INL/MIS-21-63219-Revision-0

Modeling Graphite Degradation (Oxidation and Irradiation)

July 2021

Changing the World's Energy Future

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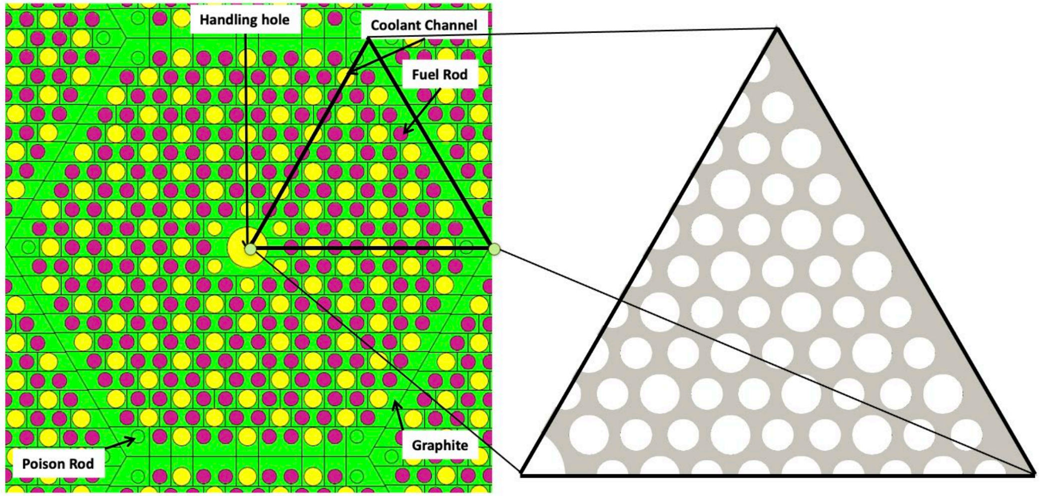
ART
Advanced Reactor Technologies

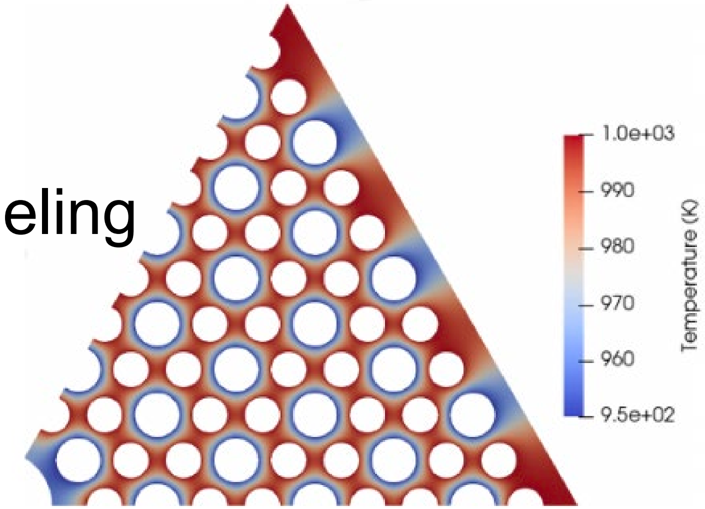
Presentation Outline

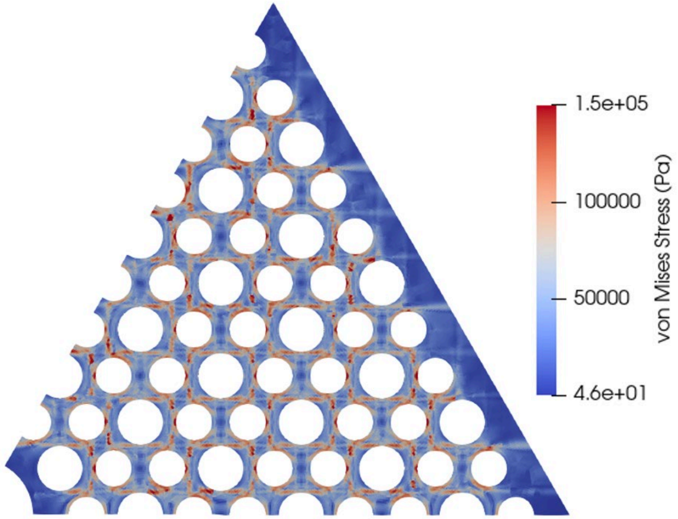
Background and motivation
- Component design (ASME rules)
- Graphite degradation
  - Oxidation
  - Irradiation

MOOSE modeling
- Oxidation modeling
- Graphite component stress modeling
  - Oxidized conditions
  - Irradiated conditions

Future work







Background and Motivation: ASME Rule for Graphite Core Component Design

The ASME BPVC Section III, Division 5 provides guidance on graphite core component design in article HHA-3000.

