



Axial Relocation Modeling in BISON: Theory, Application, and Discussion

December 2023

Changing the World's Energy Future

Kyle A Gamble, Ahmed Hamed



INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance, LLC

DISCLAIMER

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness, of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trade mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

Axial Relocation Modeling in BISON: Theory, Application, and Discussion

Kyle A Gamble, Ahmed Hamed

December 2023

**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**

December 6, 2023

Kyle A. Gamble

Computational Scientist

Ahmed Hamed

R&D Staff Scientist

Axial Relocation Modeling in BISON

Theory, Application, and Discussion

Battelle Energy Alliance manages INL for the
U.S. Department of Energy's Office of Nuclear Energy



Idaho National Laboratory

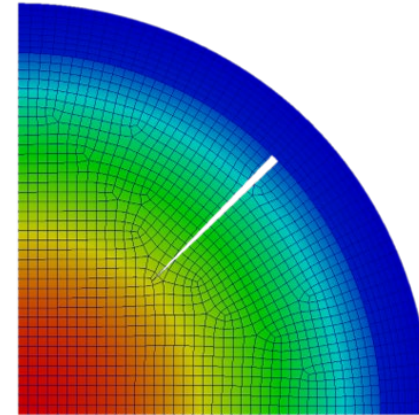
Outline

- Introduction
- Axial Relocation Model for LWR
 - Initial implementation
 - Extension to Layered2D (2.5D)
 - Multiscale advancements
 - Informing the discrete element method (DEM)
- Extension to fast reactor fuels
- Summary

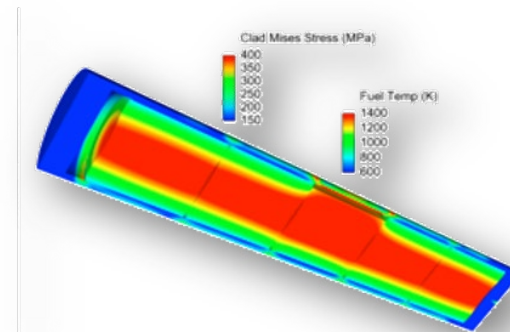
The BISON Fuel Performance Code

2D axisymmetric (or 1.5D)

- Finite element-based engineering scale fuel performance code
- Solves the fully-coupled thermo-mechanics and species diffusion equations in 1D, 1.5D, 2D axisymmetric or plane-strain, 2.5D, or full 3D
- Applicable to both steady and transient operation
- Used for LWR, ATF, TRISO, and metallic fuels
- Readily coupled to lower length scale material models
- Designed for efficient use on parallel computers
- Includes LOCA and RIA accident capability

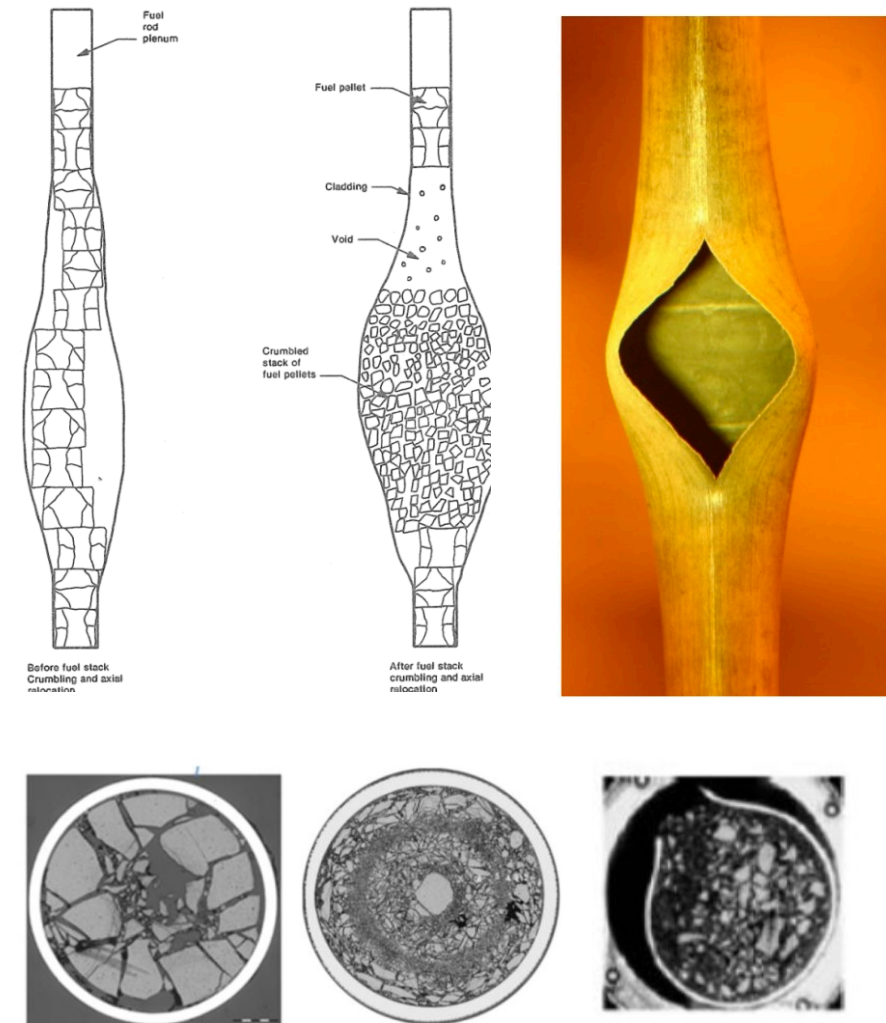


2D (or 2.5D) plane strain



Fuel Fragmentation, Relocation, and Dispersal (FFRD)

- Reactor vendors seek economic benefits associated with increasing nuclear fuel service lifetime in existing light water reactors fleet.
- Fuel fragmentation, relocation, and dispersal (FFRD) phenomena represent a major safety concern still needs to be addressed.
- Formation of high burnup structure (HBS) in conjunction with LOCA can lead to axially relocated fuel to escape fuel pin and get dispersed into the primary coolant system through cladding rupture.
- Predictive modelling of the FFRD phenomena requires capturing the synergistic impact of the fuel particle characteristics, cladding burst opening geometry, and stress level on the emergent dynamics.

