GAS-COOLED REACTOR
ADVANCED REACTOR TECHNOLOGIES PROGRAM

July 17, 2024

Overview of Graphite Model Development

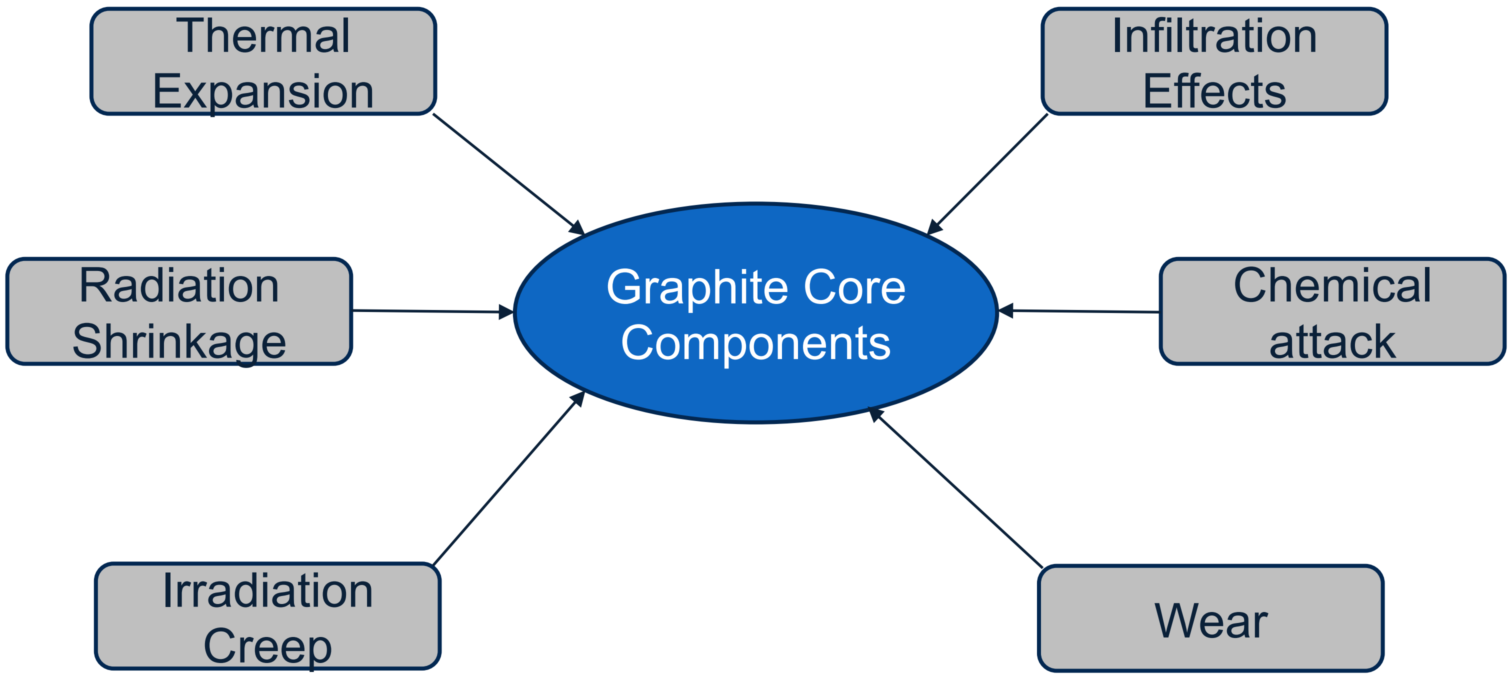
V Prithivirajan
Computational Material Scientist- INL

DOE ART GCR Review Meeting
Hybrid Meeting at INL
July 16–18, 2024

Outline

- Introduction
- Thermo-mechanical graphite models
- Oxidation modeling
- Wear modeling
- Graphite in molten salt
  - Potential degradation mechanisms
  - Stress due to volumetric heating
  - Role of different parameters
- Modeling salt infiltration into graphite
- Models for non-linear mechanical behavior of graphite
- Summary

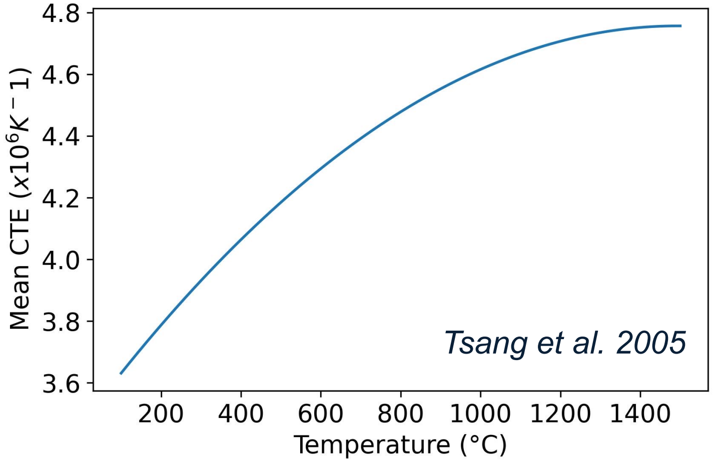
Introduction



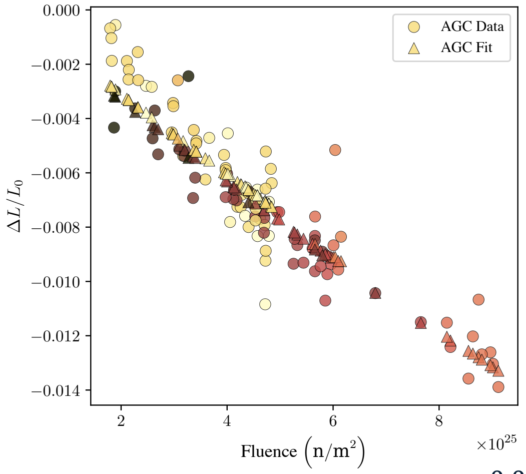
- Graphite components are subjected to multiple loading scenarios in a nuclear environment
- Build a comprehensive simulation capability for graphite

Thermo-mechanical graphite models

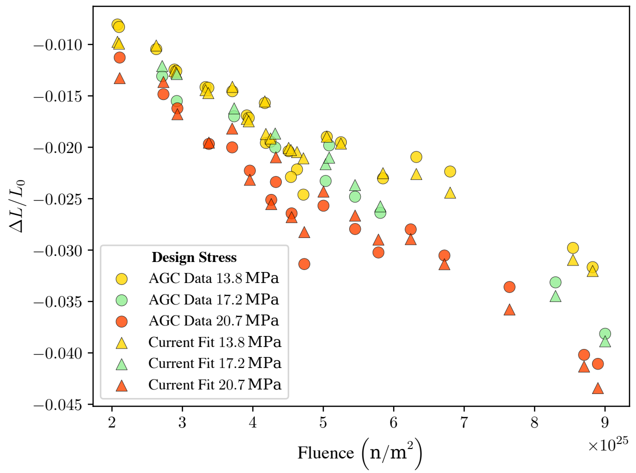
Contributor: Parikshit Bajpai (INL)



