INL/MIS-21-62431-Revision-0

TRISO Fuel Performance Modeling

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Changing the World's Energy Future

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TRISO Fuel Performance Modeling

CNSC Seminar

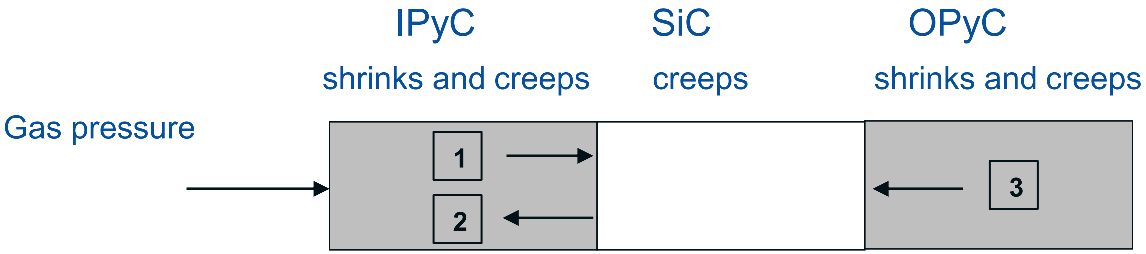
Idaho National Laboratory

Outline

- Overview of TRISO fuel performance modeling
- TRISO fuel performance code PARFUME
- TRISO fuel performance modeling with BISON
- PARFUME and BISON comparison

TRISO Fuel Performance Modeling

- **Basic fuel particle behavior**
  - Several physical phenomena influence the behavior of the particles including fission gas production and irradiation effects.

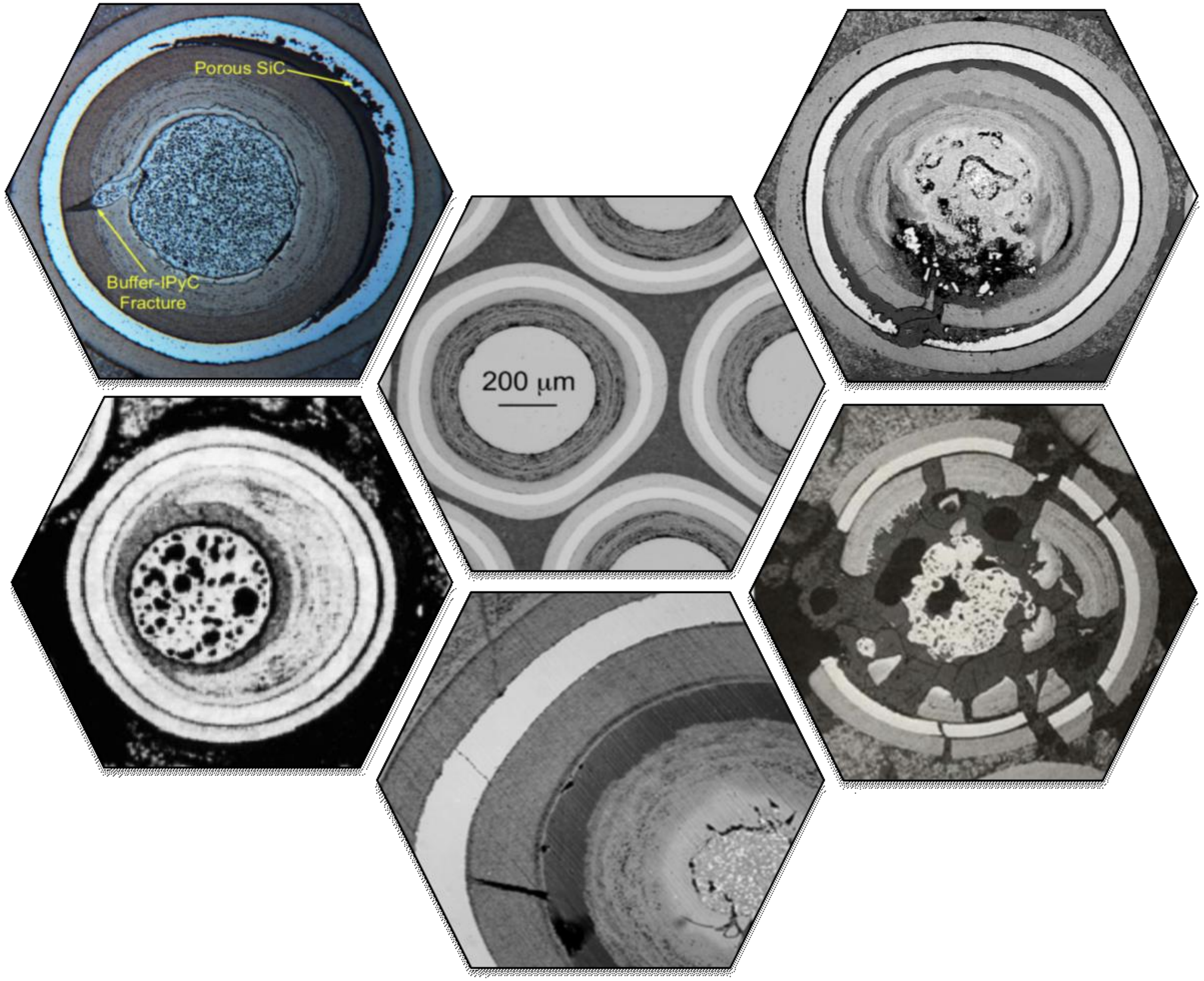


1. Gas pressure is transmitted through IPyC
2. IPyC shrinks, pulling away from the SiC
3. OPyC shrinks, pushing on the SiC

- **Fuel performance modeling**
  - Optimize particle design
  - Plan irradiation experiments (pre-test predictions)
  - Identify tolerances of specifications permissible during manufacture
  - Estimate reactor fuel performance
    - Identify critical parameters affecting particle behavior
    - Gain a scientific understanding of what is happening during irradiation or during an accident
- **Existing TRISO fuel performance model**
  - **PARFUME**/TIMCOAT: 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.

TRISO Failure Modes

- Mechanical
  - Pressure vessel failure
  - Cracking of the IPyC layer
  - Partial debonding of IPyC/SiC and Buffer/IPyC
  - Pressure vessel failure of an aspherical particle
- Thermochemical
  - Amoeba effect
  - Palladium attack of the SiC layer
  - Corrosion of SiC by CO
  - SiC thermal decomposition



PARFUME – PARticle Fuel ModEl

- **Fuel Performance Code PARFUME Highlights**
  - Captures failure mechanisms, gas release, fission product transport, etc.
  - Thermomechanics was emphasized in the early 2000's
  - Fission product transport is more stressed lately

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

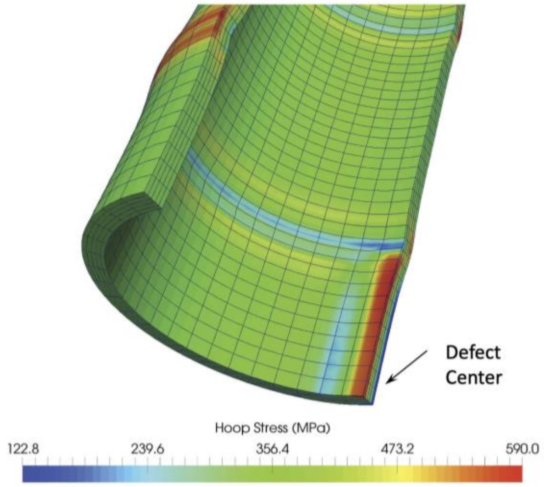
PARFUME in the AGR Program

PARFUME is routinely used for evaluations of new fuel particle designs, providing both pre and post irradiation and safety test predictions, supporting fuel fabrication specifications, and comparing model to PIE results