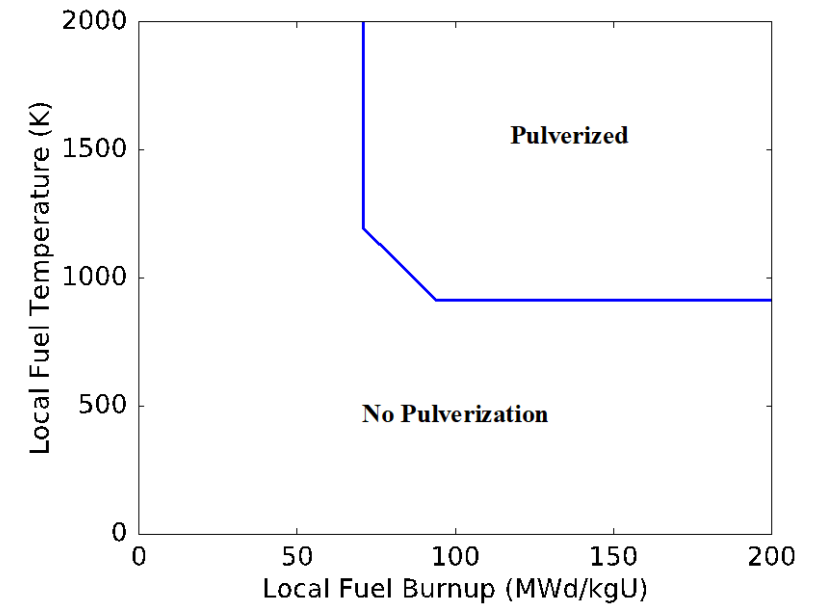


Axial Relocation Model

- Jernkvist and Massih developed a model that wraps around the FRAPTRAN-1.5 fuel performance code, which uses a Layered1D (1.5D) geometric representation of fuel rods.
- Utilizes a binary system of fragment sizes:
 - Large fragments: fragments
 - Small fragments: pulvers



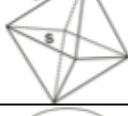
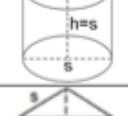

$$l_f = D_{FP} \min \left(1, \frac{\pi}{n_f} \right)$$

l_f = characteristic length of fragments
 D_{FP} = fuel outer diameter
 n_f = number of fuel fragments



**Pulvers
(default)**

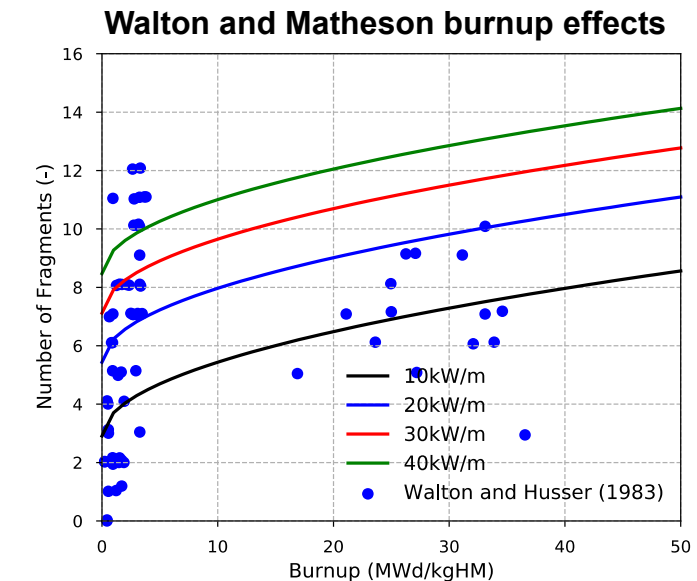
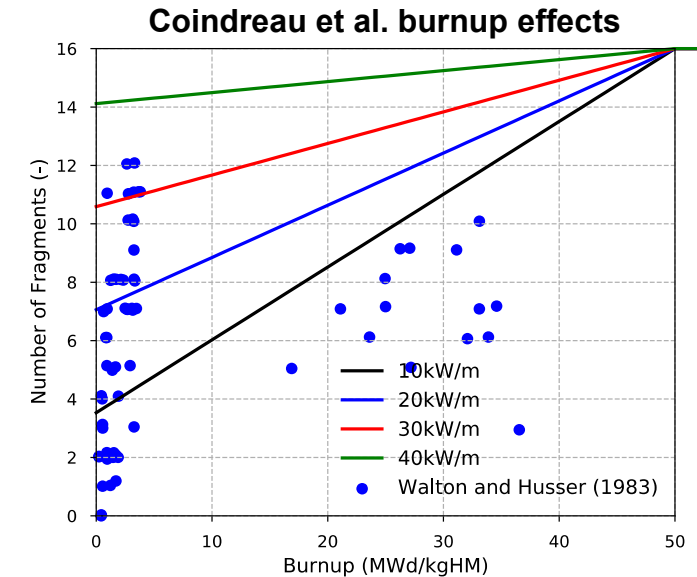
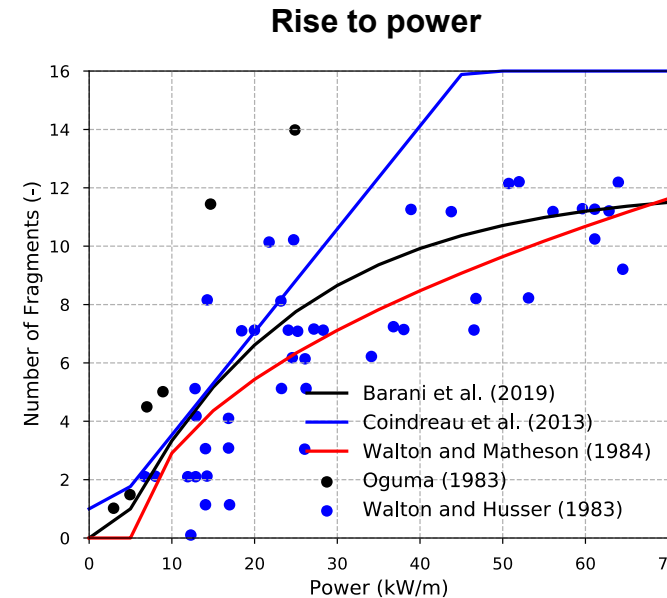
**Fragments
(default)**

Shape and dimension		ψ	D_p	V_p	A_p
Sphere with diameter s		1.000	s	$0.5236s^3$	πs^2
Cube with side s		0.806	$1.147s$	s^3	$6s^2$
Octahedron with side s		0.846	$0.895s$	$0.4714s^3$	$3.4641s^2$
Ideal cylinder, $h=s$		0.874	$1.069s$	$0.7854s^3$	$4.7124s^2$
Triangular prism, $h=s$		0.716	$0.910s$	$0.4330s^3$	$3.8660s^2$