$$\epsilon^{TE} = CTE.(T - T_{ref})\boldsymbol{I}$$



$$\epsilon^{RS} = 0.00184\gamma^2 - 0.0136e^{\frac{0.01466}{k_B T}\gamma}$$



$$\epsilon^{IC} = \frac{\sigma}{E_0} - 0.000334e^{0.0016T}\sigma\gamma$$

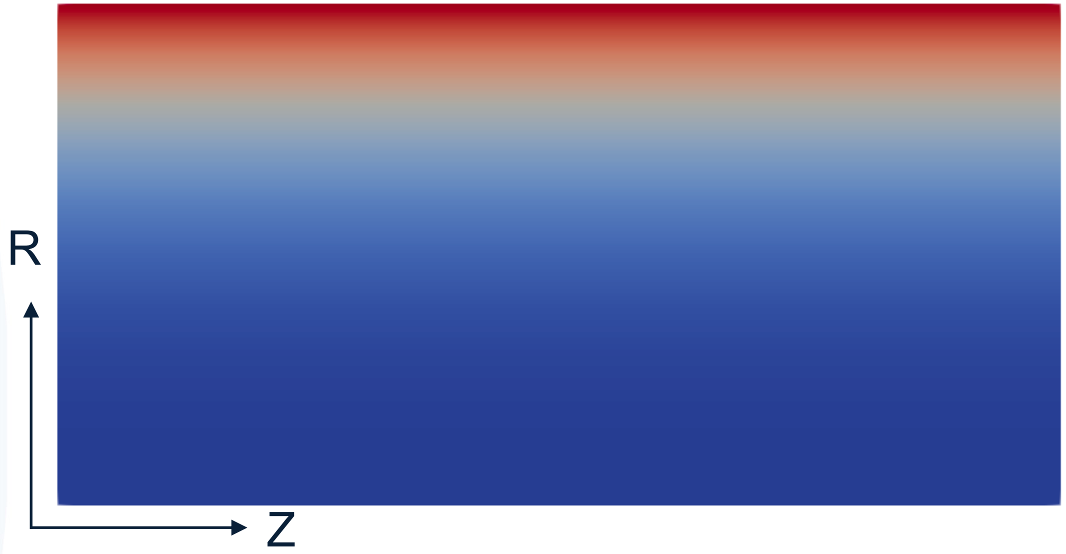
Empirical models for thermal expansion, radiation shrinkage, and irradiation creep are implemented in Grizzly* (MOOSE Application)

Available grades: H-451, IG-110, and NBG-18

*P Bajpai et al. Development of Graphite Thermal and Mechanical Modeling Capabilities in Grizzly. INL Report. 2024 [INL/RPT-24-78905]

This work was funded by NEAMS
POC: Benjamin Spencer (INL)

Oxidation Modeling



Penetration of oxygen in graphite

$$N_i \cong -[C_T]D_{eff}\nabla y_i + y_i N_i$$

$$\frac{\partial \varepsilon[CO2]}{\partial t} = -\nabla N_{CO_2} + (1-x)k_e f f'' S_A[O_2]$$

$$\frac{\partial \varepsilon[CO]}{\partial t} = -\nabla N_{CO} + x k_e f f'' S_A[O_2]$$

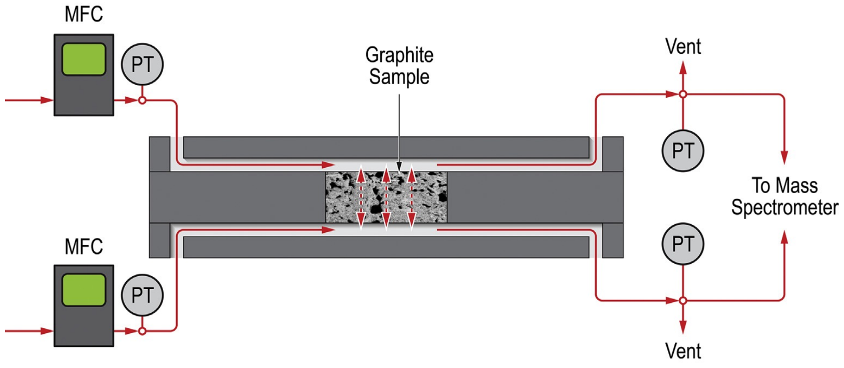
$$\frac{\partial \varepsilon[O2]}{\partial t} = -\nabla N_{O_2} + \left(1-\frac{x}{2}\right) k''_{eff} S_A[O_2]$$

$$\frac{\partial \varepsilon[I]}{\partial t} = -\nabla N_I$$

Oxidation model is available in Grizzly for IG-110 and NBG-18 grades

Joseph Bass, Graphite Degradation Modeling and Analysis, INL Report, 2022 [INL/EXT-21-65240]

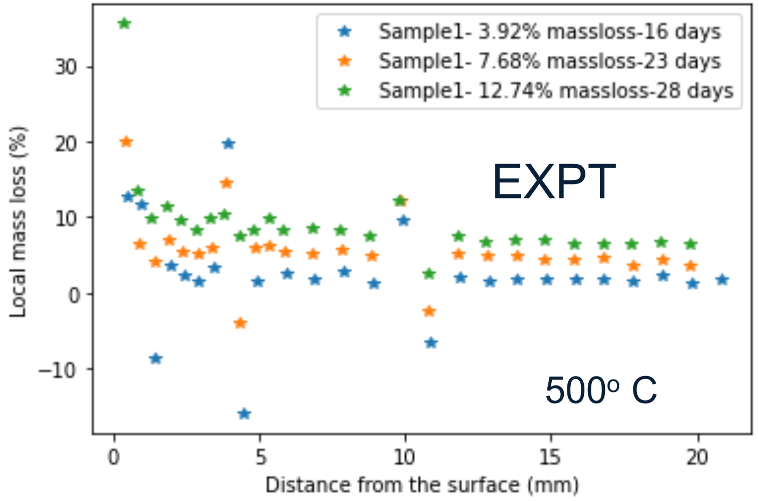
Oxidation Modeling



Diffusion experiment

$$N_i \cong -[C_T]D_{eff}\nabla y_i + y_i N_i$$

D= 2 in, L = 1 in

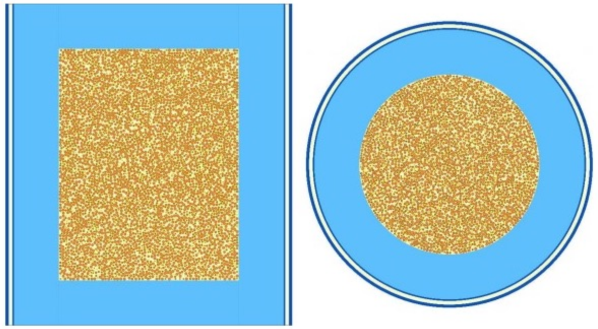


Experimental Collaborators: Rebecca Smith, Chuting Tsai, and Mayura Silva (INL)

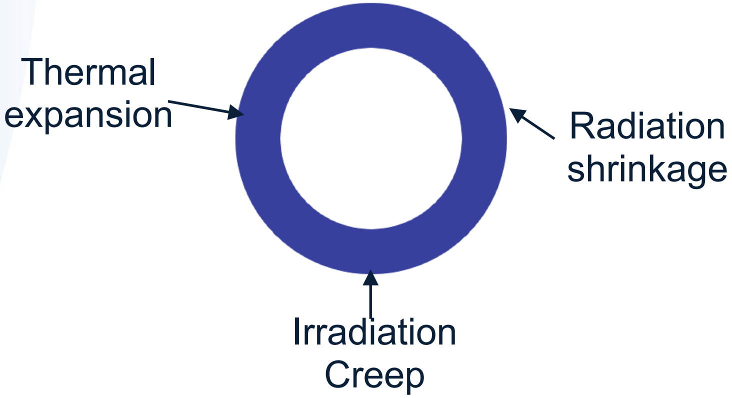
* JJ Kane et al, Carbon 136 (2018).

