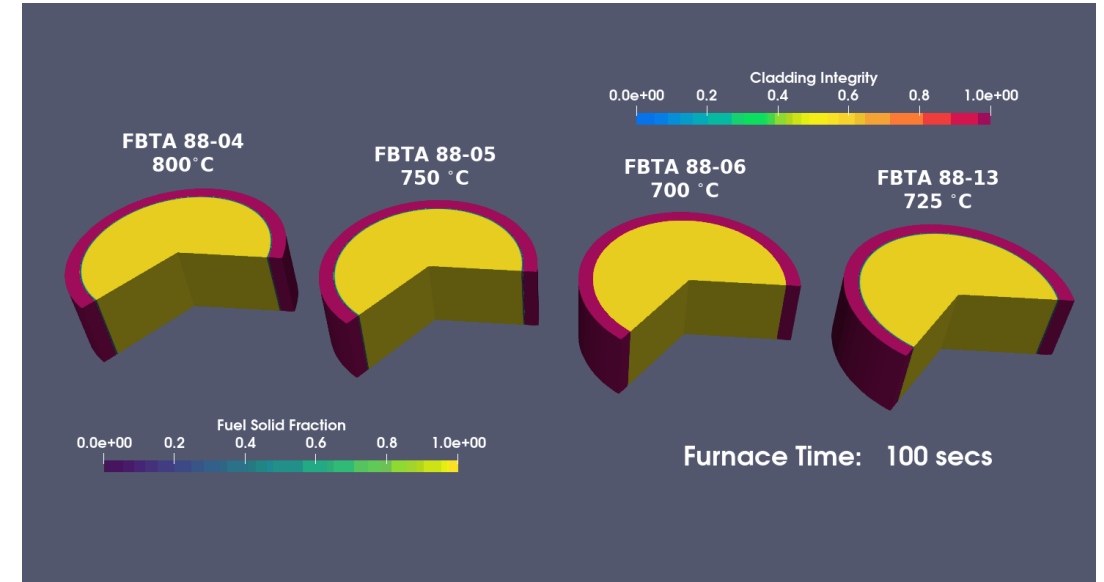
METAPHIX Series Experiments

FBTA Assessment Case

[1] Y Miao et al., ANL/NEAMS-23/6, 2023

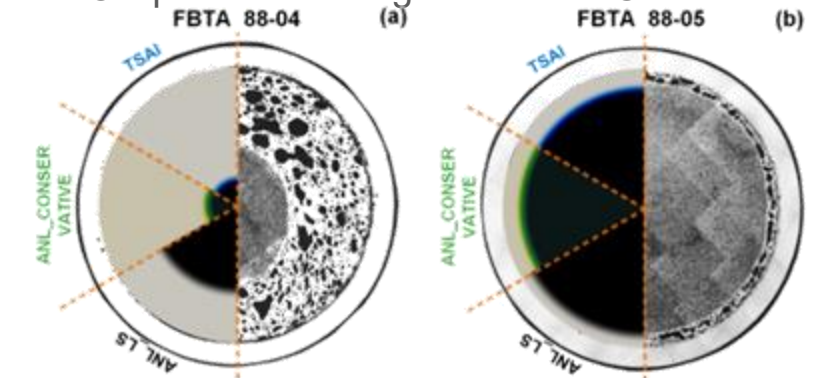
[2] https://mooseframework.inl.gov/bison/metallic_fuel/FBTA/doc/FBTA.html

- FBTA Tests Coverage
 - (Baseline) 4 tests based on X425/T437
 - (Comprehensive) 124 tests based on 23 irradiated pins
- Fuel-Cladding Interface Liquefaction
 - Legacy Tsai + updated ANL correlations for cladding
 - Improved fuel liquefaction correlation
- Impacts of the Assessment Case
 - Eutectic cladding penetration model V&V
 - Platform for statistic studies



Cladding Penetration Comparison
(four tests based on T437)