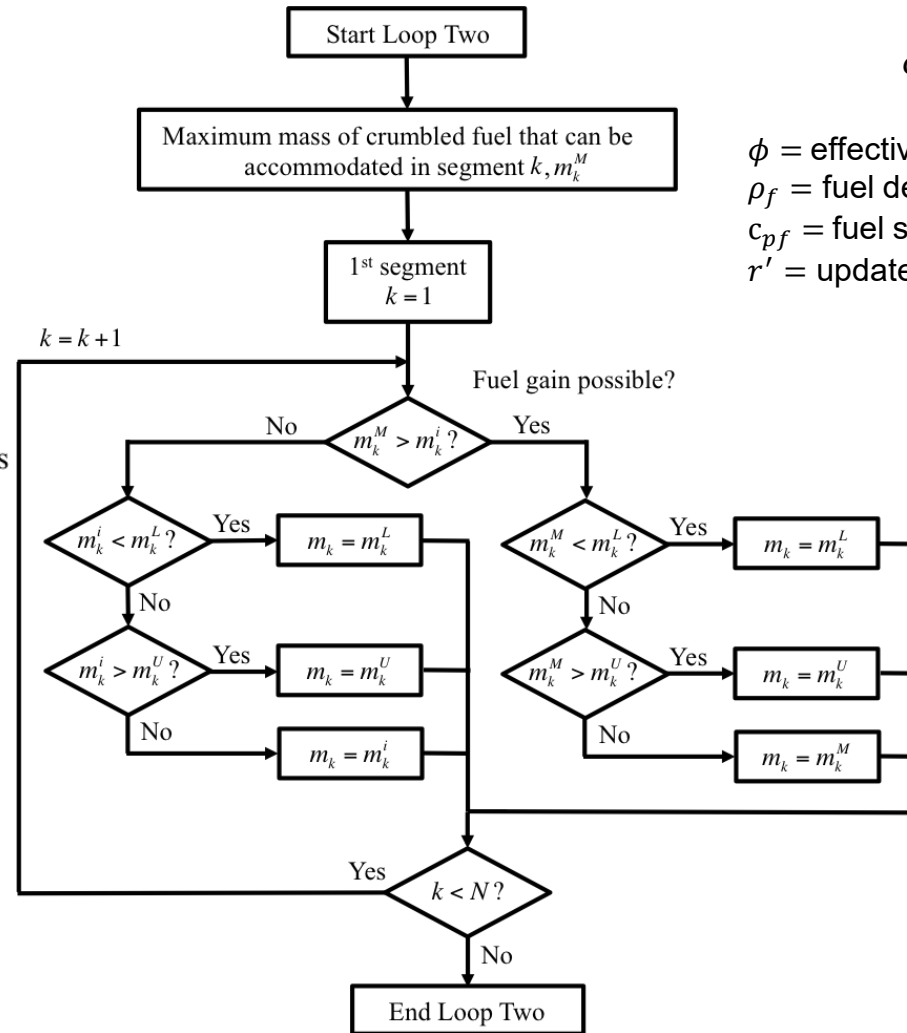
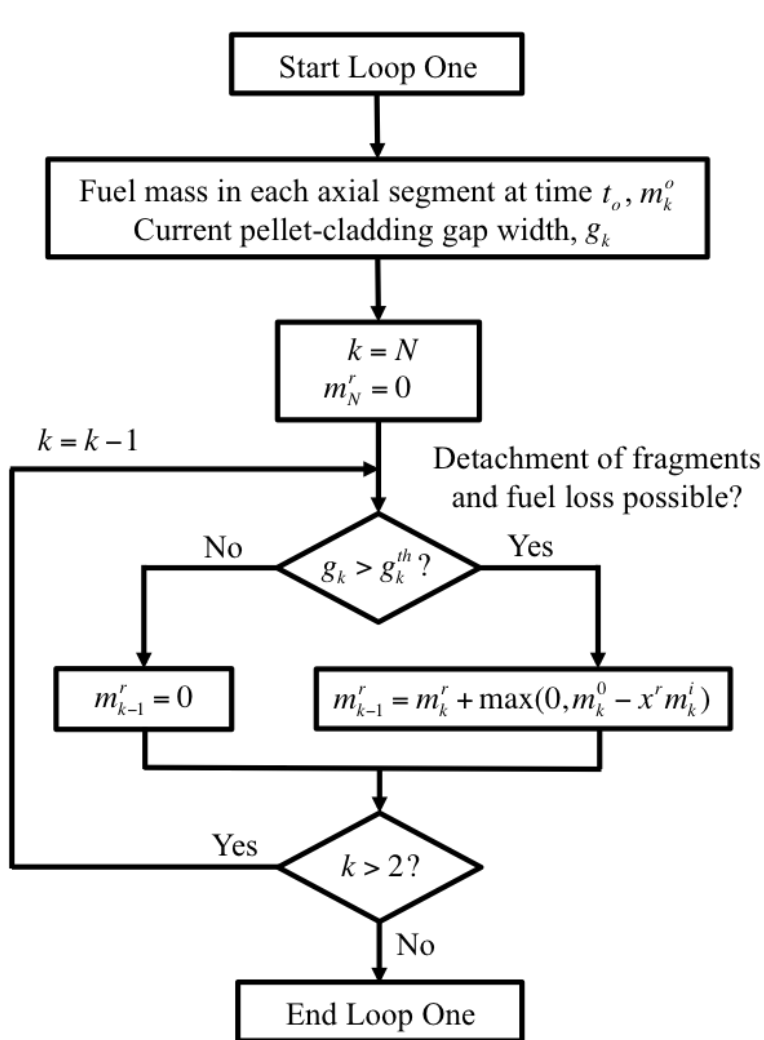
Fuel Cracking and Large-Scale Fragments

- Existing models are only a function of maximum power and rod average burnup.
 - No ramp rate dependence or impact of the material property driving fracture (i.e., tensile strength)

Model	Formulation
Coindreau et al.	$n_f^o = \max\left(1, \min\left(\frac{6q'_{max}}{17}, 16\right)\right)$ $n_f = \min\left(n_f^o + \frac{(16 - n_f^o)Bu_{av}}{50}, 16\right)$
Walton and Matheson	$n_f = 0.8(\sqrt{Bu_{av}} + \sqrt{3.3\{x\}})$ $\{x\} = \begin{cases} 0, & q'_{max} - 6.0 < 0 \\ q'_{max} - 6.0, & q'_{max} - 6.0 \geq 0 \end{cases}$
Barani et al.	$n_f = \begin{cases} 0, & q'_{max} < 5.0 \\ 1.0 + 11.0\left(1.0 - \exp\left(-\frac{q'_{max} - 5.0}{21.0}\right)\right), & q'_{max} \geq 5.0 \end{cases}$

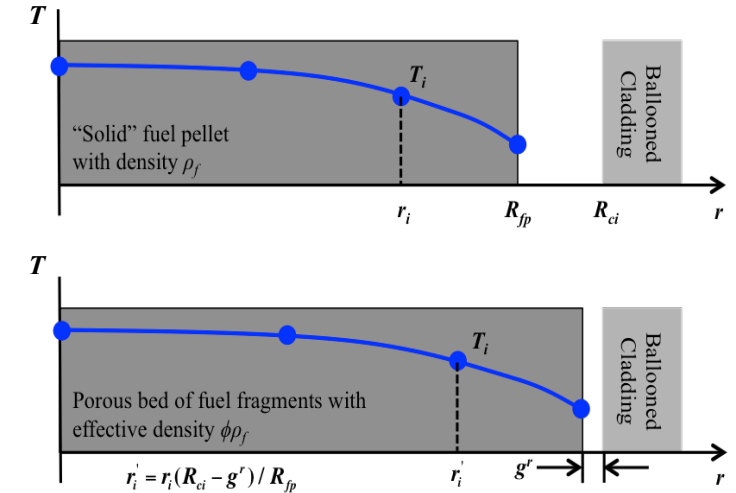


Axial Relocation Model



$$\phi \rho_f c_{pf} \frac{\partial T}{\partial t} - \frac{1}{r'} \frac{\partial}{\partial r'} \left(k_{eff} r' \frac{\partial T}{\partial r'} \right) = \phi q'''(t, r')$$

ϕ = effective packing fraction
 ρ_f = fuel density
 c_{pf} = fuel specific heat
 r' = updated radial position
 k_{eff} = effective thermal conductivity
 T = temperature
 $q'''(t, r')$ = volumetric heat generation