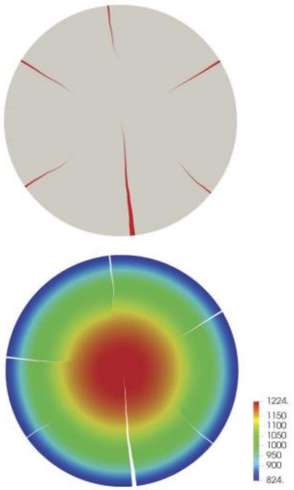
- **IAEA normal and accident benchmarks**
- **AGR-1**
  - Predictions
    - Irradiation
    - Safety Testing on 18 compacts
    - Palladium penetration (SiC failure)
  - Comparison to PIE
    - Fission product release during irradiation and during safety testing
    - Kernel swelling and buffer densification
  - Accident Benchmark (about to begin through GIF)
- **AGR-2**
  - Predictions
    - Irradiation
    - Safety Testing on 8 compacts
- **AGR-3/4 and AGR-5/6**
  - Predictions
    - Fuel specification basis evaluation
    - Fission product transport (AGR-3/4)

BISON – Nuclear Fuel Performance Code

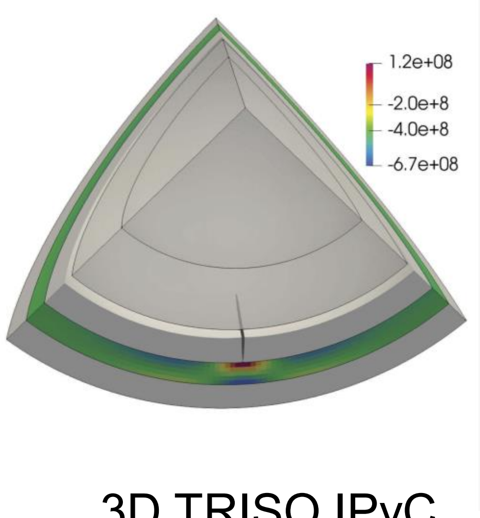
- Overarching objective to deliver an integrated set of **predictive** computational tools for nuclear fuel performance analysis and design.
- One of its major goals is to have a great amount of **flexibility** in how it is used, including in the types of fuel it can analyze, the geometry of the fuel 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.



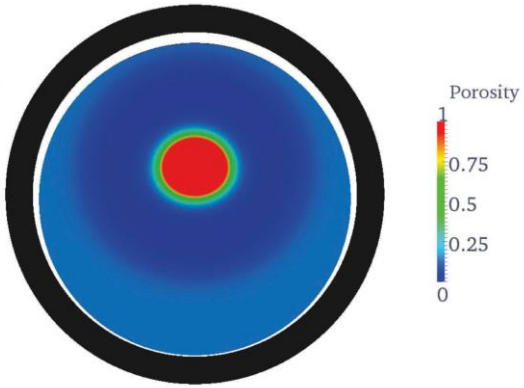
Hoop stress in the cladding near an MPS defect



LWR fuel radial cracks prediction



3D TRISO IPyC cracking modeling



Porosity contours in a restructured fuel pellet

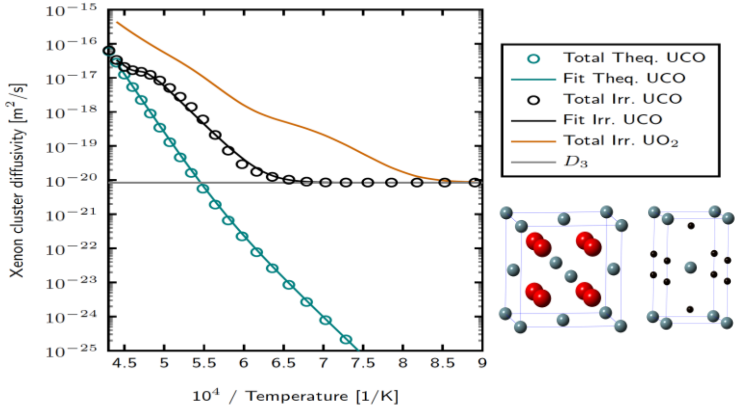
WILLIAMSON et al. · BISONS: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms, Nuclear Technology, DOI:10.1080/00295450.2020.1836940

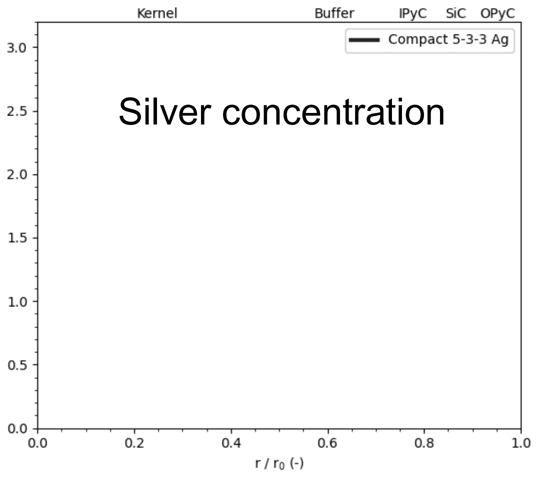
TRISO Fission Product Diffusion

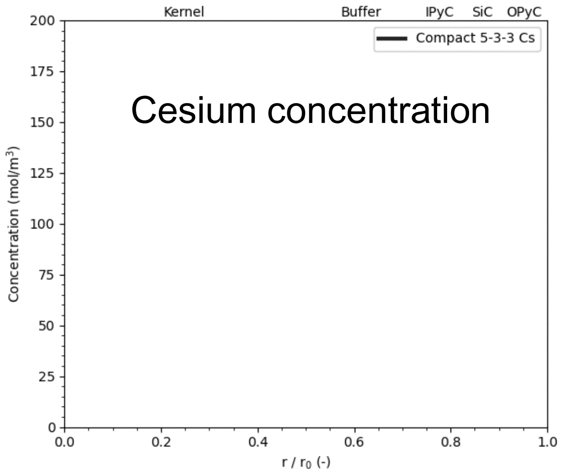
- Fission product diffusion modeling for TRISO fuel follows the same pattern as for any other fuel:

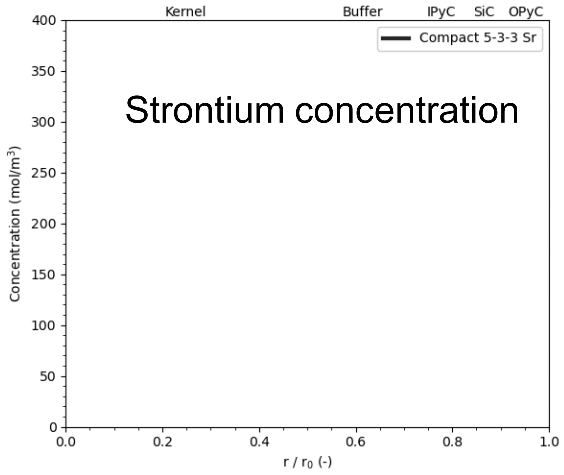
$$\frac{\partial C}{\partial t} = \nabla \cdot D\nabla C - \lambda C + S$$

- BISON provides two models for fission gas production and release:
  1. Sifgrs (Simple Integrated Fission Gas Release and Swelling)
     - For use with UO_2 and used in all our LWR cases.
  2. UCOFGR (Booth model)
     - For use with UCO. Diffusivities are obtained from **lower-length scale modeling** by LANL