Three design approaches are provided:

1) Simplified Assessment (requires computing stresses)

- compares the peak equivalent stress to an allowable stress value

2) Full Assessment (requires computing stresses)

-uses computed stresses to determine a probability of failure and ensure it is sufficiently low.

3) Design-by-Test

-Requires experimental testing of a component to show acceptable performance.

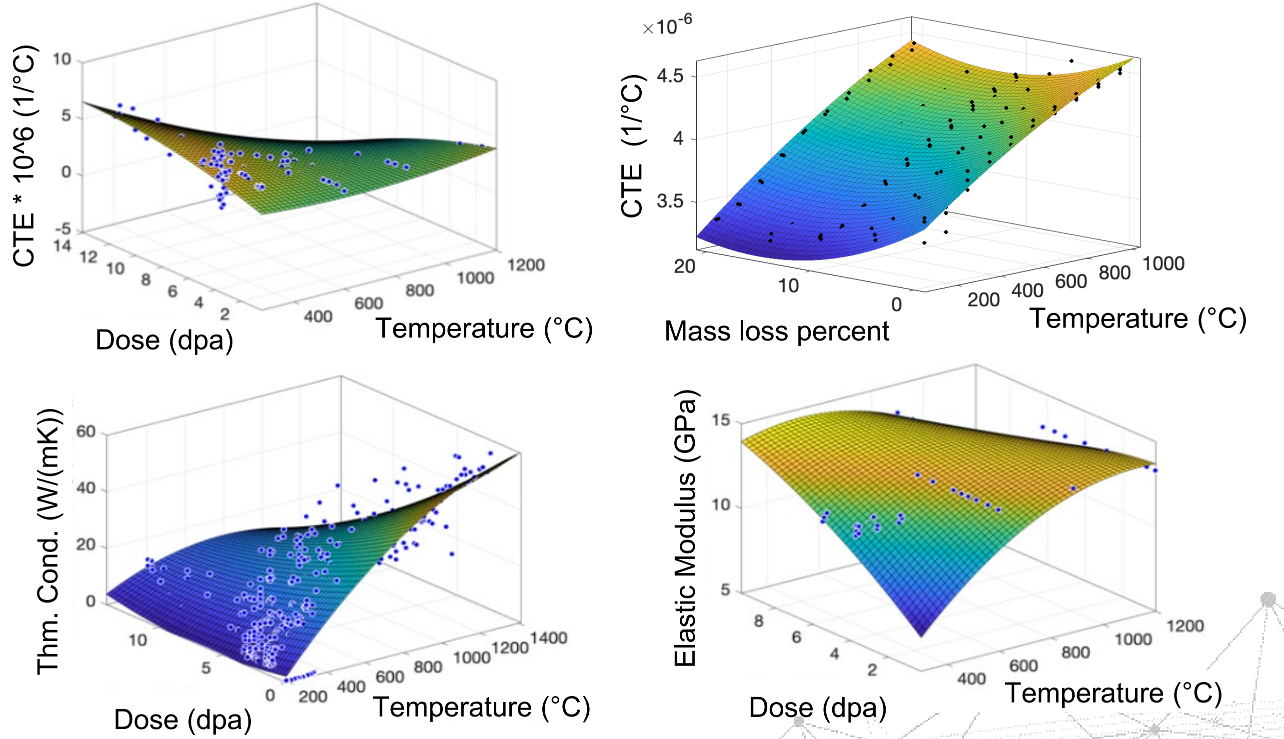
Experimental verification of a design in many cases may be an unattractive or infeasible option. In this case, designing a graphite component based on ASME rules requires determining stresses which will invariably require utilizing computational models.

Background and Motivation: Graphite Degradation (oxidation and irradiation)

Graphite behavior in a reactor environment can be heavily influenced by oxidation and irradiation. These mechanisms must be accounted for when analyzing a graphite component.