R_{ci} = cladding inner radius
 R_{fp} = fuel outer radius
 g^r = residual gap

Axial Relocation: Double Balloon Testing

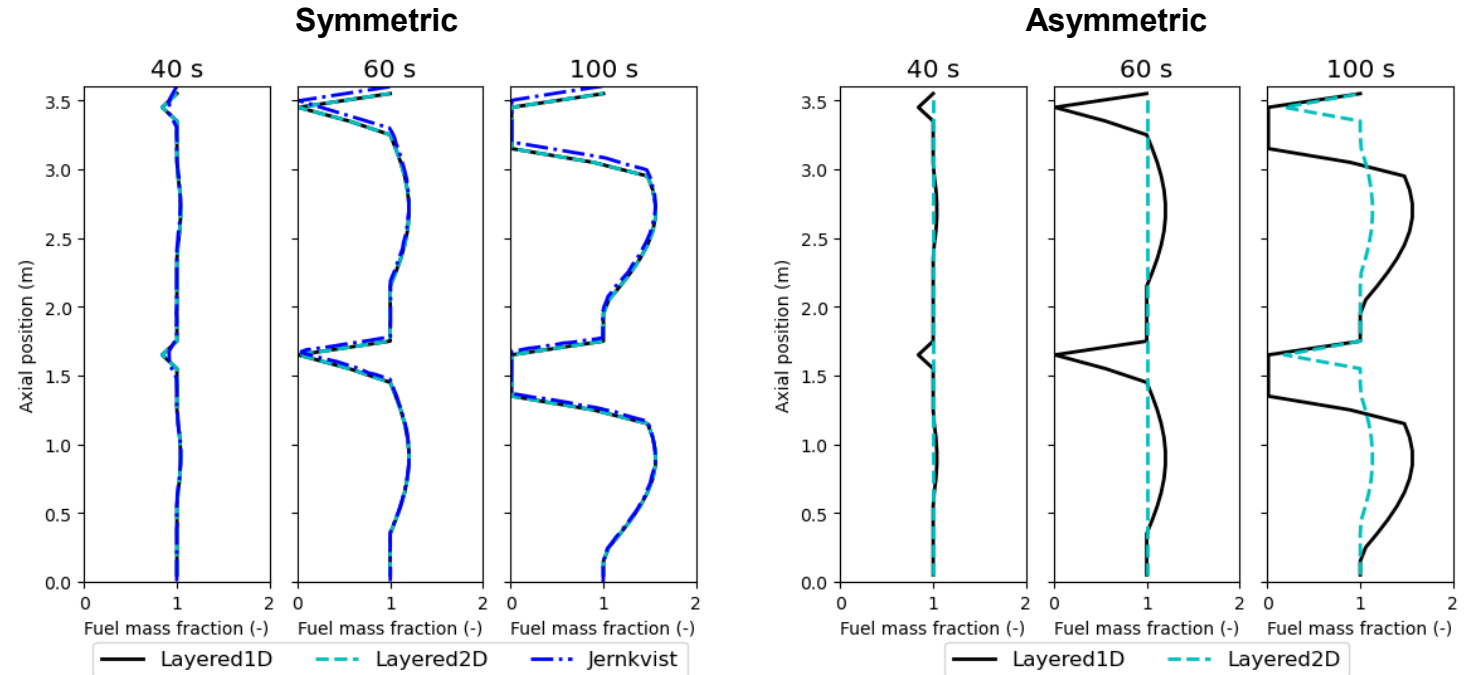
- The active fuel length is 3.6 m with fuel pellet diameter of 9.0 mm. The fuel-to-clad gap is closed, and the effective packing fraction is set to 0.75 in crumbled layers.
- The inner radius of the cladding is then displaced as a function of time and position to induce a double balloon.

– Symmetric:

$$R_{ci}(t, z) = 4.5 \times 10^{-3} + 2.0 \times 10^{-5} t \left| \sin \left(\frac{\pi z}{2L_a} \right) \right|$$

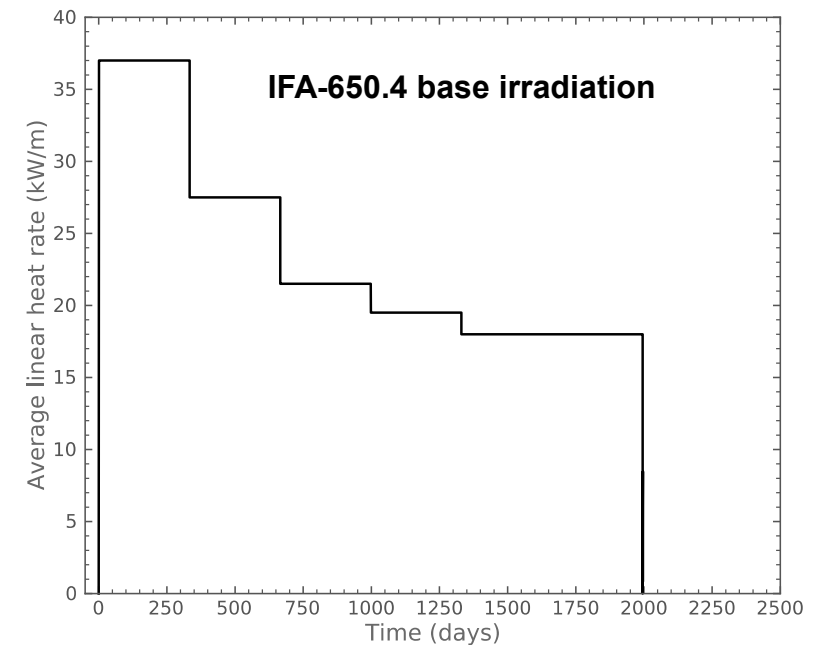
– Asymmetric:

$$R_{ci}(t, z) = 4.5 \times 10^{-3} + 2.0 \times 10^{-5} t \sin \left(\frac{\theta}{2} \right) \left| \sin \left(\frac{\pi z}{2L_a} \right) \right|$$



Axial Relocation Validation (Halden IFA-650 Series)

- IFA-650.4: The experiment that reignited industry's interest FFRD.
 - Very high burnup (~ 92 MWd/kgU), single balloon, severe pulverization and fuel relocation.
- IFA-650.9: Designed to confirm observations from IFA-650.4
 - Very high burnup (~ 89.9 MWd/kgU), double balloon, severe pulverization and fuel relocation.
- IFA-650.14: An experiment on a rodlet with a small plenum
 - High burnup (70.8 MWd/kgU), moderate pulverization and fuel relocation, large single balloon, no rupture.
- Each experiment consisted of the following phases:
 - Preparatory phases
 - Blowdown phase
 - Heat-up phases



Sensitivity of Axial Relocation Model

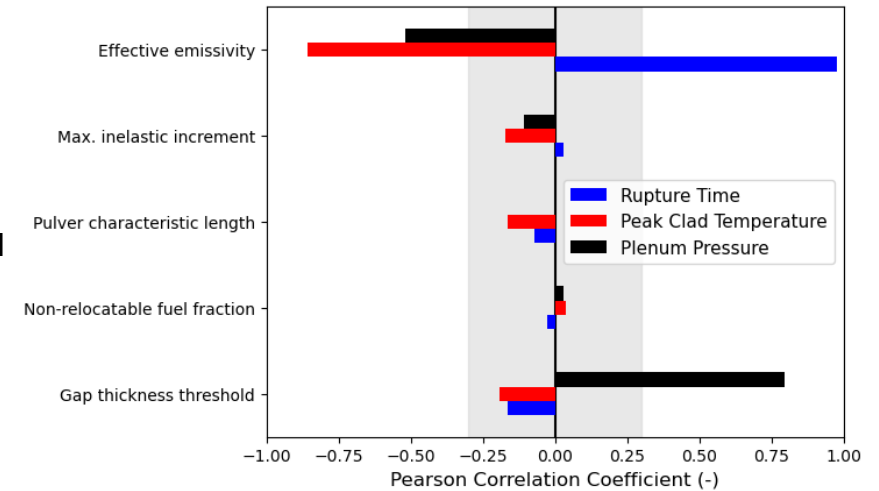
- Assess the impact of some modeling assumptions regarding the axial relocation and LOCA modeling capabilities.
- Both a plastic instability (PI) and overstrain (OS) cladding failure criteria were studied.
- The effective emissivity during radiation is the most important parameter.