BISON prediction using Tsai-Bauer Correlation



Post-FBTA metallographs of the four tested sections

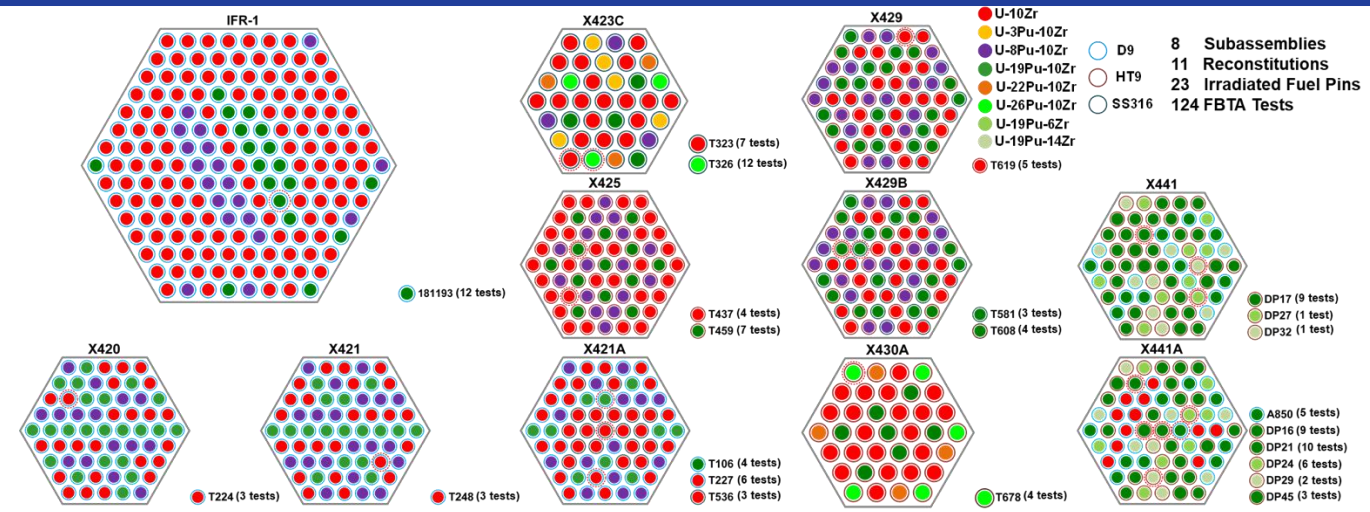


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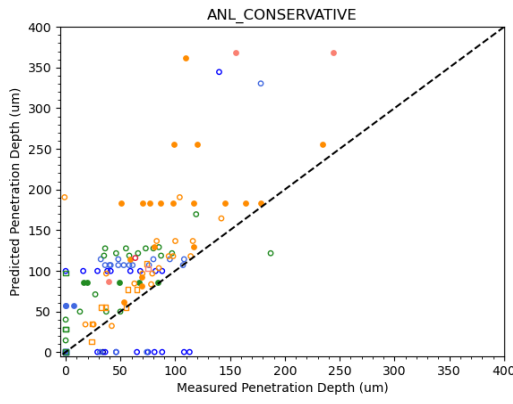
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FBTA Assessment Case

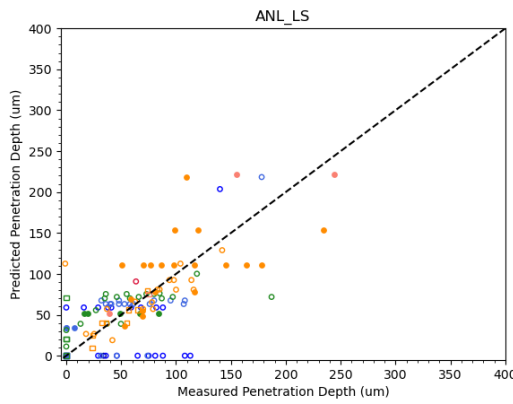
- Full FBTA coverage
 - 23 irradiated pins → 124 FBTA tests
 - Binary + 5 Pu contents
 - HT9, CWD9, CW316SS
- Comprehensive validation platform
 - Empirical models
 - Mechanistic and AI/ML models



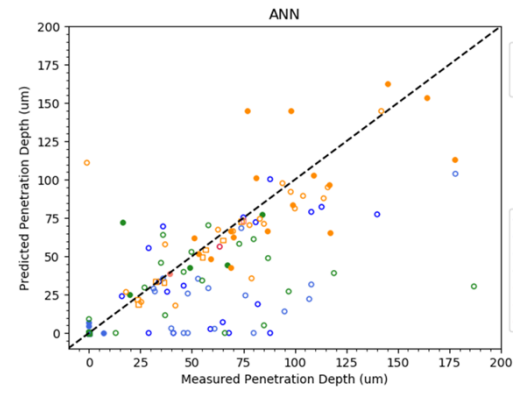
Summary of covered FBTA tests and used irradiated pins