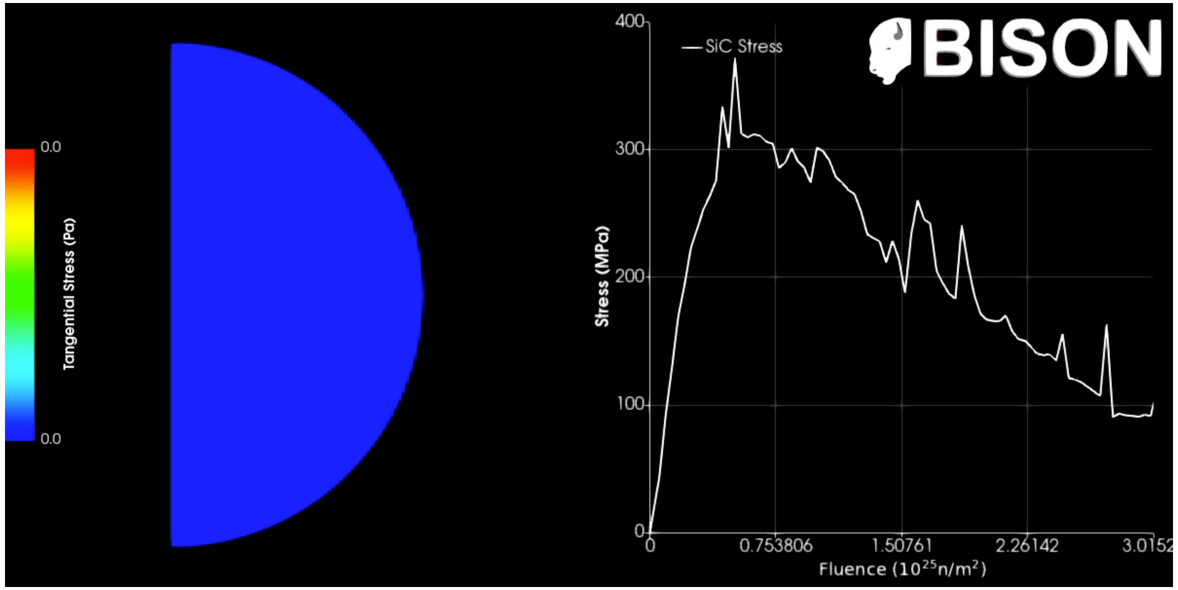


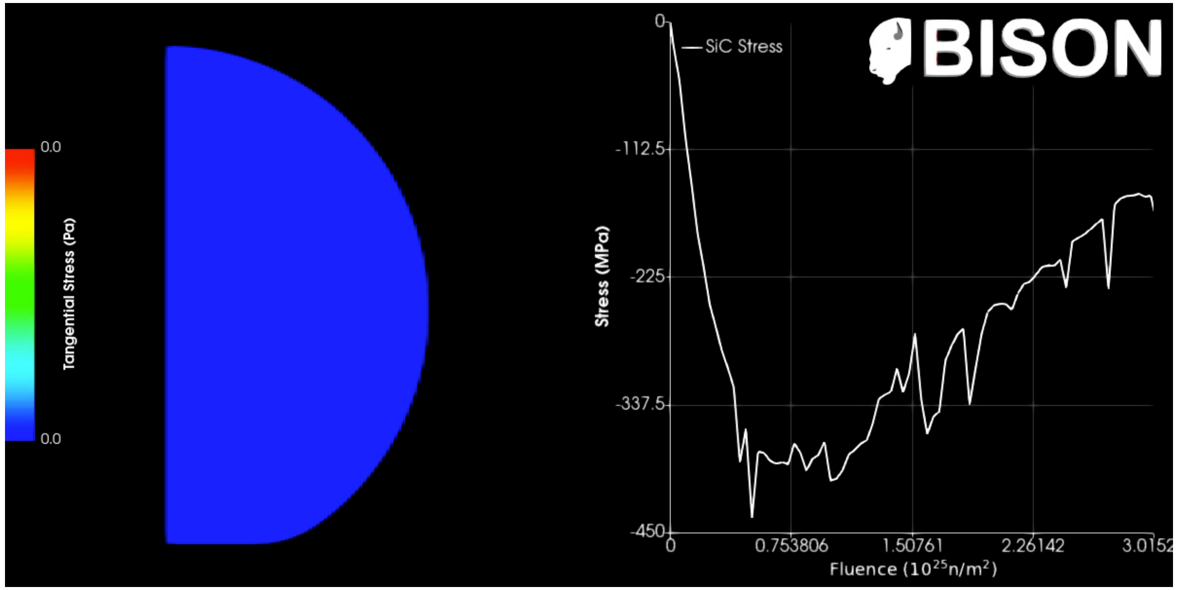




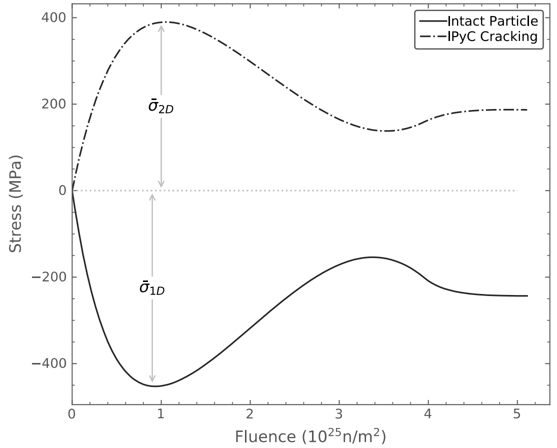
TRISO Multi-dimensional Failure Analysis

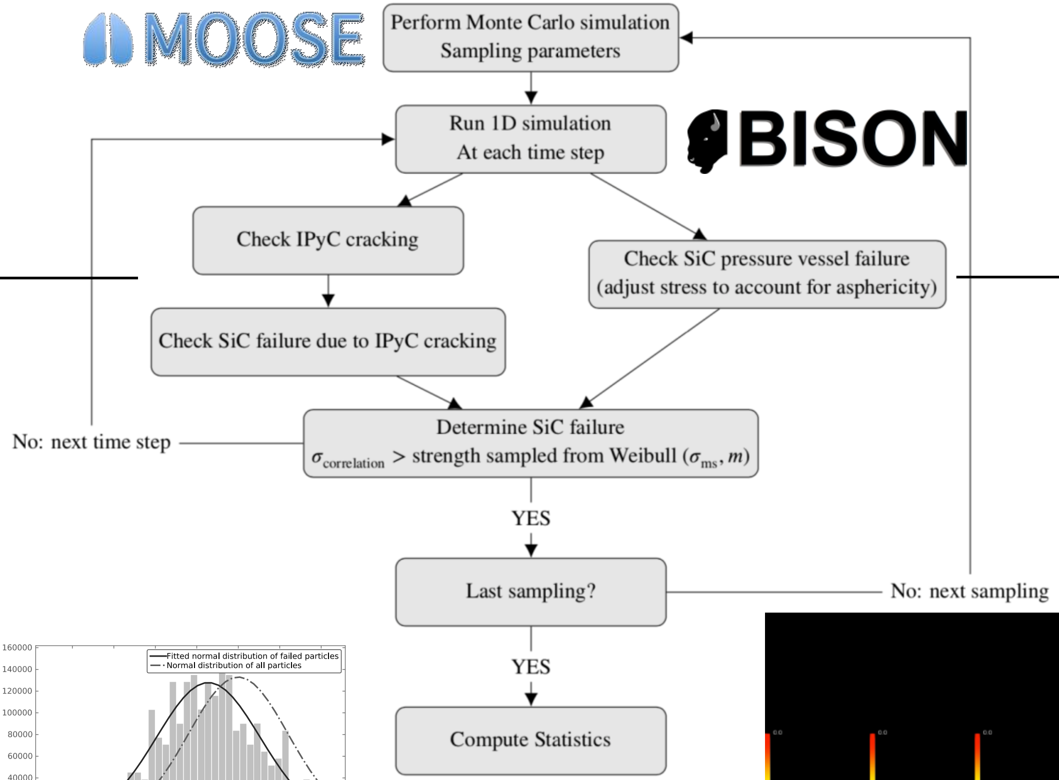
- BISON can model the following mechanical and thermochemical failures
  - Pressure vessel failure of spherical and aspherical particles
  - Irradiation-induced PyC failure leading to SiC cracking
  - IPyC-SiC and Buffer-IPyC debonding (on-going in FY21)
  - Palladium penetration of SiC