$$h_r = \epsilon \sigma (T_c^2 + T_h^2)(T_c + T_h) \quad \epsilon = \epsilon_c \epsilon_h R_h (\epsilon_c R_c + \epsilon_h R_h - \epsilon_c \epsilon_h R_c)^{-1}$$

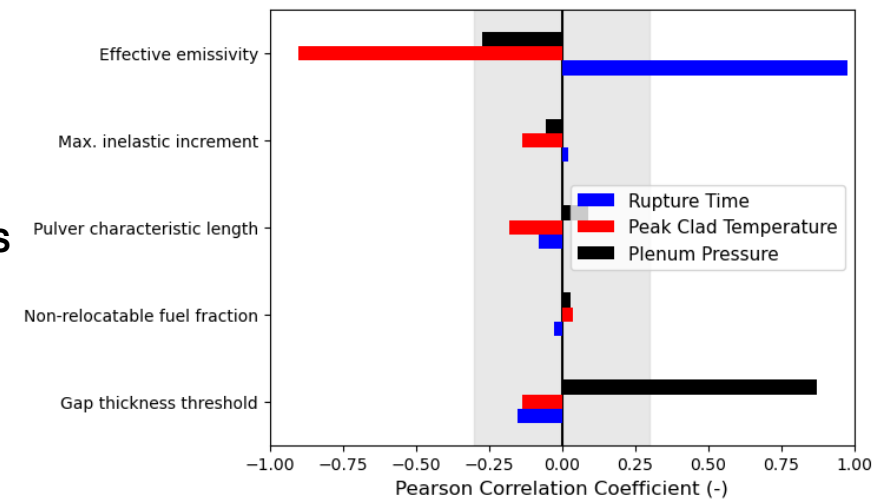
Parameter	Uncertainty Range	Distribution
Gap thickness threshold (m)	$[0.1 \times 10^{-3}; 0.5 \times 10^{-3}]$	Uniform
Non-relocatable fuel fraction (-)	[0.005:0.05]	Uniform
Pulver characteristic length (μm)	[50:500]	Uniform
Maximum inelastic increment (-)	[0.0001:0.01]	Uniform
Effective emissivity during radiation (-)	[0.4:0.75]	Uniform

In addition to the uncertain parameters provided in the table, three large fragment models were analyzed: Barani et al., Coindreau et al., and Walton and Matheseon as well as three different number of layers representing the fuel in the mesh: 15, 30, and 60.

60 layers, PI

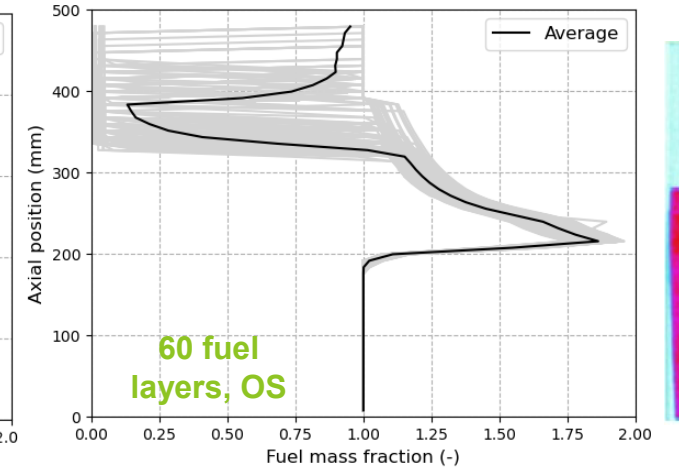
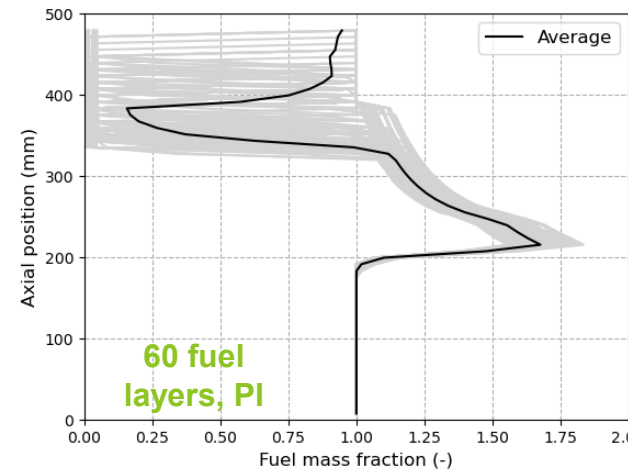
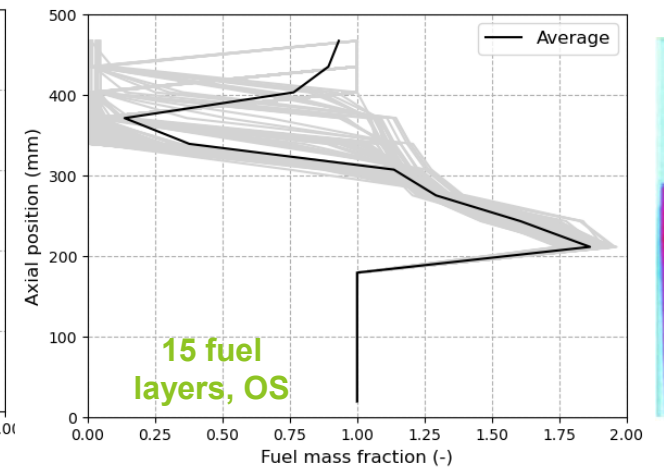
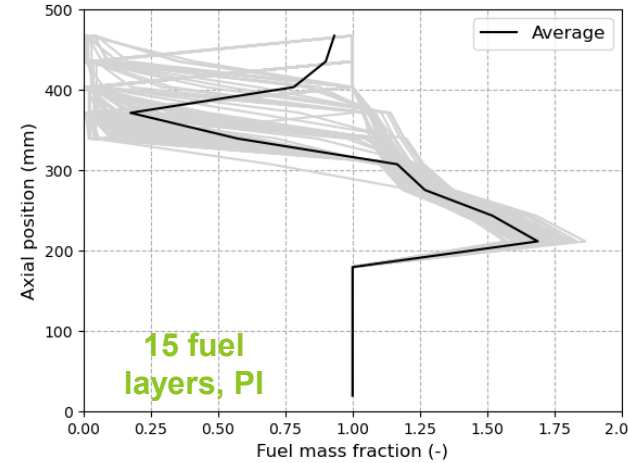


60 layers, OS



Axial Relocation IFA-650.4 Validation

- Some of the 200 realizations predict complete fuel loss at the top of the rod.
- Limited mesh dependence on predictions.
- The overstrain criterion leads to slightly larger balloons.