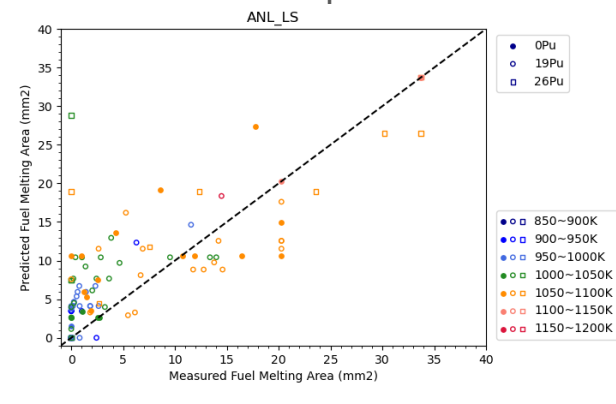
ANL conservative cladding penetration model



ANL best fitting cladding penetration model



Demo of a preliminary artificial neural network surrogate model (MOOSE-libTorch)



ANL best fitting cladding penetration model in fuel liquefaction prediction

Conclusions

- Databases-Powered Validation Achievements Highlight
 - Established BISON-FIPD and BISON-OPTD integration for metallic fuel models validation.
 - Steady-state
 - X447: FCCI & cladding degradation at high temperatures ([milestone report](#), [assessment](#), [paper](#), [VTB](#))
 - X423: fuel volumetric swelling ([milestone report](#), [assessment](#), [paper](#))
 - X425: fuel-cladding mechanical interaction (assessment in preparation)
 - Transient performance
 - FBTA: systematic fuel-cladding liquefaction ([milestone report](#), [assessment](#), paper in preparation)
 - WPF FM-1: run-to-breach furnace test ([milestone report](#), [assessment](#))
- Future Work
 - Expand the coverage of the databases-powered validation platforms
 - Investigate an extensive set of mechanistic models using such platforms
 - Go beyond the current axisymmetric single-pin scheme to support assembly level assessment



An overview of mechanistic cladding-side FCCI model development and preliminary validation

Jacob Hirschhorn, Larry Agesen, Chao Jiang, and Boone Beausoleil

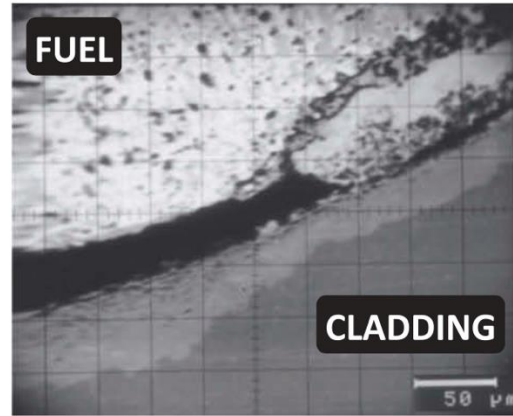


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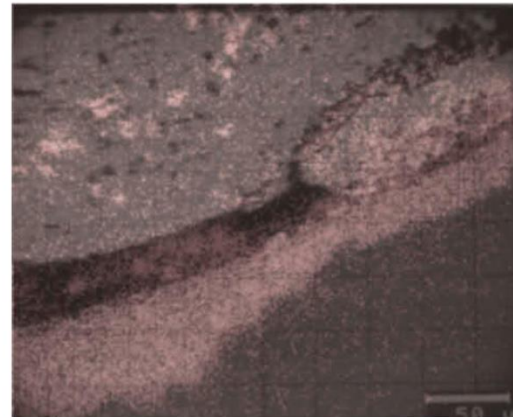
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Cladding-side FCCI background

- Lanthanide fission products migrate to the cladding to form brittle intermetallic phases, which are considered strengthless wastage
- Experimental observations have correlated the axial distributions of radial cladding deformation, lanthanide activity, power density, and temperature, hinting at the impacts of lanthanide production and transport
- Other observations have linked FCCI to fuel cracking
- Observations hint at transport mechanisms and the roles of various microstructural features