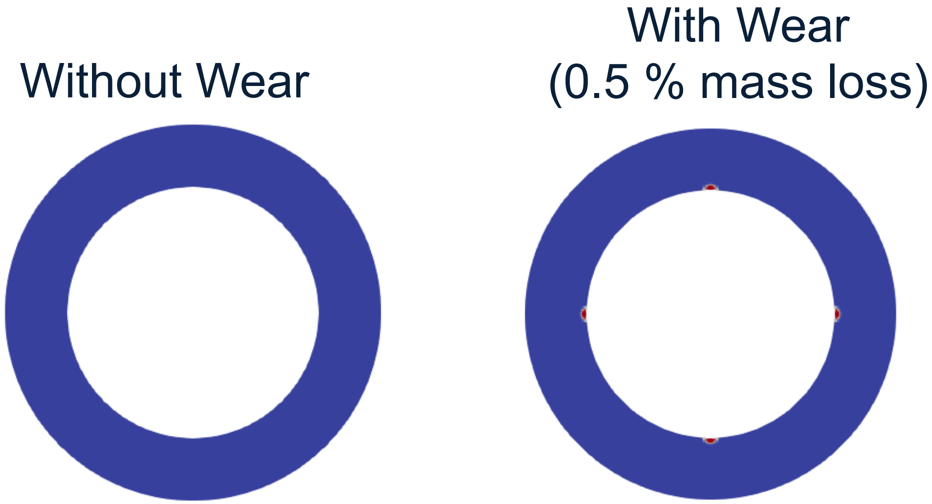
This work was funded by DOE ART
POC: William Windes (INL)

Wear Modeling



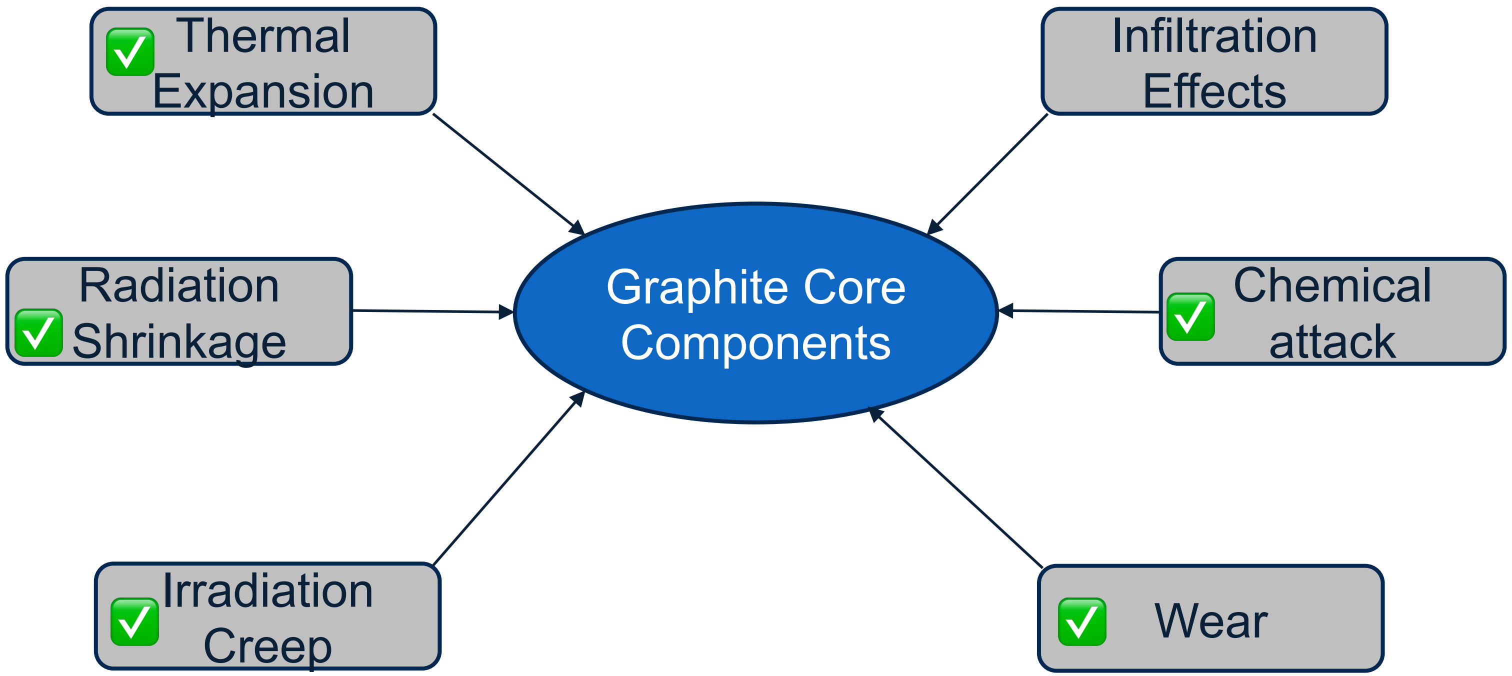
Axial (left) and Radial (right) section views of the gFHR model





This work was funded by Nuclear Regulatory Commission (NRC)
POC: Joseph Bass (NRC)

Quick Recap


✅ Thermal Expansion
Infiltration Effects
Radiation ✅ Shrinkage
Graphite Core Components
✅ Chemical attack
✅ Irradiation Creep
✅ Wear