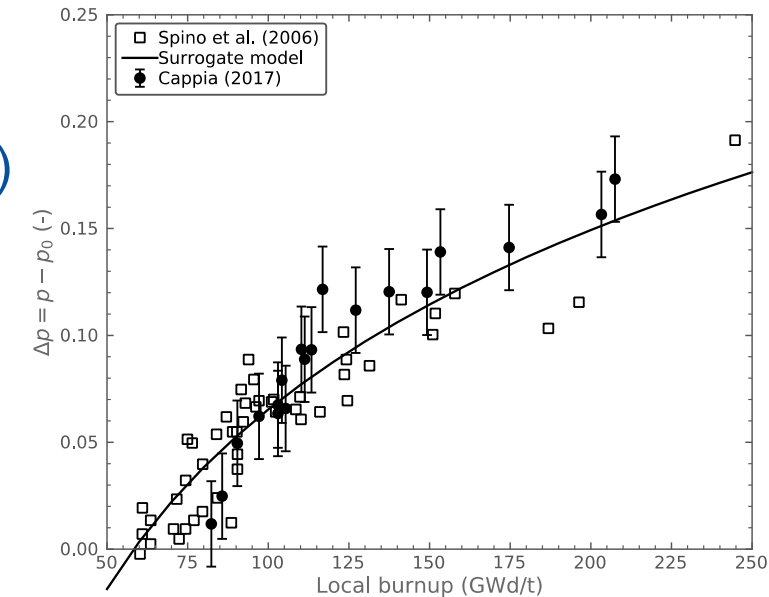
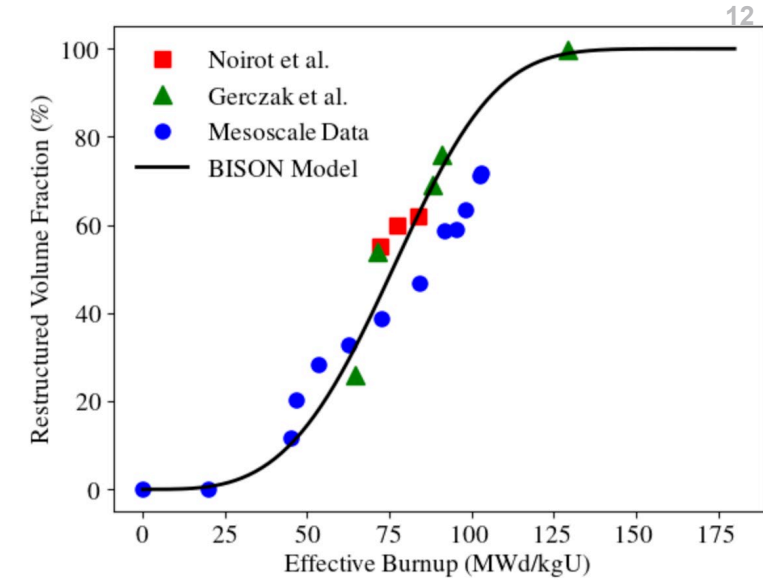
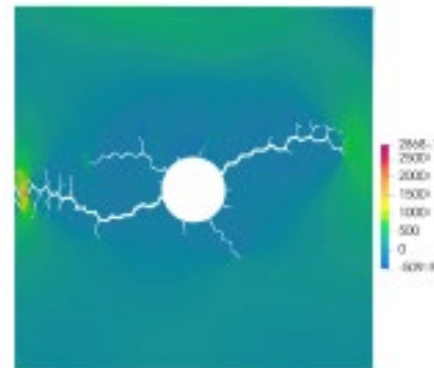
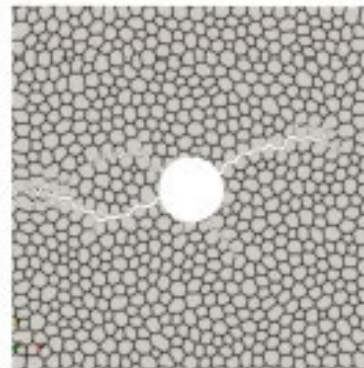
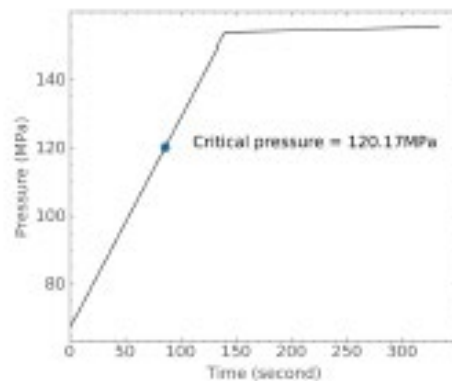
Lower Length Scale Informed Pulverization Models

Phase-field

- Developed by fitting an equation to multiple phase-field fracture calculations in high burnup fuel.

$$P_g^{cr} = 1 \times 10^6 [124.17 + 1.43858(\sigma_{gb}^{cr} - 130)(1 - p) - 1.0178\sigma_H] \quad (2D)$$

$$P_g^{cr} = 1 \times 10^6 [175.987 + 0.5035(\sigma_{gb}^{cr} - 130)(1 - 1.582p) - 1.089\sigma_H] \quad (3D)$$

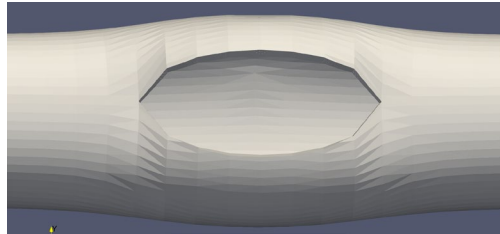


Methodology and Approach: Proposed Work

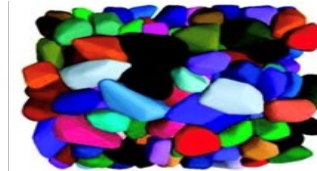
- BISON informed DEM analyses for the development of a phenomenological model for predicting fuel relocation and dispersal
- Enable a framework for coupling or informing DEM simulations from Multiphysics Object-Oriented Simulation Environment (MOOSE) based applications.

BISON

- Simulated existing loss-of-coolant-accident experiments.
 - Halden, Studsvik, Severe Accident Test Station (SATS)
- Extract final cladding dimensions and burnup and pass to LIGGGHTS-INL



DEM



LIGGGHTS-INL

- Perform DEM simulations assuming uniform particle sizes and shapes
- Perform DEM simulations accounting for particle size and shape distributions

Phenomenological Model

- Regression techniques and statistical methods available in the stochastic tools module (STM) of MOOSE
 - Particle shape, particle size distribution, burnup, and cladding distension (strain).
- Functions for packing fraction and quantity of fuel dispersed.



FEM-informed DEM modeling and simulation of fuel axial relocation and dispersal — Developed metrics

- BISON is used to simulate experimentally observed scenarios leading to FFRD.
- BISON-informed Discrete Element Method is used to simulate FFRD dynamics and analyze controlling parameters.