The behavior and properties effected by oxidation and irradiation include:

- Thermal Conductivity
  - Oxidation causes a dramatic decrease
  - Irradiation causes a dramatic decrease
- Young's Modulus and Strength
  - Oxidation causes a decrease
  - Irradiation causes an increase
- Coefficient of thermal expansion
  - Oxidation causes a decrease
  - Irradiation causes an increase
- Density
  - Oxidation causes a decrease
  - Irradiation causes an increase



Note the behavior above only necessarily applies prior to turnaround and other properties not addressed above may experience change.

MOOSE Modeling: Oxidation

Model Purpose:

The graphite oxidation model developed at INL by Kane[1] and implemented in MOOSE can compute **where**, **when** and to **what extent** oxidation has occurred in a graphite component.

Model Physics:

The primary physical considerations in the model are the **diffusivity** of the chemical species and local **reaction kinetics.** Each of these aspects are temperature and mass loss dependent, and their interaction dictates the computed oxidation profile.

The partial differential equations which describe this physics and are implemented in MOOSE are shown below.

$$\frac{\partial \varepsilon[CO_2]}{\partial t} = -\nabla \boldsymbol{N_{CO_2}} + (1 - x)k''_{eff}\boldsymbol{S_A}[O_2]$$

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

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

$$\frac{\partial \rho}{\partial t} = k''_{eff}\boldsymbol{S_A}[O_2] \qquad \boldsymbol{N_i} \cong -[C_T]D_{eff}\nabla y_i + y_i\,(\boldsymbol{N_i} + \boldsymbol{N_m})$$

$$\frac{\partial(\rho C_p T)}{\partial t} = \nabla \cdot (\boldsymbol{k_T}\nabla T) + k''_{eff}\boldsymbol{S_A}[O_2]\,\Delta H_{rx}(x)$$

$$\frac{\partial \varepsilon[CO]}{\partial t} = -\nabla \boldsymbol{N_{CO}} + x\,k''_{eff}\boldsymbol{S_A}[O_2]$$

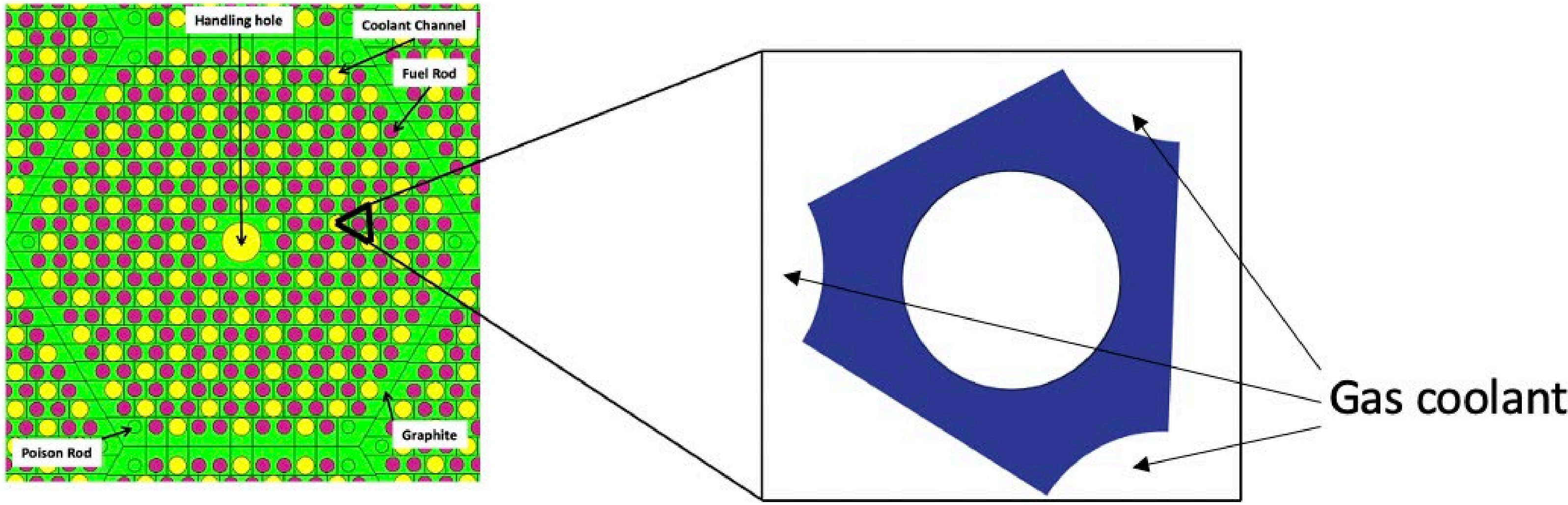
[1] J. Kane et al. (2017). Understanding the reaction of nuclear graphite with molecular oxygen: Kinetics, transport, and structural evolution. *Journal of Nuclear Materials,* Volume (493), pp. 343-367.