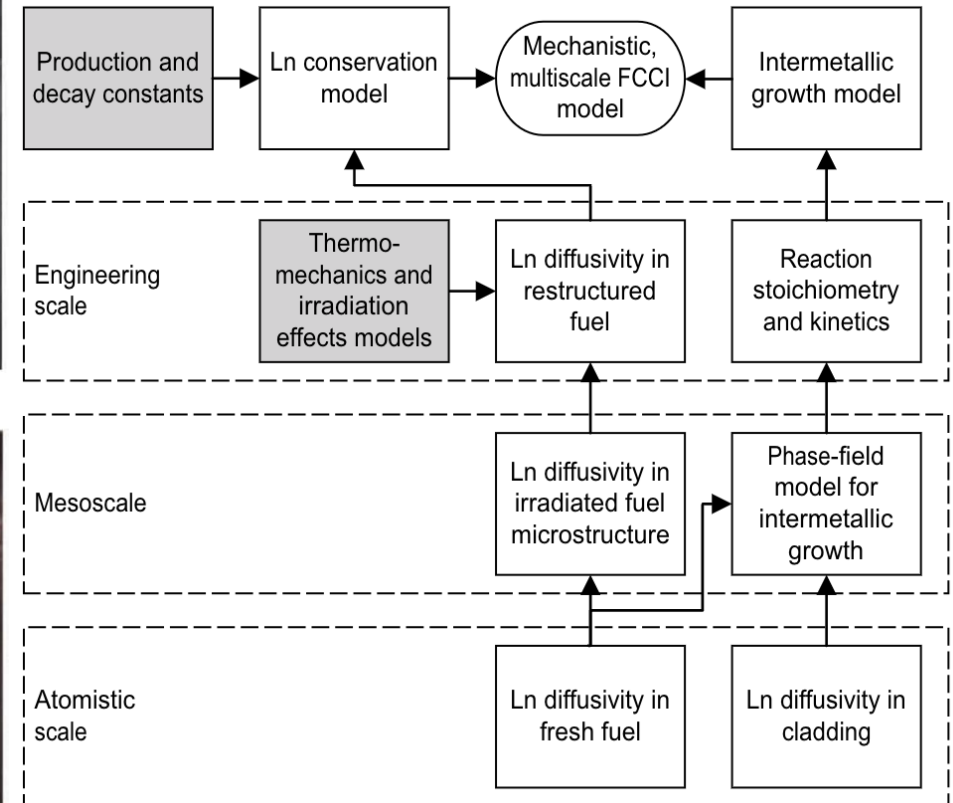


(a) Micrograph



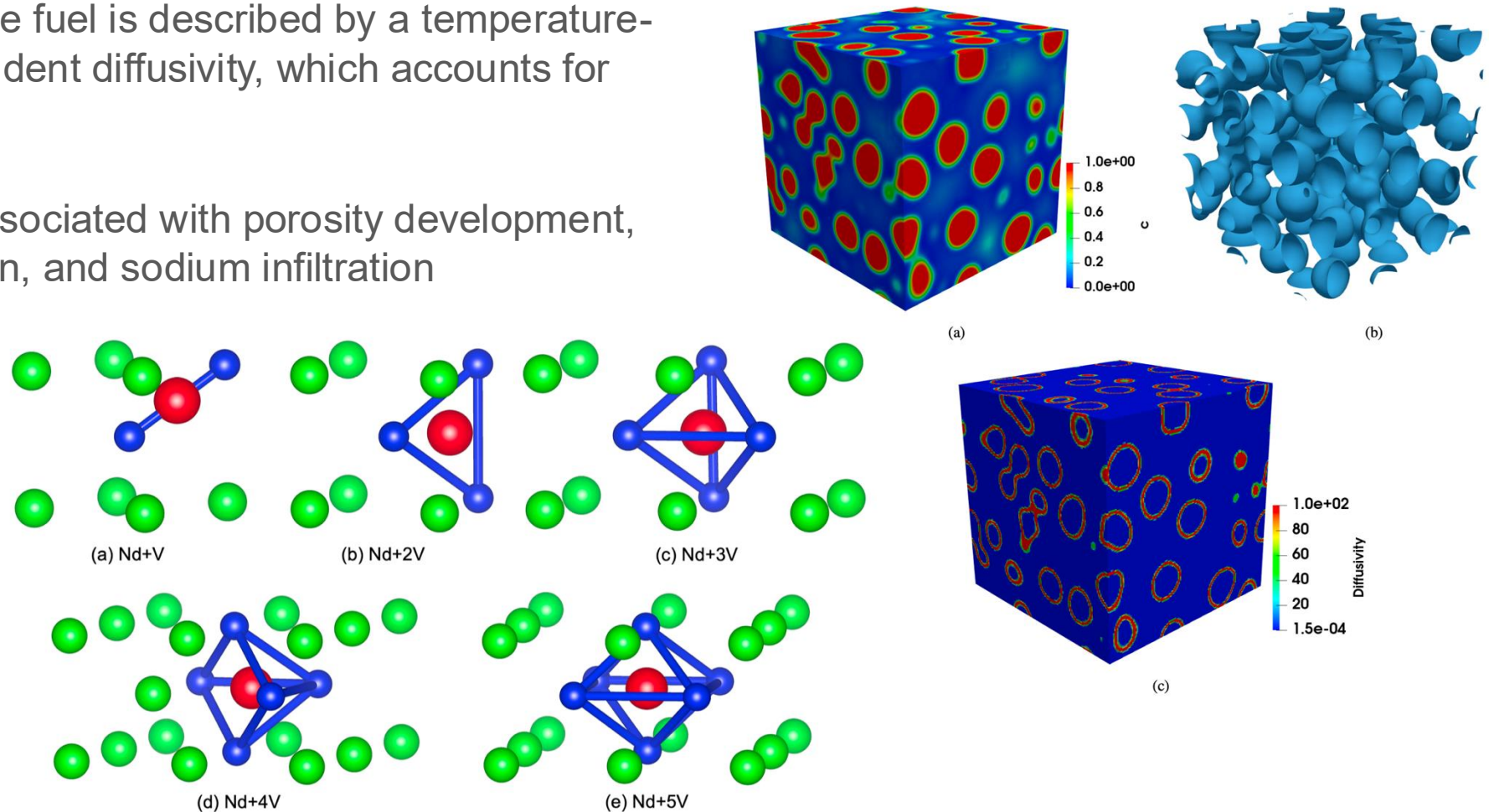
(d) Neodymium overlaid on micrograph

Cladding-side FCCI framework:



Atomistic parameters are weighted in mesoscale simulations

- Lanthanide transport in the fuel is described by a temperature- and microstructure-dependent diffusivity, which accounts for
 - Solid-state diffusion
 - Liquid-like transport associated with porosity development, porosity interconnection, and sodium infiltration
- These features account for temperature and energy deposition (through dependence on microstructure)



Preliminary model demonstration and validation

- A 1D phase-field model of the fuel-intermetallic-cladding was developed to study growth kinetics
- The engineering scale model considers
 - Lanthanide conservation in the fuel using a source term from the literature
 - Reaction using a boundary condition on the fuel surface
- Predicted wastage can be coupled back into the cladding mechanics solve by modifying the cladding stress or elastic properties
- Multiscale coupling was used to guide engineering scale development