Material Properties:

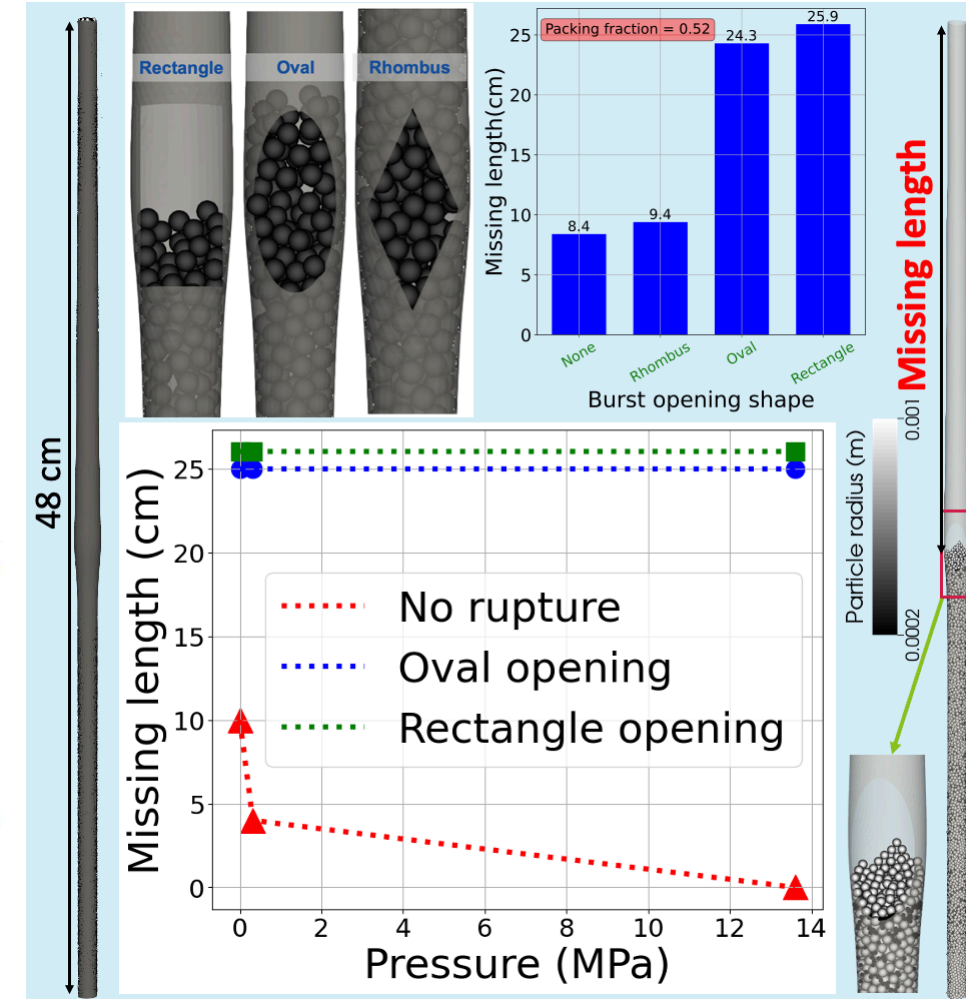
- Density
- Friction coefficient
- Coefficient of restitution
- Young's modulus
- Poisson's ratio

BISON/Halden IFA Experiments:

- Particle size & distribution
- Geometry of ballooned and ruptured fuel cladding tube (surface mesh)
- Initial packing fraction/**stress state**
- **Temporal evolution of the fuel clad**
- **Burst opening shape**
- **Fuel fragment shape**

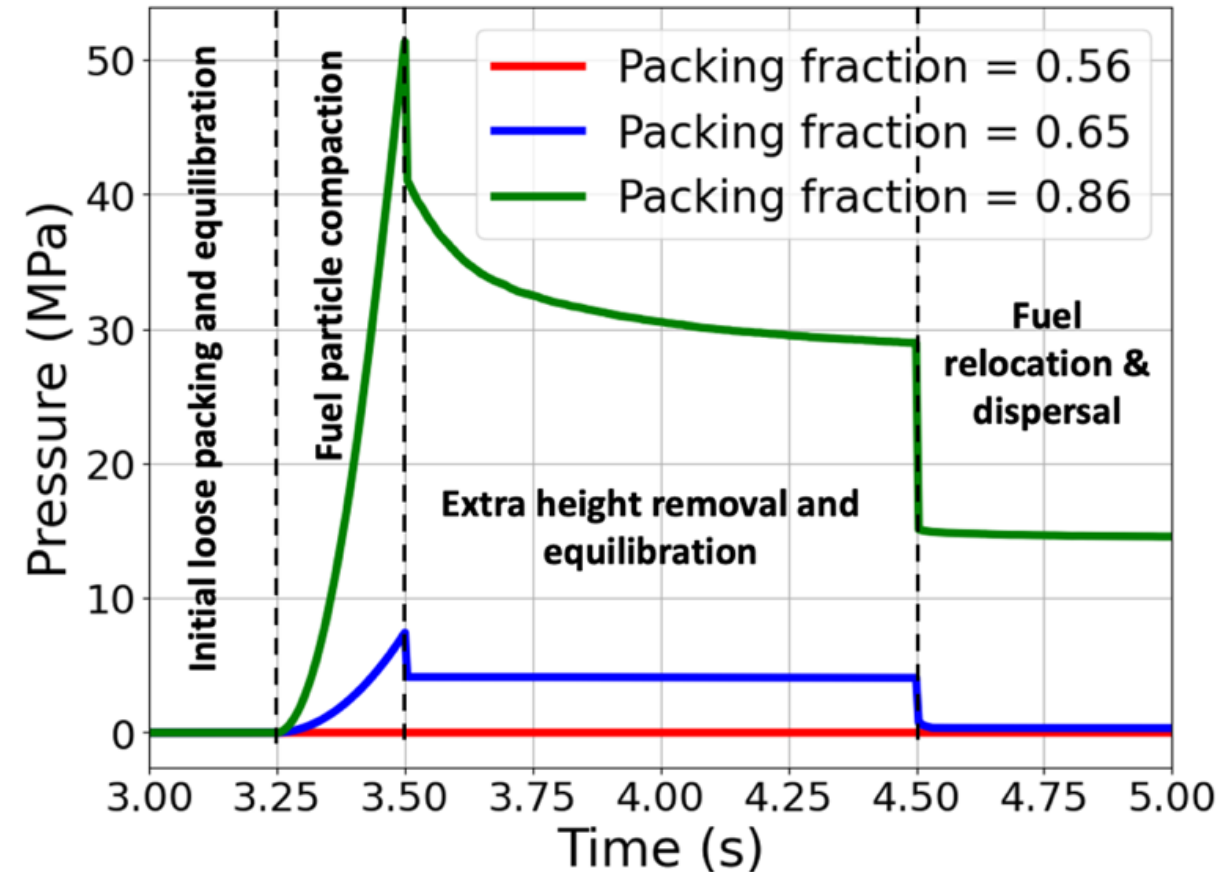
Model prediction:

- Missing fuel length
- Mass fraction
- Filling ratio
- Circumferential strain threshold