Graphite in molten salt

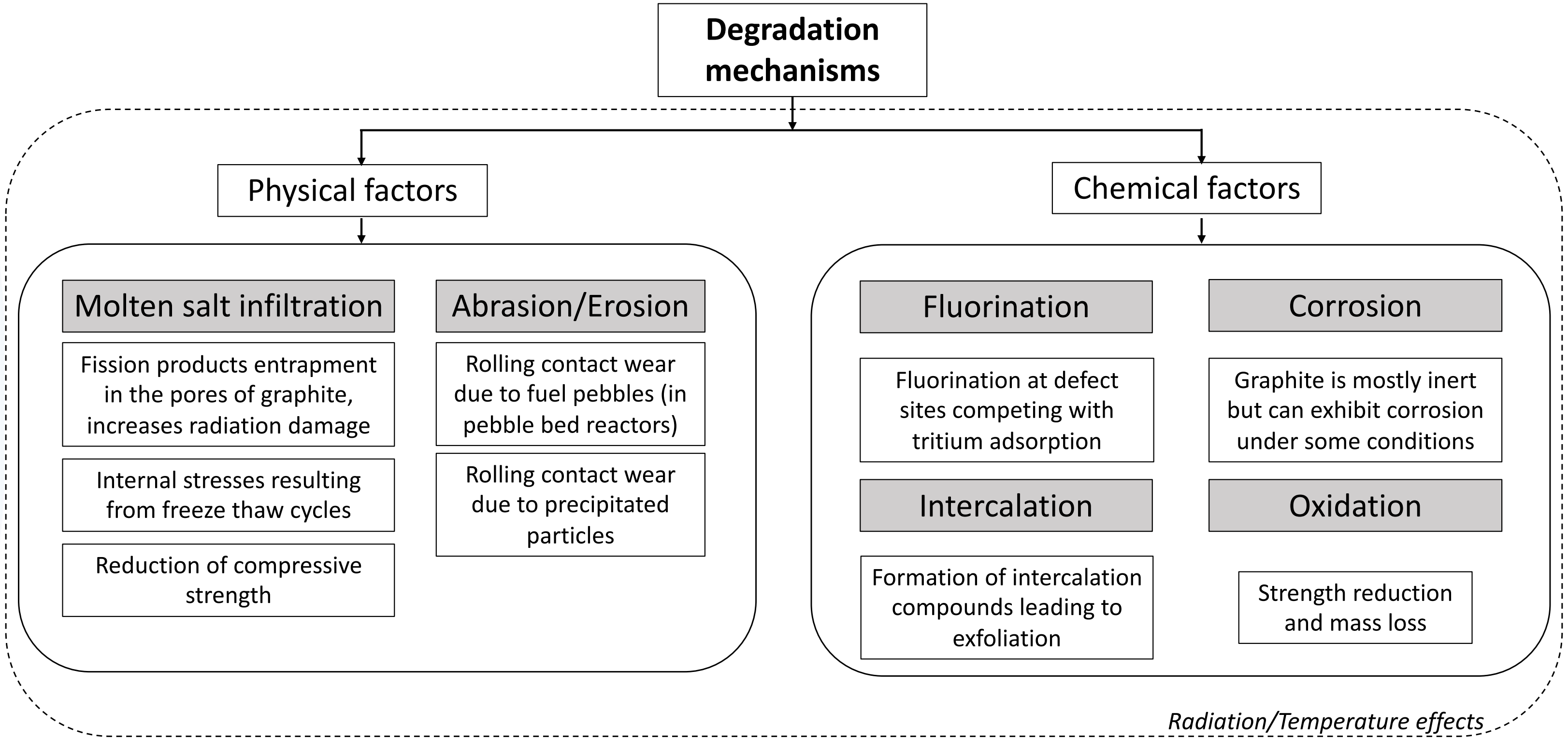
Analysis of graphite's interaction with molten salt has several associated challenges:

- Limited experimental data and operation experience
  - Limited knowledge of degradation factors and their potential impact
- Limited analysis methods (MSR specific considerations are very limited in the ASME Code)
- Limited modeling capabilities have been developed for graphite-molten salt interactions

The NRC recognizes the importance developing computational tools for modeling graphite-molten salt interactions.

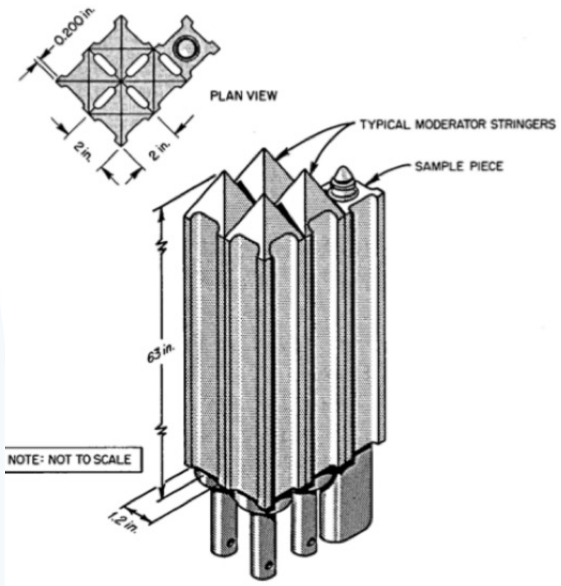
The following molten salt computations work is intended to support the NRC in assessment of vendor applications.

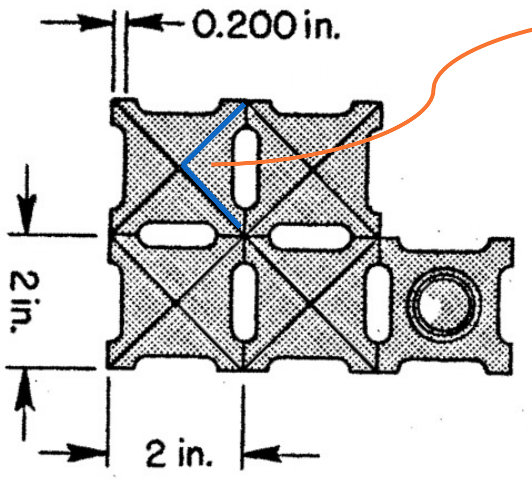
Potential degradation mechanisms

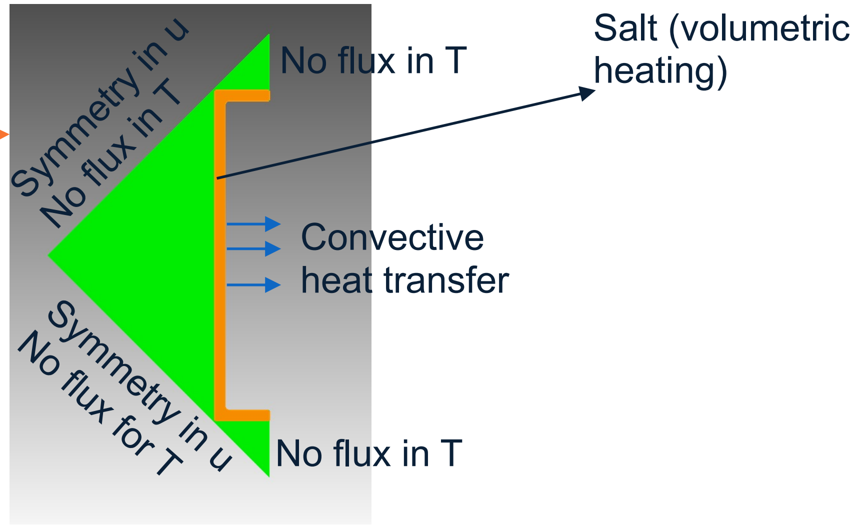


V.Prithivirajan, Examining Graphite Degradation in Molten Salt Environments: A Chemical, Physical, and Material Analysis, NRC Technical Letter Reports, August 2024.