- Simulations used EBR-II experiment X447 fuel rod DP75
- Optimization was used to account for uncertainties related to which process(es) limit wastage formation, e.g., reactant availability (fission source and fuel transport), fuel cracking and potential Zr rind disruption, reactant transport through the gap, and reactant transport through the reaction layer and the rate of reaction

$$\text{Lanthanide conservation} \quad \frac{\partial c}{\partial t} = \nabla \cdot D \nabla c + \dot{F} \gamma - \lambda c,$$

$$\text{Reaction boundary condition} \quad J = -D \nabla c = M_0 \exp \left(\frac{-E_a}{kT} \right) (c - c_{eq}),$$

$$\text{Wastage velocity} \quad v = f_S V_m f_G f_{TV} J,$$

$$\text{Geometry factor} \quad f_G = \frac{R_f}{R_f + t_g + \delta},$$

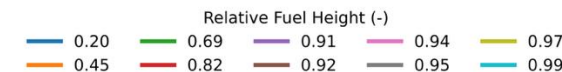
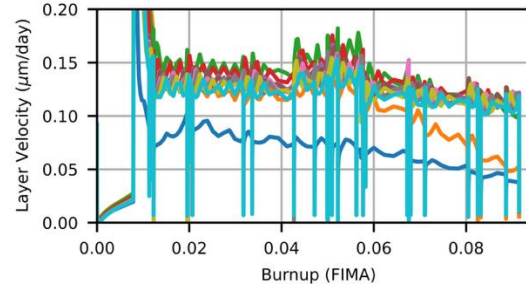
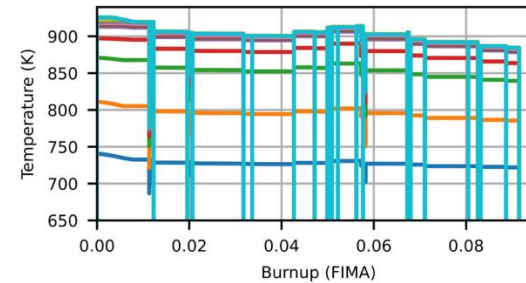
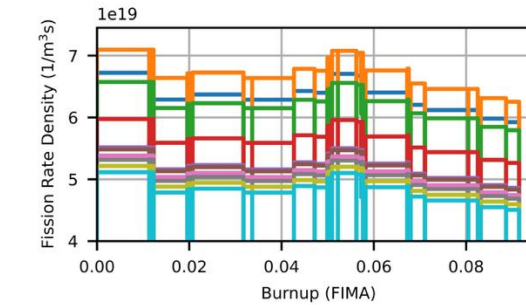
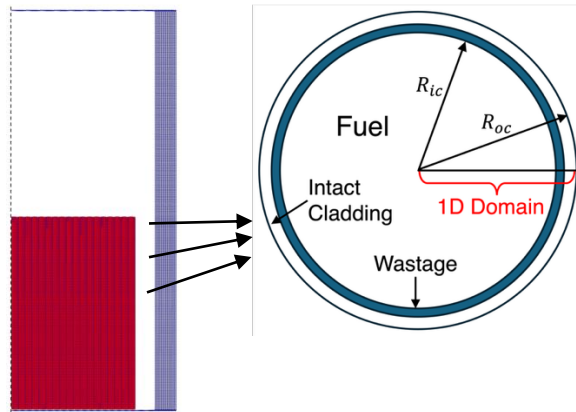
$$\text{Azimuthal heterogeneity} \quad f_{TV} = \frac{\delta_{max}}{\delta_{uniform}},$$