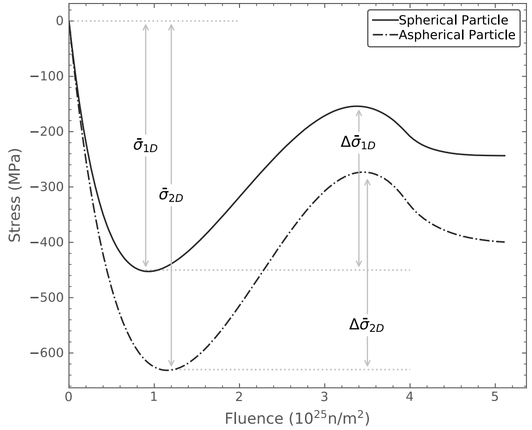


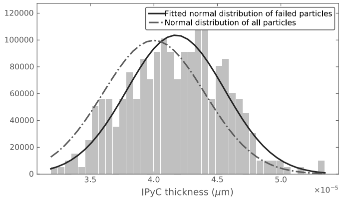


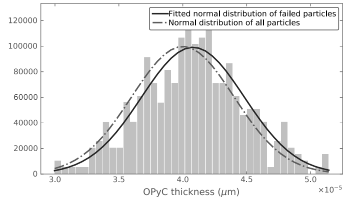
TRISO Monte Carlo Failure Probability Calculation

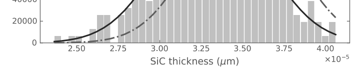




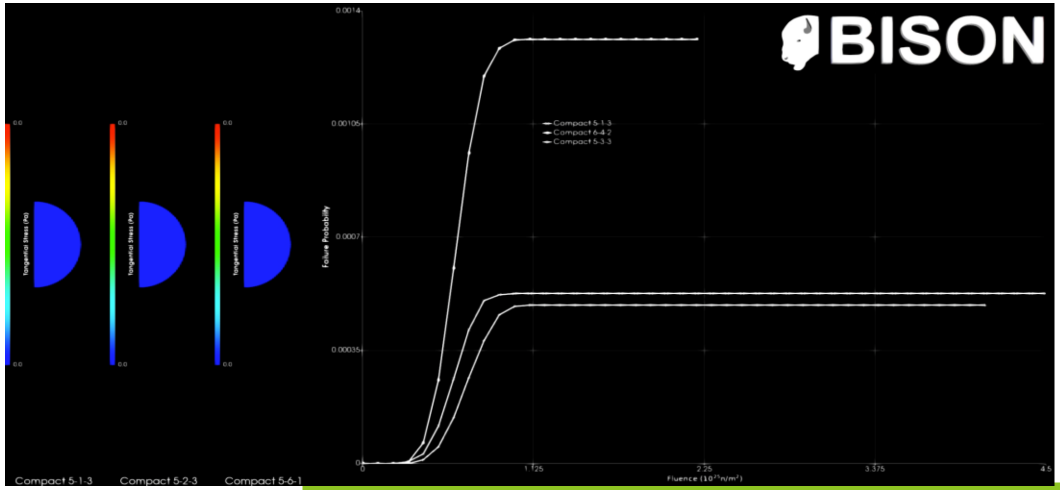








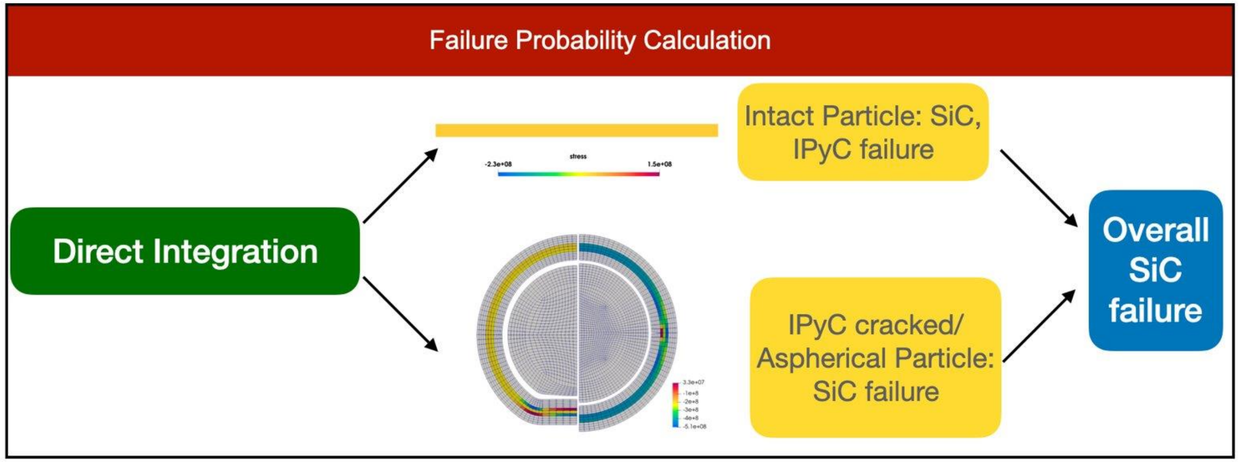
AGR5/6/7 Compact	BISON		PARFUME	
	IPyC cracking	SiC failure	IPyC cracking	SiC failure
5-1-3	7.45 x 10^{-1}	7.34 x 10^{-4}	5.96 x 10^{-1}	5.88 x 10^{-4}
5-2-3	6.55 x 10^{-1}	4.9 x 10^{-4}	5.62 x 10^{-1}	5.26 x 10^{-4}
5-6-1	9.15 x 10^{-1}	1.31 x 10^{-3}	8.52 x 10^{-1}	1.33 x 10^{-3}



Fast Integration to Compute Failure Probability

- Although BISON/MOOSE's build-in Monte Carlo sampling incurs very minimal computational overhead, it is still very expensive to run a very large number of Monte Carlo samples (more than 100 millions).
- We have been developing (almost done) a fast integration approach to calculate failure probability that needs much less time than the Monte Carlo approach.
  - It performs direct integration of failure probability density using sparse grid method.
  - It allows to directly run 2D high-fidelity analysis without relying on stress correlation factors.