Does salt infiltration induce stress ? – simulation setup



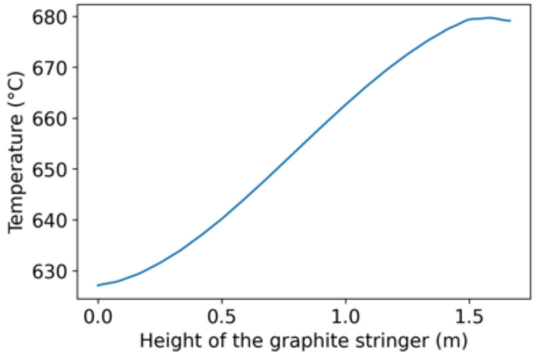


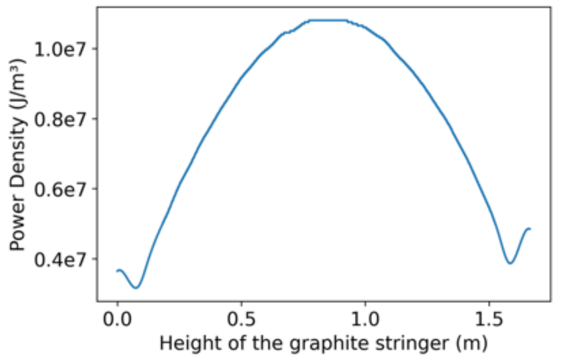


#	Property	Unit	Value
1	Young's modulus	GPa	9.8
2	Poisson's ratio		0.14
3	Thermal conductivity	W/mK	63
4	Specific heat (@ 600°C)	J/kg	1400
5	Density	kg/m³	1760
6	CTE	/K	4.50E-06

Heat source is applied over continuous space, so it has been scaled by porosity fraction to keep the total heat consistent

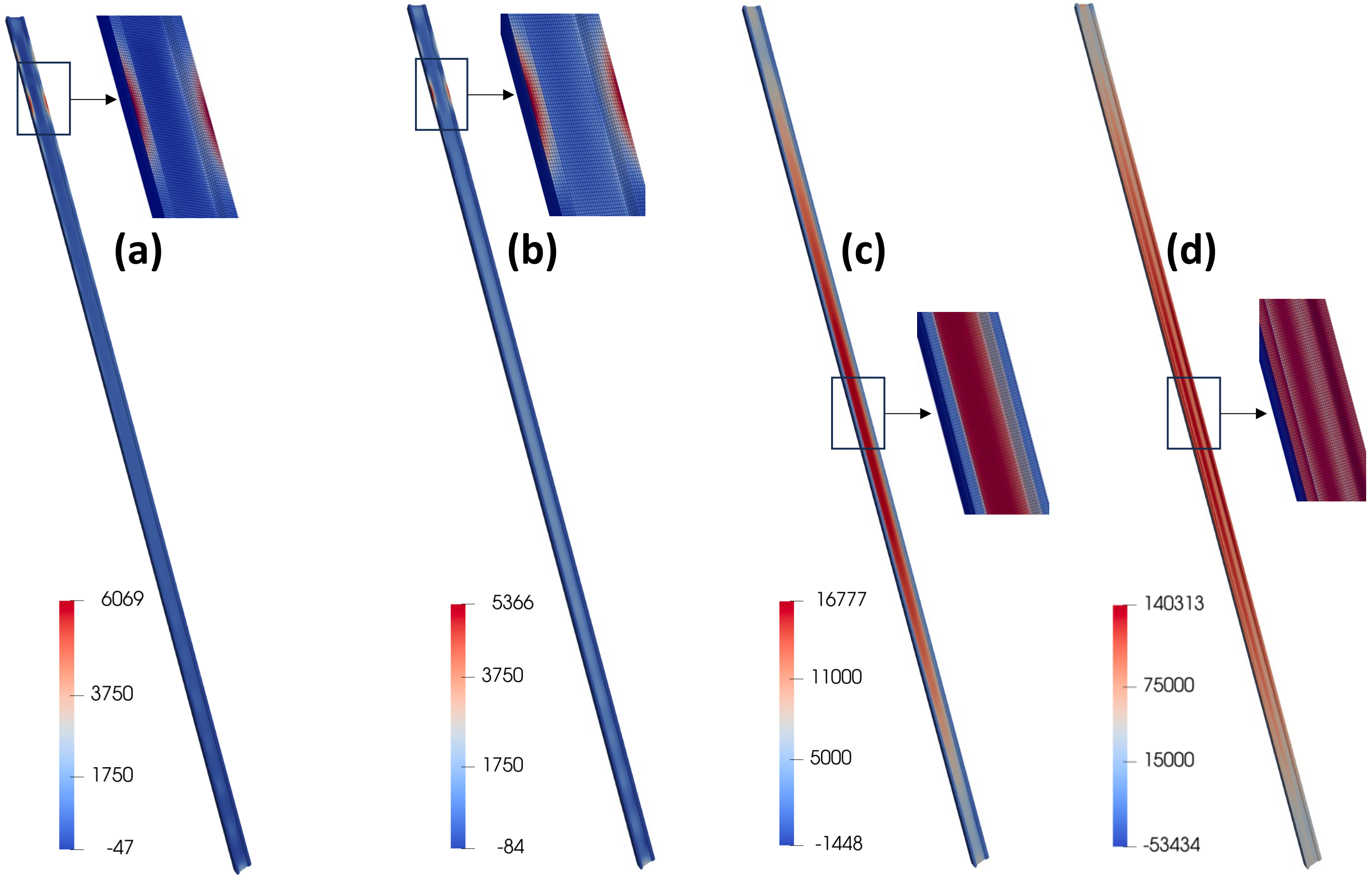
*Mustafa et al. Thermal Spectrum Molten Salt-Fueled Reactor Reference Plant Model. 2023



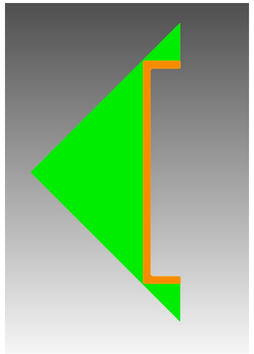


This work was funded by Nuclear Regulatory Commission (NRC)
POC: Joseph Bass (NRC)

Does salt infiltration induce stress ? – Simulation results

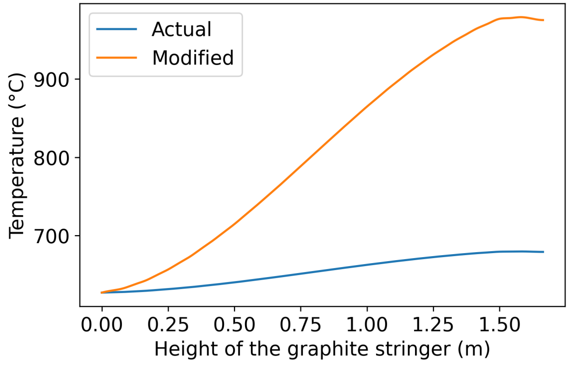


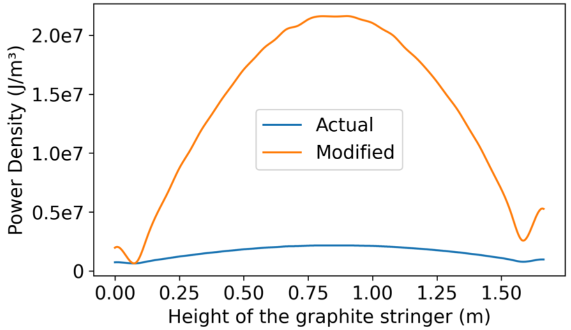
Variation of maximum principal stress (Pa) induced by volumetric heating because of salt infiltration at different levels: (a) 0%, (b) 10%, (c) 50%, and (d) 100%.