$$\text{Incremental growth} \quad \delta = \sum_{i=1}^I \delta_{i-1} + v_i \Delta t_i.$$

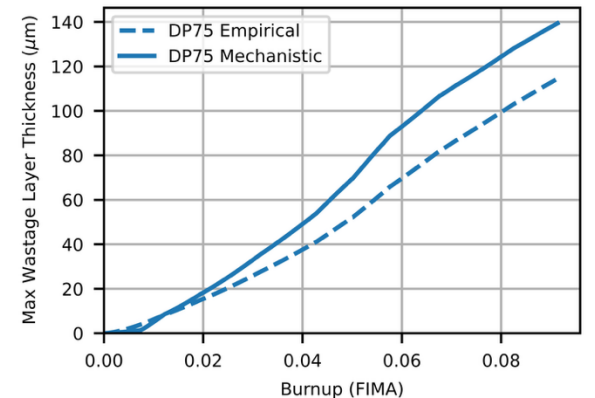
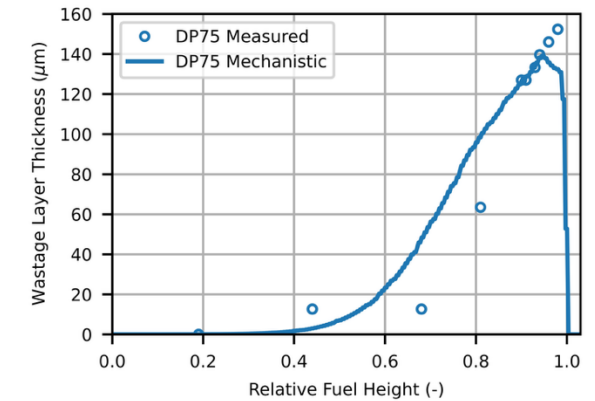
Multiscale coupling and optimization using fuel rod DP75

- Wastage thickness was measured at 10 heights
- Existing engineering scale BISON assessments provided realistic irradiation conditions and microstructural evolution, i.e., fission rate density, temperature, porosity, and pore sodium content
- Local phase-field intermetallic growth simulations predicted resulting layer velocities
- Flux boundary condition parameters were optimized to match observed wastage profiles

EBR-II X447 DP75
(radius × 100)