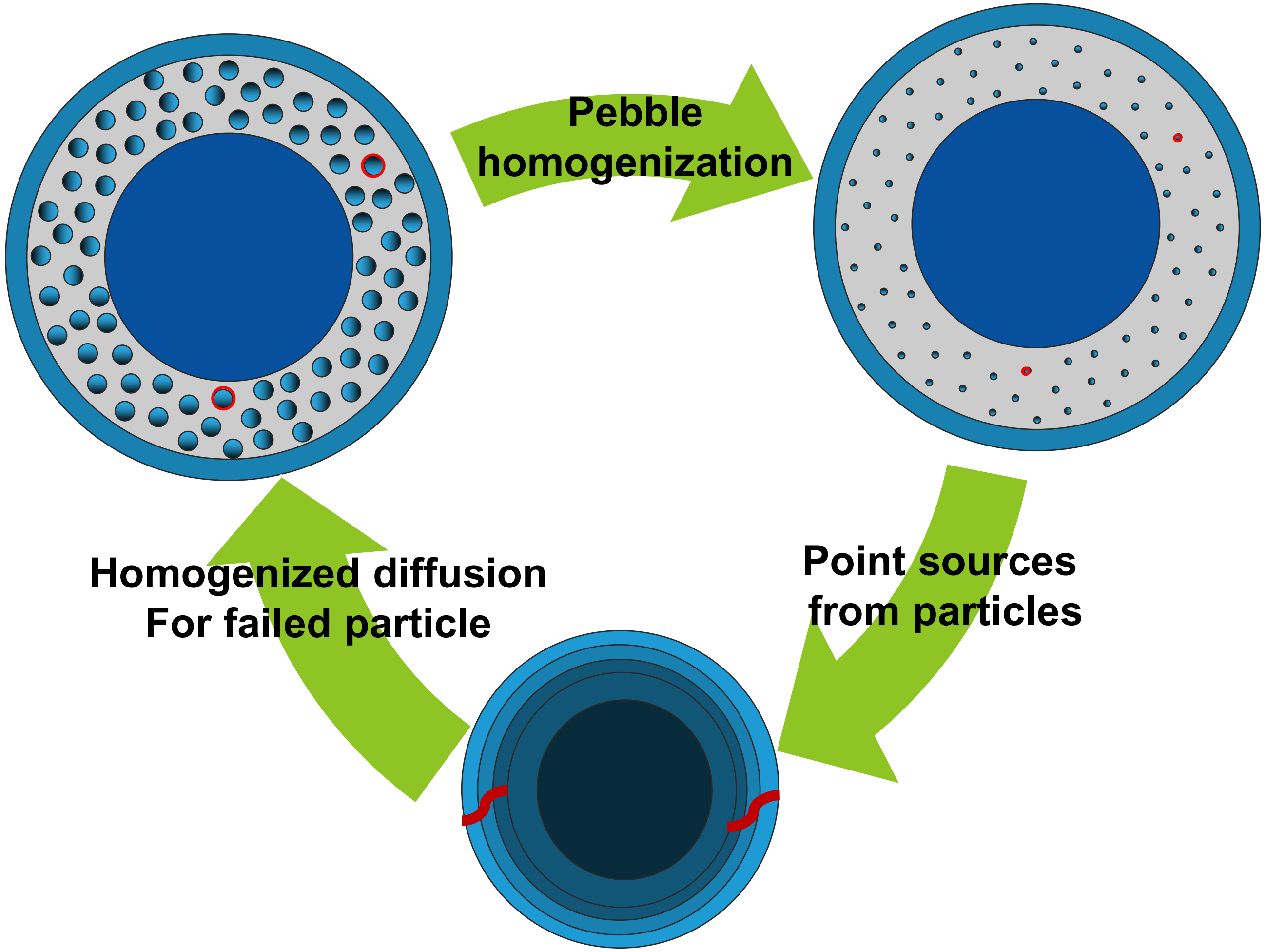
$$P = \frac{1}{\sqrt{2\pi}^n D_j D_k \ldots} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \ldots \exp\left(-\frac{(-v_j - \mu_j)^2}{2D_j^2}\right) \left[1 - \exp\left(-\left(\frac{\sigma_c(v_j, v_k \ldots)}{\sigma_{ms}}\right)^m\right)\right]$$

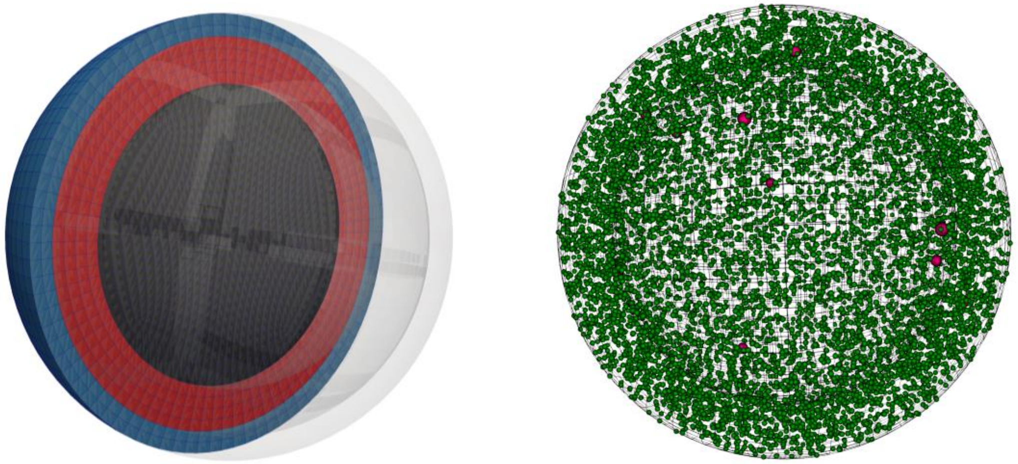


New flow chart using fast integration approach (higher accurate and less time)

AGR-2 Compact	Monte Carlo		Fast Integration	
	IPyC cracking	SiC failure	IPyC cracking	SiC failure
5-1-3	2.23×10^{-1}	9.75×10^{-5}	2.28×10^{-1}	1.08×10^{-4}
5-3-3	1.25×10^{-1}	4.53×10^{-5}	1.31×10^{-1}	5.05×10^{-5}
6-4-2	3.59×10^{-1}	1.16×10^{-4}	4.02×10^{-1}	1.42×10^{-4}
6-4-3	3.15×10^{-1}	1.12×10^{-4}	3.00×10^{-1}	1.11×10^{-4}

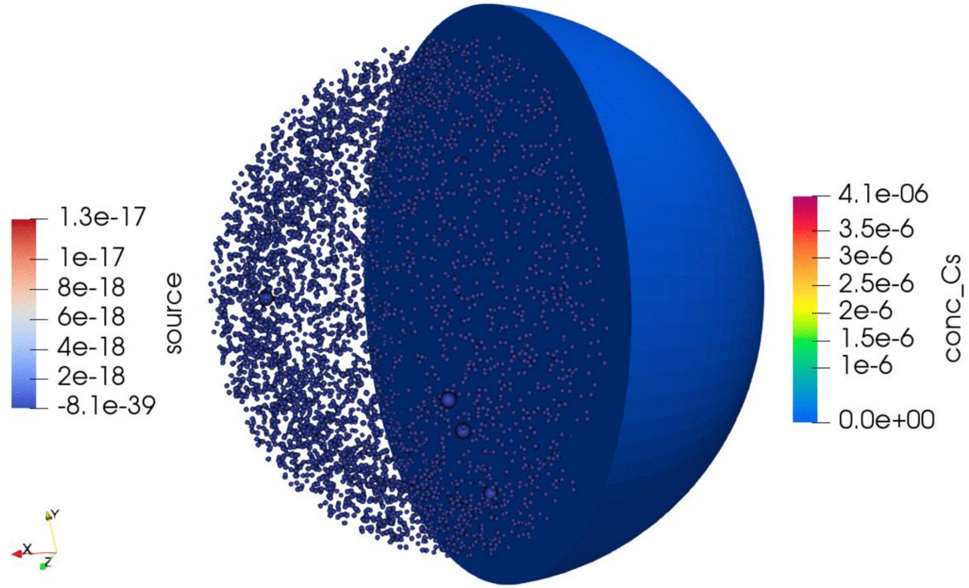
Pebble/Compact Modeling





Multi-Scale Pebble and Particle Simulation:

1. Monte Carlo calculation of particle point sources
2. 3D pebble/compact modeling



Cs concentration

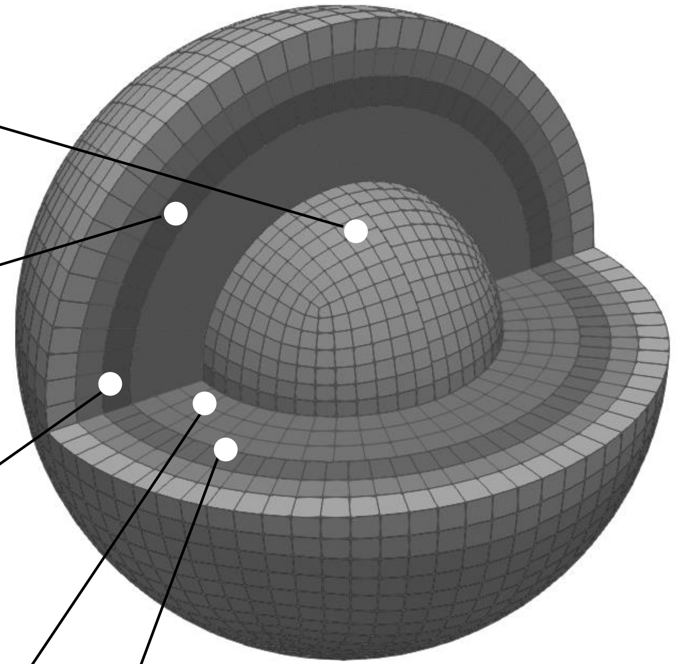
UCO-TRISO Thermal-mechanical Models

UCOThermal
UCOBurnup
UCOElasticityTensor
UCOVolumetricSwellingEigenstrain
UCOFGR

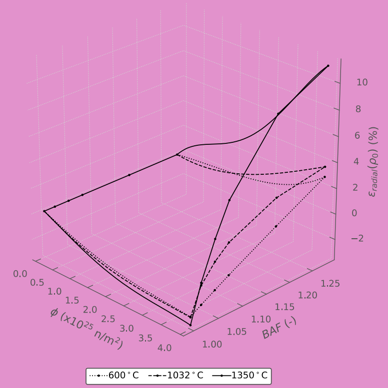
BufferThermal
BufferElasticityTensor
BufferCEGACreep
BufferThermalExpansionEigenstrain
BufferCEGAIrradiationEigenstrain

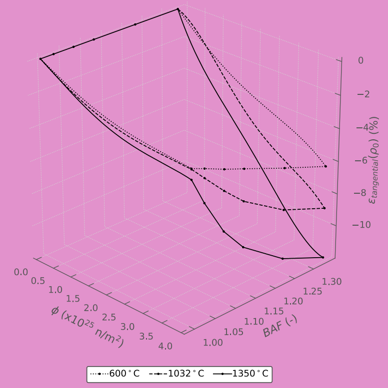
MonolithicSiCElasticityTensor
MonolithicSiCThermal
SiCPdPenetration

GraphiteMatrixThermal



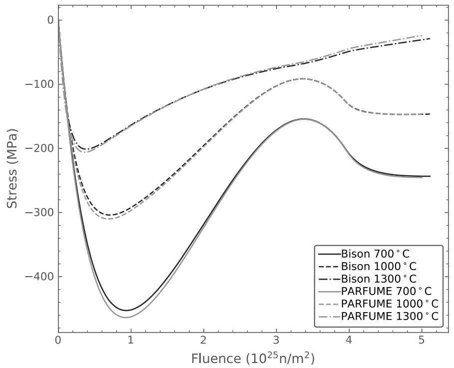
PyCThermalExpansionEigenstrain
PyCElasticityTensor
PyCCEGACreep
PyCCEGAIrradiationEigenstrain
PyCCharacteristicStrength
BaconAnisotropyFactor



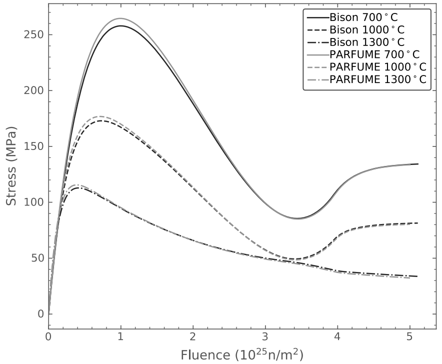


BISON and PARFUME Comparison

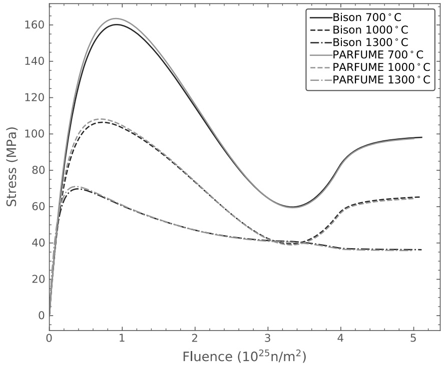
Condition	EFPD	Burnup (%FIMA)	Fast fluence (10^{25} n/m^2, E>0.18 Mev)	Irradiation Temperature (℃)
1	500	13.5	5	700
2	500	13.5	5	1000
3	500	13.5	5	1300