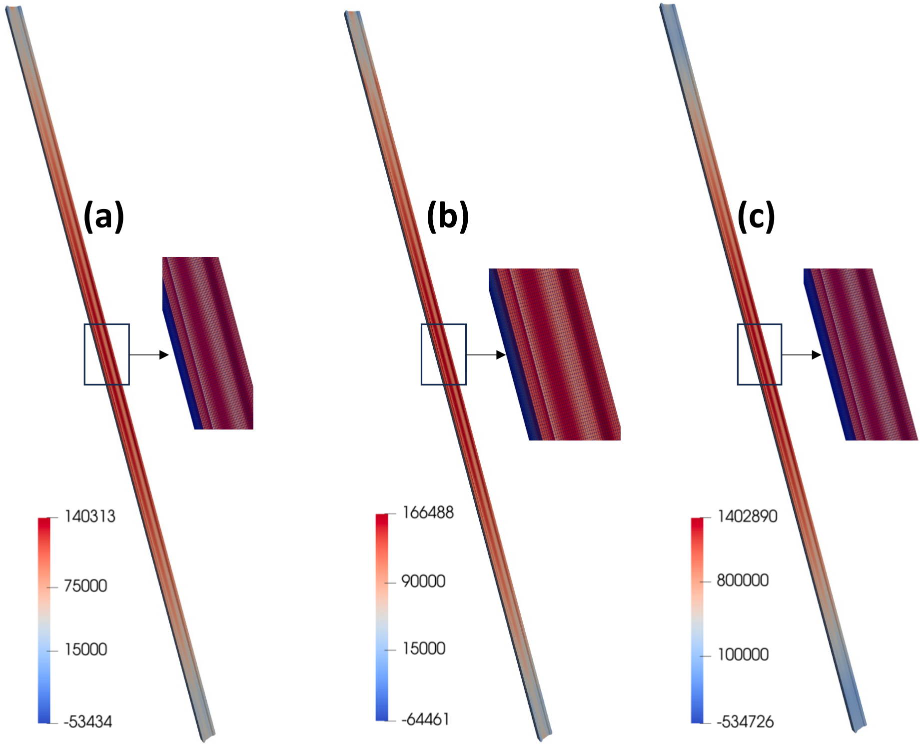


This work was funded by Nuclear Regulatory Commission (NRC)
POC: Joseph Bass (NRC)

Role of temperature and power density variations



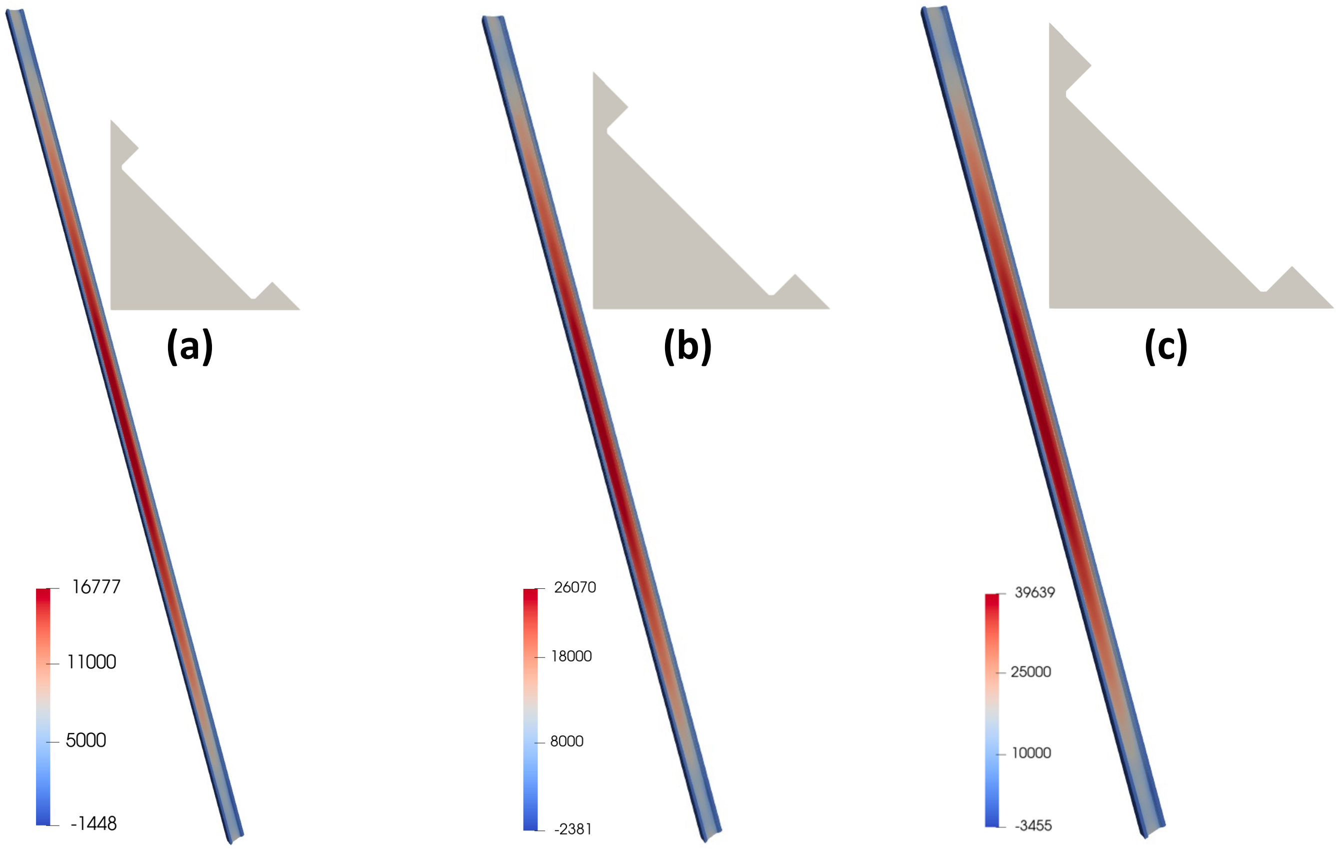




Maximum principal stress induced by volumetric heating with variations in (b) temperature distribution and (c) power density compared to the baseline case (a)

This work was funded by Nuclear Regulatory Commission (NRC)
POC: Joseph Bass (NRC)