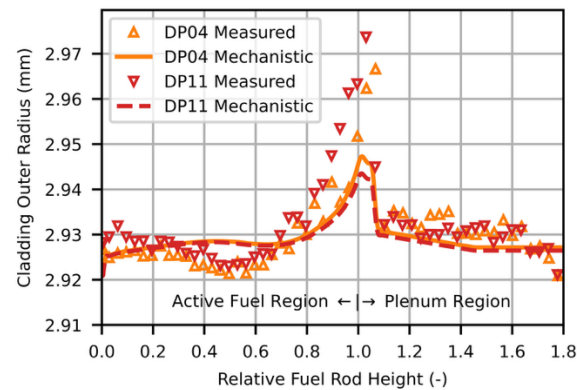


$$J = -D \nabla c = M_0 \exp \left(\frac{-E_a}{kT} \right) (c - c_{eq}),$$

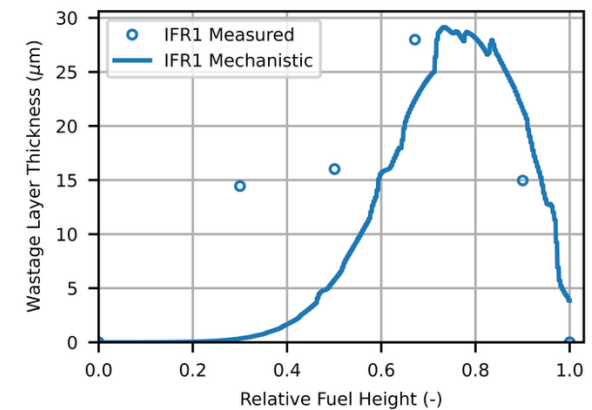
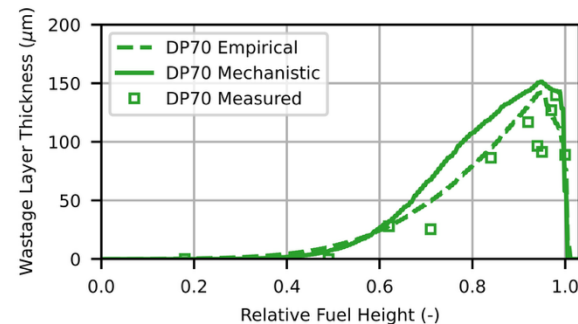
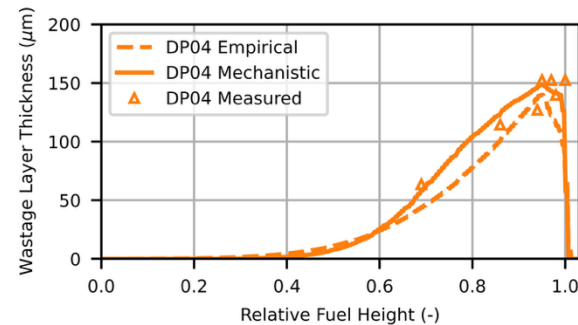