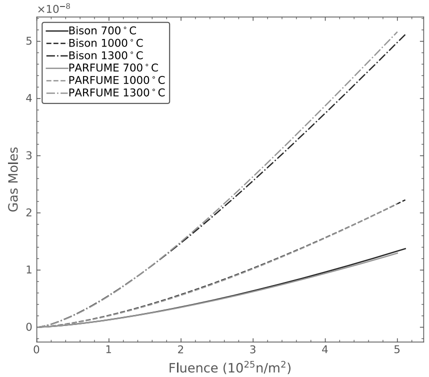
Tangential stress in SiC



Tangential stress in IPyC

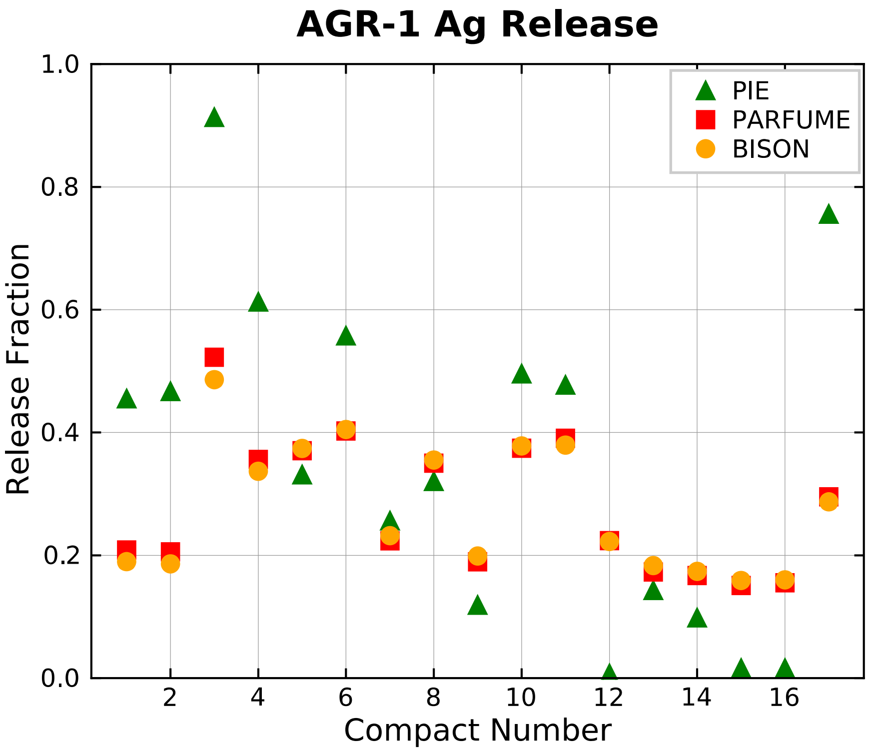


Tangential stress in OPyC

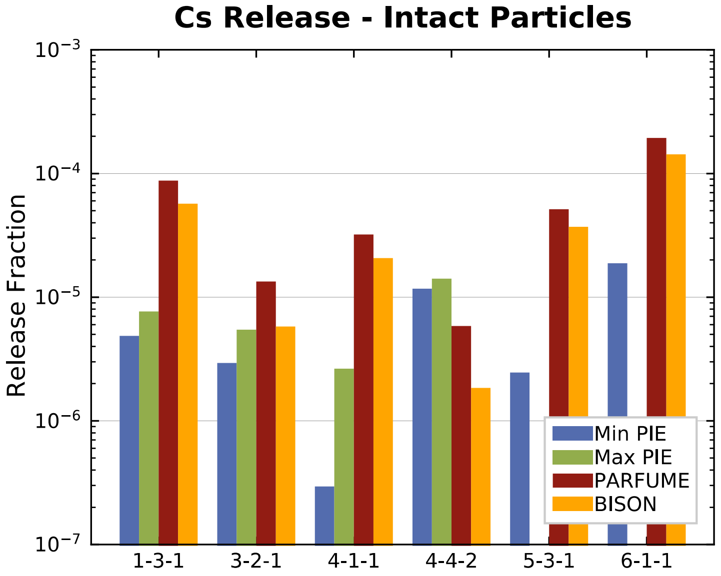


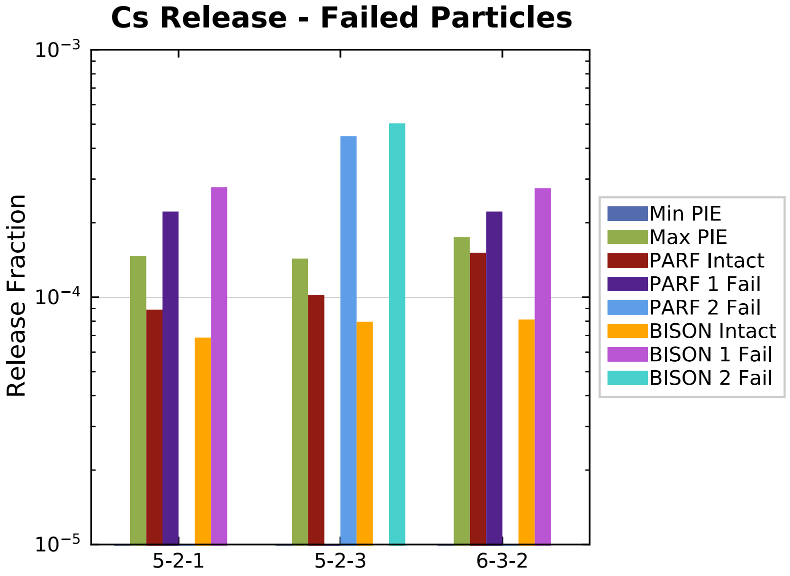
Gas Moles

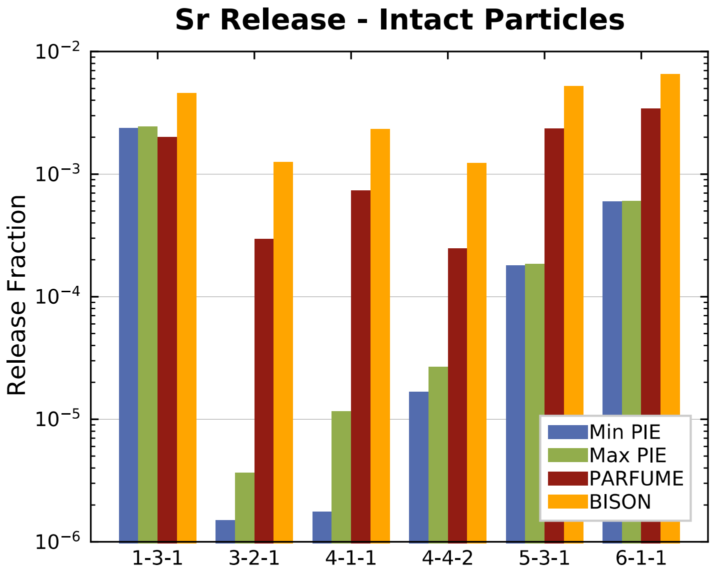
TRISO AGR-1 Validation

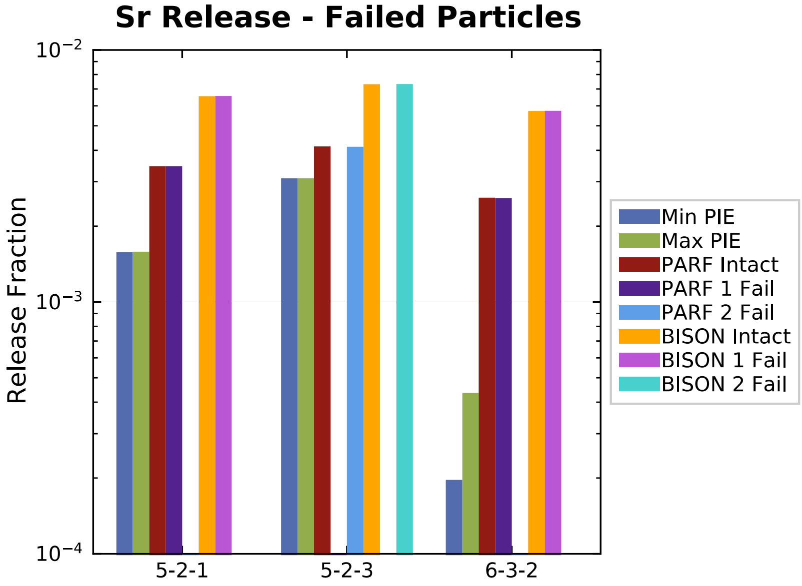


Comparison of measured and computed silver release fractions for seventeen compacts