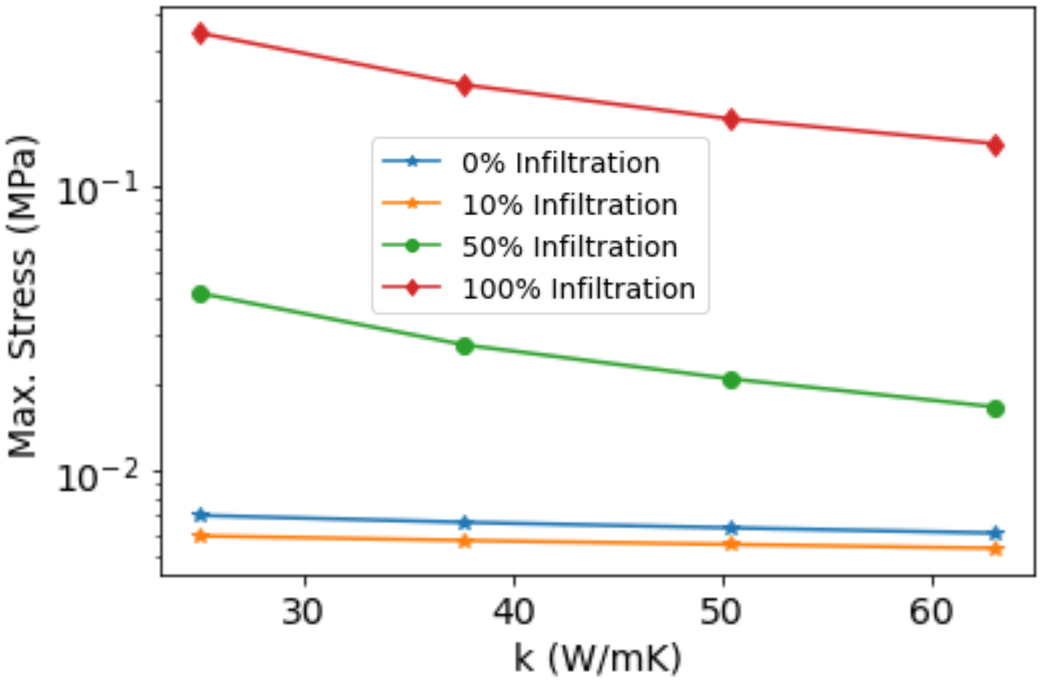
Role of cross-section geometry



Maximum principal stress induced by volumetric heating for different cross-sectional variations compared to the baseline (a): (b) 1.25X and (c) 1.5X.

This work was funded by Nuclear Regulatory Commission (NRC)
POC: Joseph Bass (NRC)

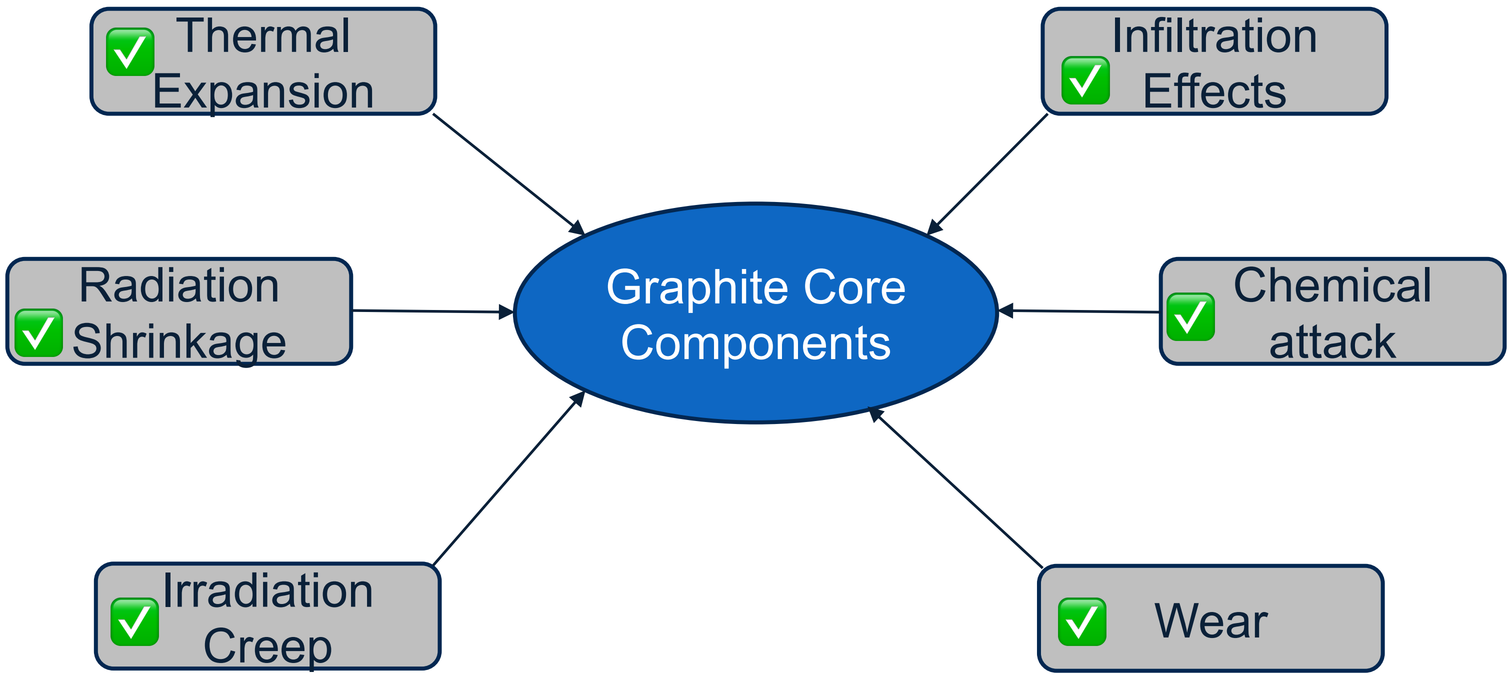
Role of thermal conductivity



Influence of graphite's thermal conductivity on maximum stresses induced by volumetric heating across different levels of salt infiltration

This work was funded by Nuclear Regulatory Commission (NRC)
POC: Joseph Bass (NRC)

Quick Recap

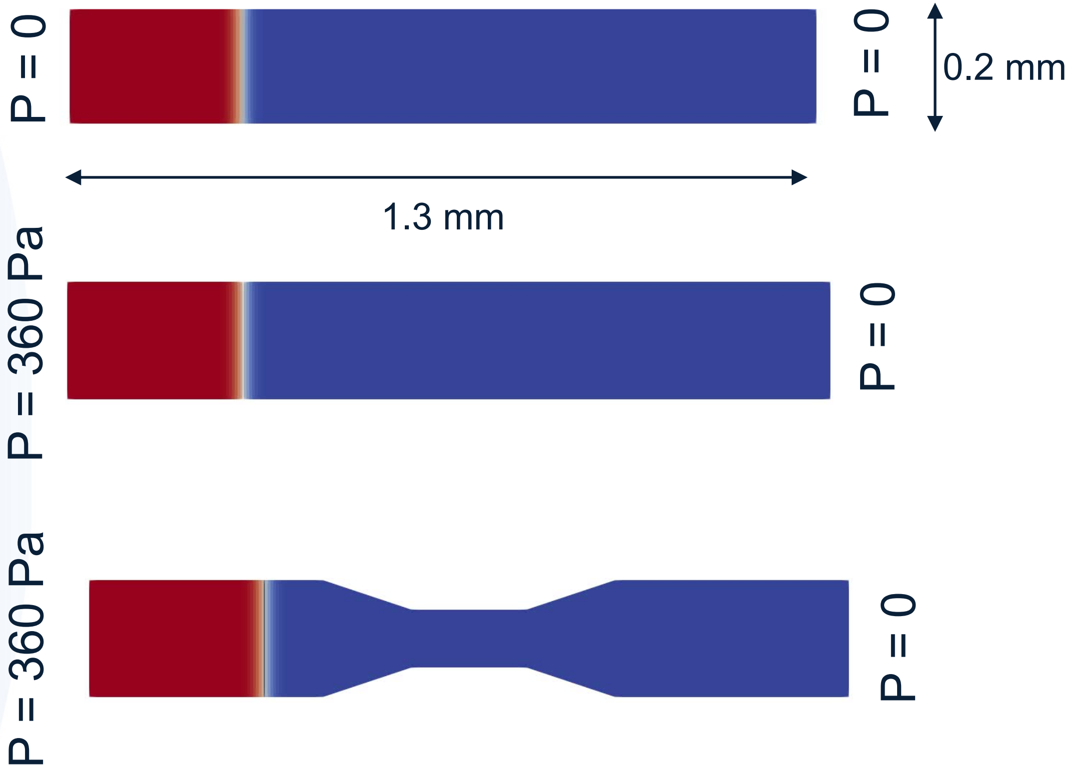


Thermal Expansion
Infiltration Effects
Radiation Shrinkage
Graphite Core Components
Chemical attack
Irradiation Creep
Wear