Preliminary model demonstration and validation

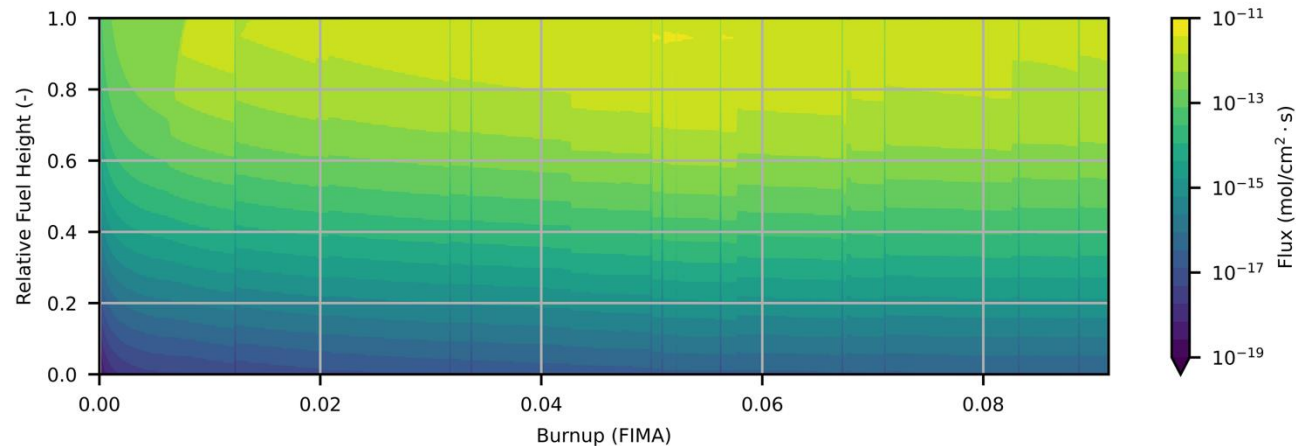
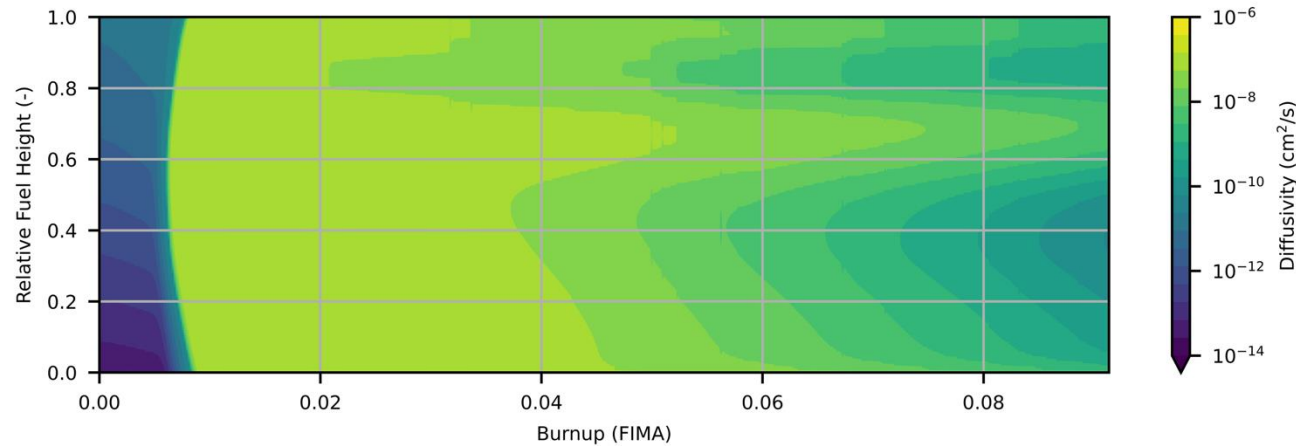
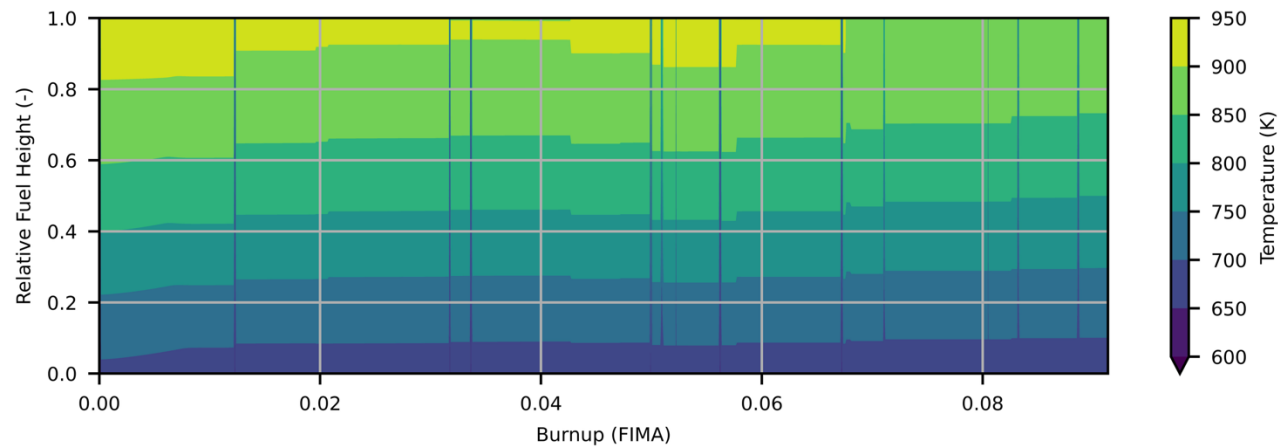
- The optimized model was validated against radial cladding dilation and wastage thickness measurements from 3 additional fuel rods from EBR-II experiment X447
- It was then applied to predict wastage for a commercial-length fuel rod from FFTF experiment IFR1, where it predicted the expected magnitude of peak wastage and the shift in its axial position toward the fuel midplane, potentially due to the impacts of varying fission rate density and temperature (and the spatial distributions thereof)



FFTF IFR1 fuel rod (left)
EBR-II X447 fuel rod (right)
(radius $\times 100$)



A closer look at DP75



- The spatial and temporal temperature surface reveals the high fidelity of operating conditions sourced from the Metallic Fuel Irradiation & Physics Database
- The diffusivity surface illustrates changes in lanthanide transport due to solid state diffusion; porosity development, interconnection, and sodium infiltration; and porosity collapse due to hot pressing
- The flux surface illustrates how lanthanides might behave in the fuel to produce the observed wastage behaviors
- This modular framework yields observables that can be compared to experiments

NEAMS Outlook: Metallic fuel

Summary

- Baseline capabilities in place
- V&V through BISON-FIPD/OPTD integration
 - Maintenance and enhancement of X447 Assessment Case
 - Establishment of X423/X425 Case
 - Improvement of liquid phase penetration models
- New mechanistic FCCI model ready for use
- Continued assessment support

Next Steps

- Prioritized tasks by stake-holder interest:
 - Improvement of hot-pressing model using mechanistically sound models?
 - Implementation of new HT9 LaRomance models as available (coupled with FCCI)?
 - Resurrect fast running 1.5D simulations?
 - Incorporation of minor actinides?
 - Transient fuel modeling?

Overall status for metallic fuel: Good progress we can stand on
Need to: 1) grow assessments based on FIPD,
2) start executing the next challenge problem





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