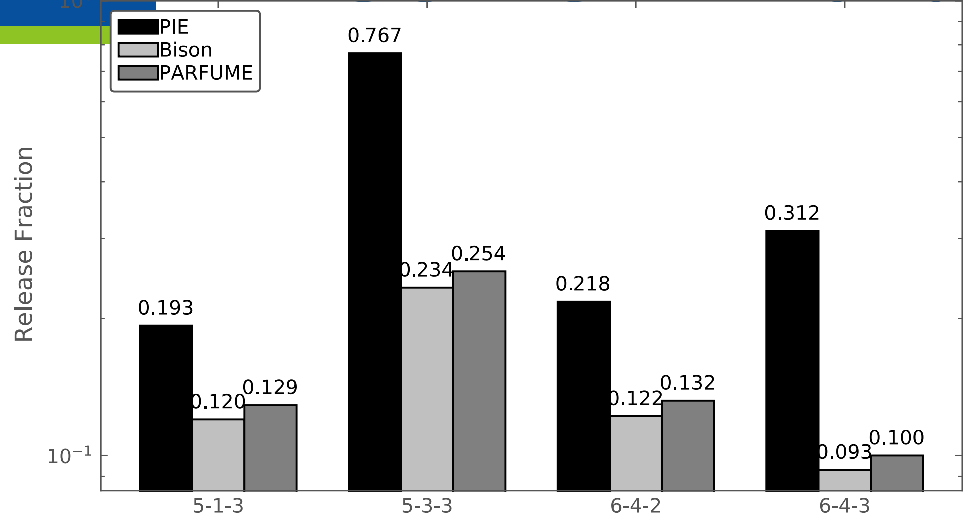




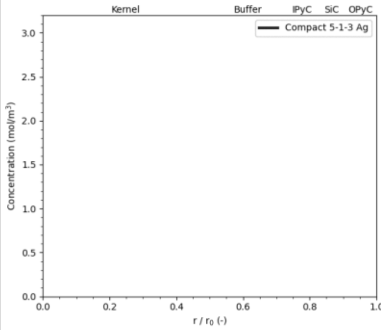




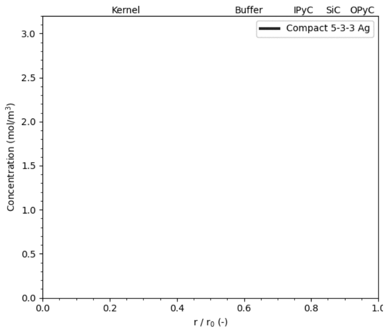
TRISO AGR-2 Validation



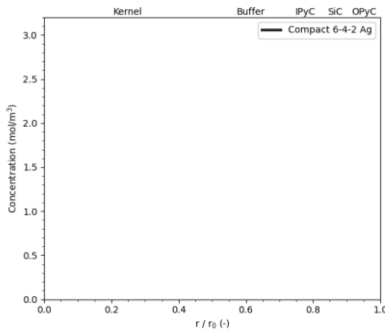
Silver release fractions



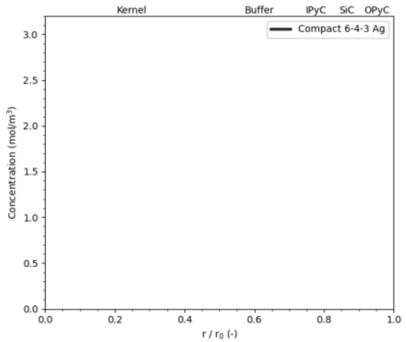
Silver compact 5-1-3



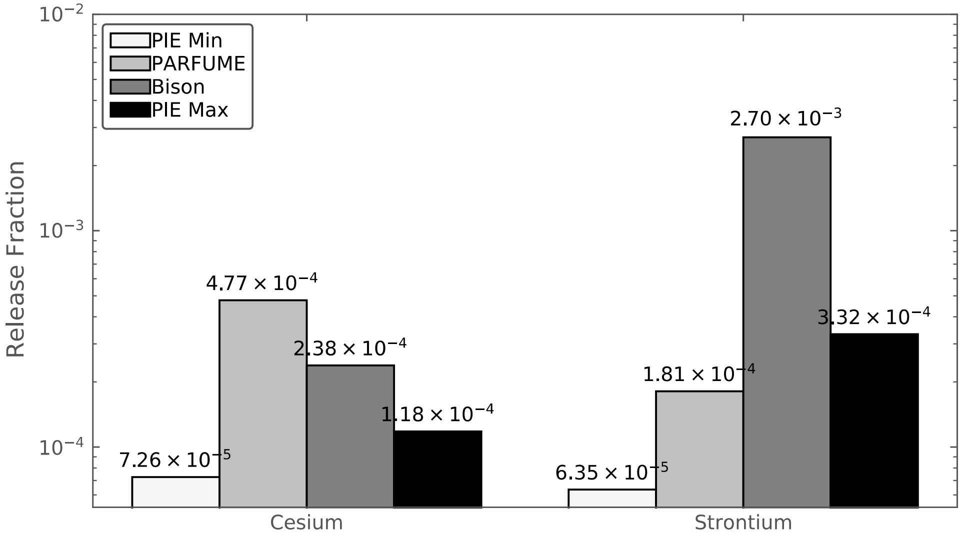
Silver compact 5-3-3



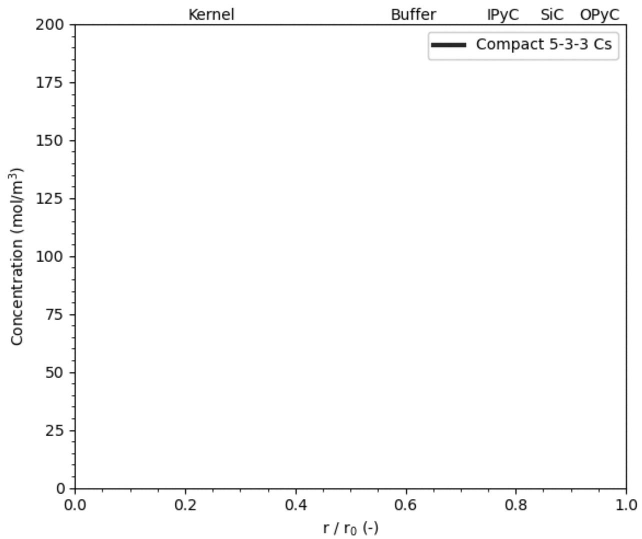
Silver compact 6-4-2



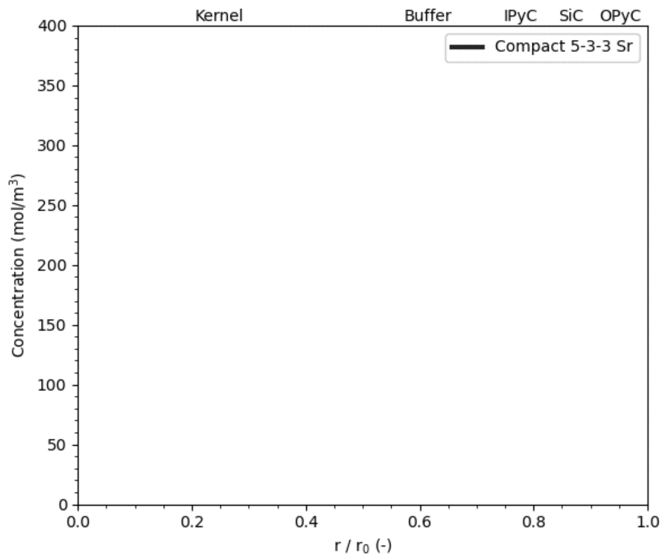
Silver compact 6-4-3



Cesium and Strontium release fractions (Compact 5-3-3)



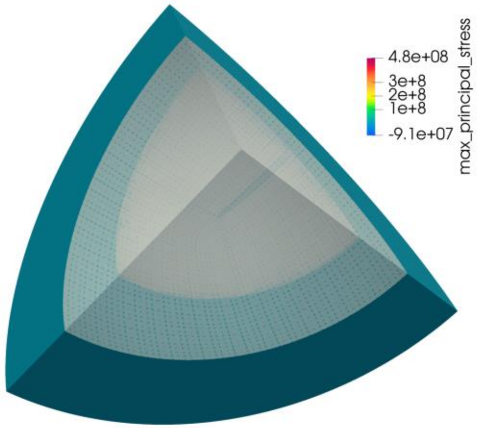
Cesium compact 5-3-3

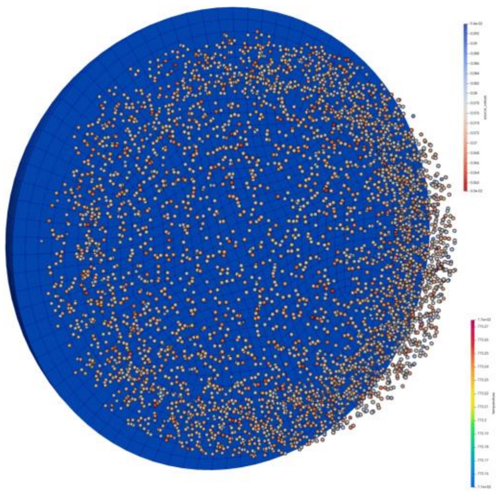


Strontium compact 5-3-3

Conclusion

- **PARFUME**
  - captures failure mechanisms, gas release, fission product transport, etc.
  - used in the AGR program
  - reliable prediction tool, models fine tuned with PIE results
- **BISON**
  - has almost all PARFUME models and their capabilities (failure probability calculation)
  - utilize **multidimensional**, multi-physics, **multiscale** approach





Suggested Reading

- Fuel Performance and Fission Product Transport Modeling
  - J.J. Powers, B.D. Wirth, A review of TRISO fuel performance models, J. Nucl. Mater. 405 (2010) 74-82
  - G.K. Miller et al., PARFUME Theory and Model Basis Report, INL/EXT-08-14497, September 2018
  - W. F. Skerjanc, B. P. Collin, Assessment of Material Properties for TRISO Fuel Particles used in PARFUME, INL/EXT-18-44631, August 2018
- BISON TRISO Fuel Performance Modeling
  - J.D. Hales et al, Multidimensional multiphysics simulation of TRISO particle fuel, JNM, 2013
  - W. Jiang et al, TRISO particle fuel performance and failure analysis with BISON, JNM, 2021
  - J.D. Hales et al, Modeling fission product diffusion in TRISO fuel particles with BISON, JNM 2021
  - WILLIAMSON et al. BISONS: A Flexible Code for Advanced Simulation of the Performance of Multiple Nuclear Fuel Forms, Nuclear Technology, DOI:10.1080/00295450.2020.1836940

Idaho National Laboratory