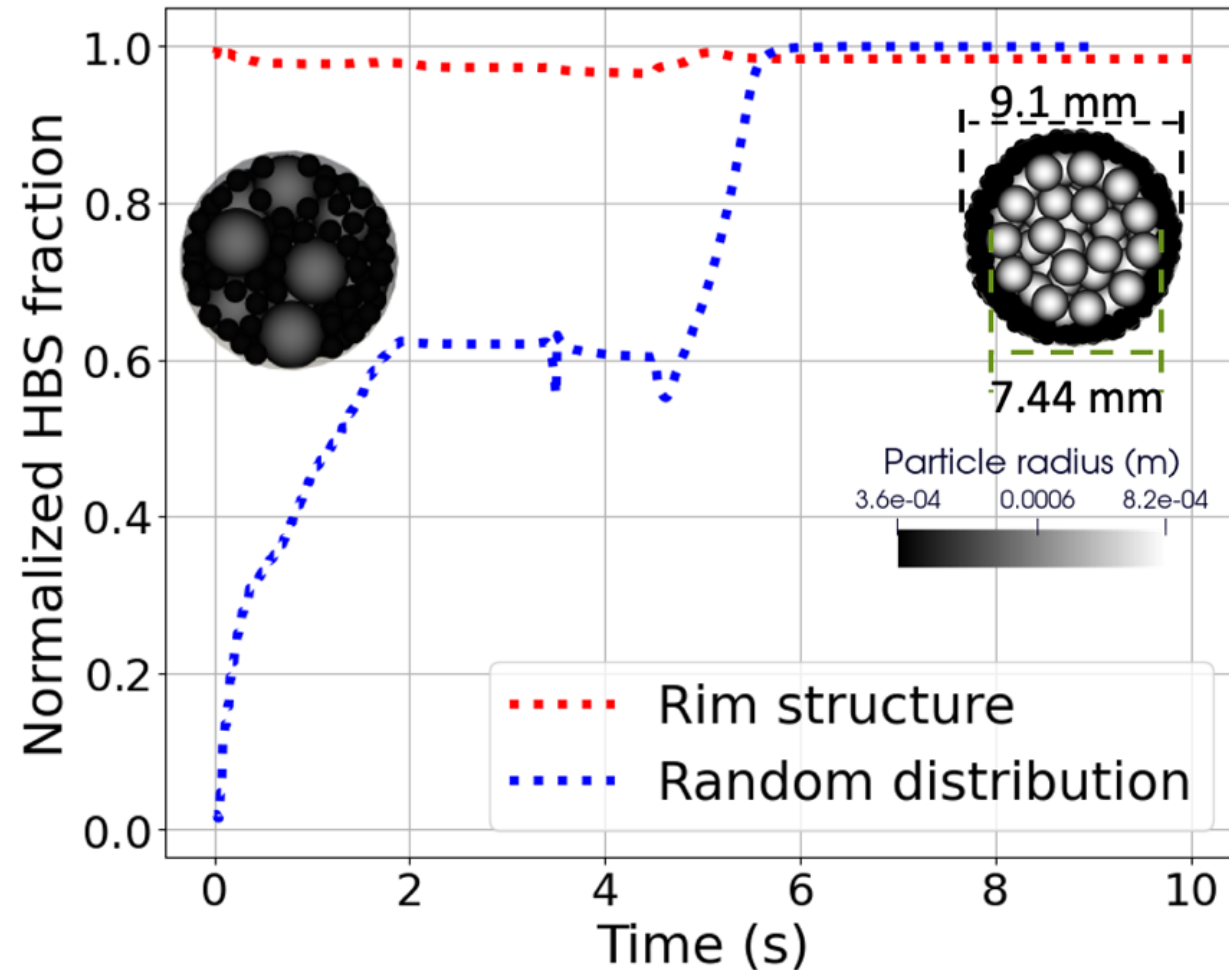
Internal pressure temporal evolution during different simulation stages

- Initial packing fraction and the internal pressure are positively correlated.
- Random loose packing can achieve a packing fraction as high as (0.5–0.6), so compaction is needed for higher fraction.
- Relocation and dispersal are treated as avalanche phenomena (needs to be revisited).
- In the absence of cladding rupture, fuel relocation and dispersal are predominantly driven by internal pressure relief rather than the gravity forces for the prestressed cases (radial relocation outweighs axial relocation).



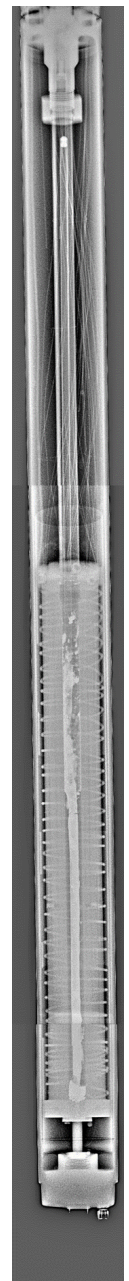
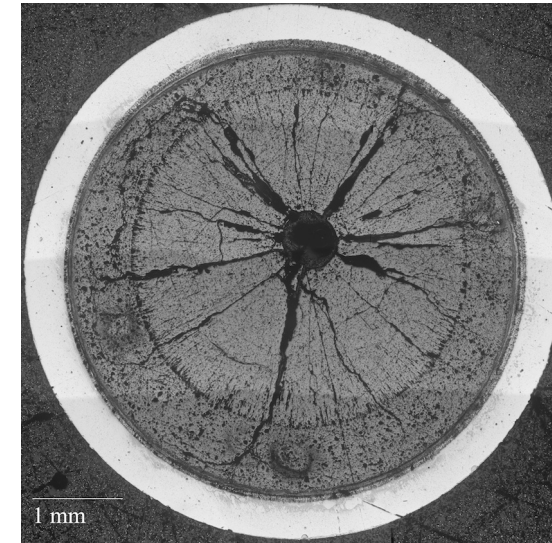
Impact of particle size distribution and radial arrangements on the observed dynamics

- Larger fuel fragments are more resisting to fuel relocation and more sensitive to the cladding burst opening shape.
- Finer particles, associated with HBS, have higher flowability and are not affected by the opening shape.
- Dynamics obtained from the rim structure is completely different from the random packing structure:
 - Rim structure leads to a layer-by-layer fuel dispersal behavior (consistent with a one-dimensional mass flow).
 - Random structure shows accumulation of fine particles over time.



Axial Relocation in Fast Reactor Fuels

- MOX
 - Existing algorithm can readily be extended with minor modifications.
 - Need to update fracture/pulverization models as needed
 - Modify mesh movement to also account for filling of central hole.
- Metallic
 - Modifications to existing algorithm are more involved.
 - Extension to 2D-RZ
 - Triggering relocation based on whether fuel is melted rather than fragmented.



Summary

- The axial relocation model used for LWR analysis in BISON was presented.
- Ongoing activities to improve the models used in axial relocation analysis from the lower-length scale were described.
- Recent activities in discrete element modeling of axial relocation were highlighted.
- A discussion on how to modify the capabilities for LWR axial relocation modeling and apply it to fast reactor fuels such as MOX and metallic were provided.

Acknowledgments

- This research was conducted by a contractor of the U.S. Government under contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a non-exclusive, royalty-free license to publish or reproduce the published form of this report, or allow others to do so, for U.S. Government purposes. Funding was provided by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program as well as Laboratory Directed Research and Development (LDRD) funds.
- This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.



Idaho National Laboratory

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy. INL is the nation's center for nuclear energy research and development, and also performs research in each of DOE's strategic goal areas: energy, national security, science and the environment.

WWW.INL.GOV