Two Phase Flow

FLiNaK (Non-Wetting)

Gas (Wetting)



Fluid Equations

$$\frac{\partial u}{\partial t} + \rho(u.\nabla)u + \nabla \mathrm{P} - \nabla.\tau - \rho g - \frac{\nu}{\epsilon^2}\psi\nabla\phi = 0$$

$$\nabla.u = 0$$

Phase-Field Equations

$$\frac{\partial \phi}{\partial t} + u.\nabla\phi - \frac{\nu\lambda}{\epsilon^2}\nabla^2\phi = 0$$

$$\psi + \epsilon^2\nabla^2\psi - \phi(\phi^2 - 1) = 0$$

Boundary Conditions

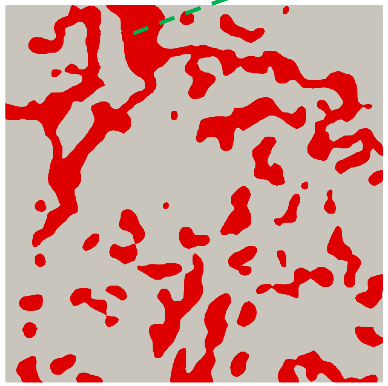
$$u = 0\ (\partial\Omega)$$

$$\nabla\phi.n = \frac{1}{\lambda}\left(\frac{3\sigma}{4}\right)\cos(\theta)\,(1 - \phi^2)$$

Develop two-phase flow capability within MOOSE to model salt infiltration into graphite

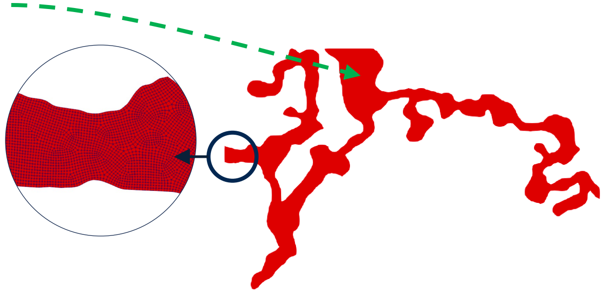
This work was funded by DOE ART
POC: William Windes (INL)

Modeling salt infiltration into graphite



50 µm

CT slice of IG-110 graphite*



Extracted 2D
Geometry and Mesh
(QUAD9)

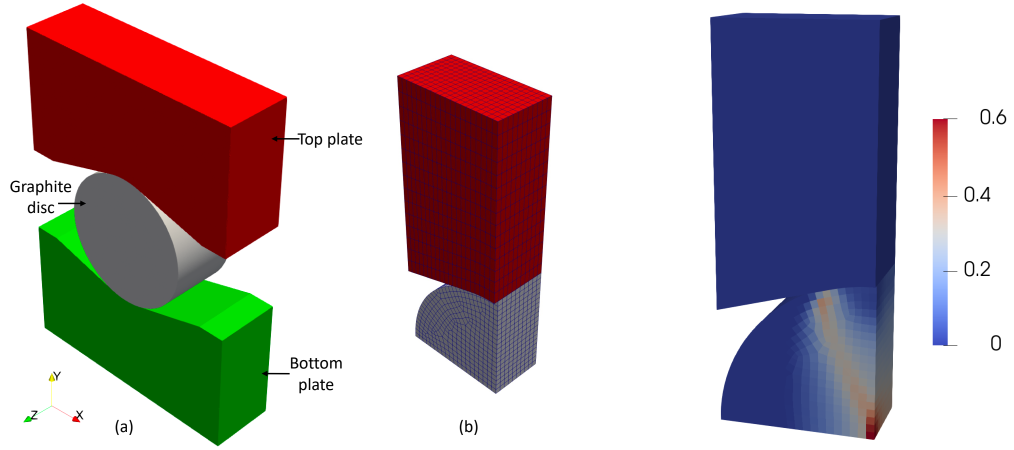
*CT slice provided by J. David Arregui Mena (ORNL)

Experimental Collaborators: J. David Arregui Mena, Nidia Gallego (ORNL)

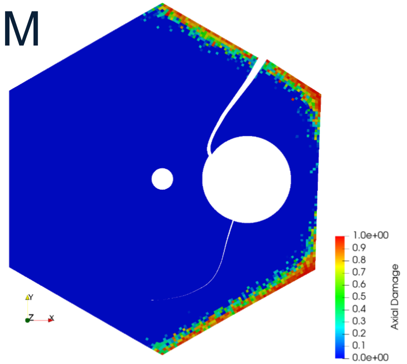
This work was funded by DOE ART
POC: William Windes (INL)

Models for non-linear mechanical behavior of graphite

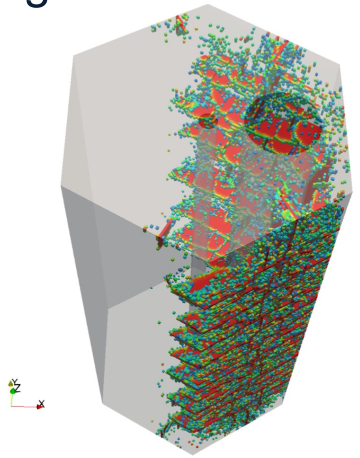
Damage plasticity model



XFEM



Smeared cracking model



Models for non-linear mechanical behavior are implemented in Blackbear

Experimental Collaborators: Arvin Cunningham (INL) and Lianshan Lin (ORNL)

B.Spencer et al. Initial Fracture Propagation Modeling of Graphite Components with Grizzly. INL Report. 2023 [INL/RPT-23-74062]

This work was funded by NEAMS
POC: Benjamin Spencer (INL)

Summary

- Thermo-mechanical models in Grizzly
- Efforts on low temperature oxidation behavior of graphite using Grizzly
- Approach to wear modeling
- Molten salt infiltration
  - Predicted stress-induced due to volumetric heating caused by fuel-salt infiltration
  - Studied role of temperature- and power density distributions, and thermal conductivity
- Developed a two-phase flow model to study molten salt infiltration into graphite
- Existing structural models in Blackbear

GAS-COOLED REACTOR

ADVANCED REACTOR TECHNOLOGIES PROGRAM

U.S. DEPARTMENT OF ENERGY

GAS-COOLED REACTOR

ADVANCED REACTOR TECHNOLOGIES PROGRAM

Thank You!

V Prithivirajan

veerappan.prithivirajan@inl.gov

U.S. DEPARTMENT OF ENERGY