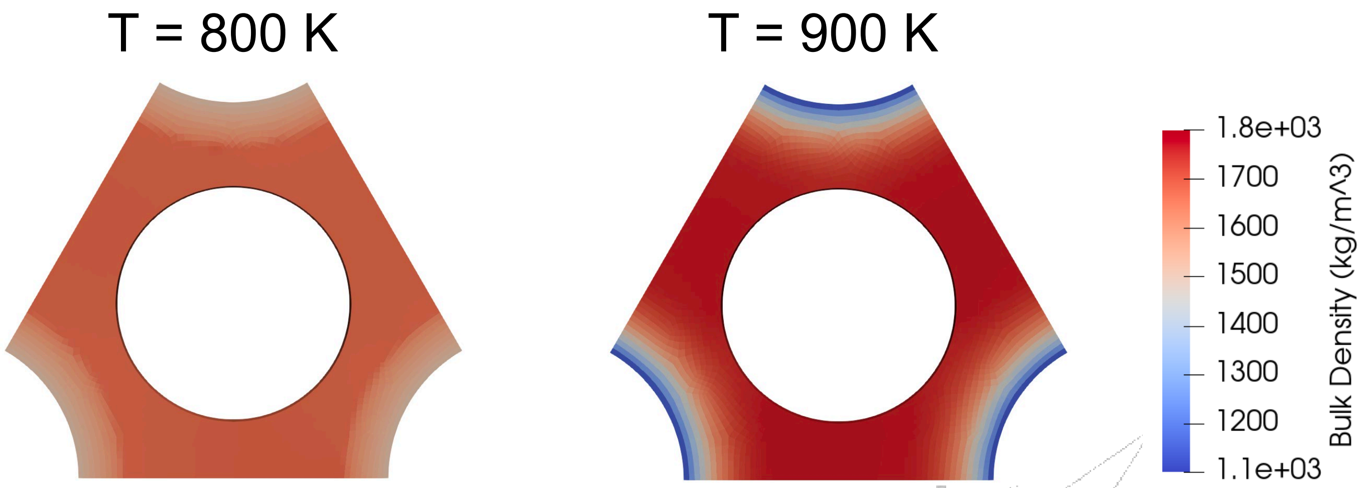
MOOSE Modeling: Oxidized Component Example Problem

The oxidation model requires grade specific parameters and has been parameterized for IG-110 and NGB-18.

As an example, problem, we consider the section of a prismatic fuel block shown to the right. In an accident scenario, oxidants may be present in the gas coolant. Simulations were run to predict the density profiles for a total mass loss of 10% at 900 K and 800 K in IG-110.

The primary take away from these results is, at higher temperature, the damage profile is narrower than the profile at the lower temperature.





Prismatic core geometry from: Sterbentz, J., et al., “High Temperature Gas-Cooled Test Reactor Point Design: Summary Report”. INL/EXT- 16-37661. March 2016

MOOSE Modeling: Stresses in Graphite Generated from Nuclear Applications

Model Purpose:

This model computes stresses in graphite which are generated in a nuclear reactor environment. These stresses can be implemented in the ASME code to assess a graphite component.

Model Physics:

The state variables in the system are the strain, temperature and mass loss.

To compute the strain the following are incorporated:

1) Thermal expansion, 2) irradiation induced swelling 3) irradiation induced creep 4) elastic strain

$$\epsilon_{total} = \epsilon_{therm} + \epsilon_{irr} + \epsilon_{creep} + \epsilon_{elastic}$$

To compute the temperature, the thermal conduction is incorporated.

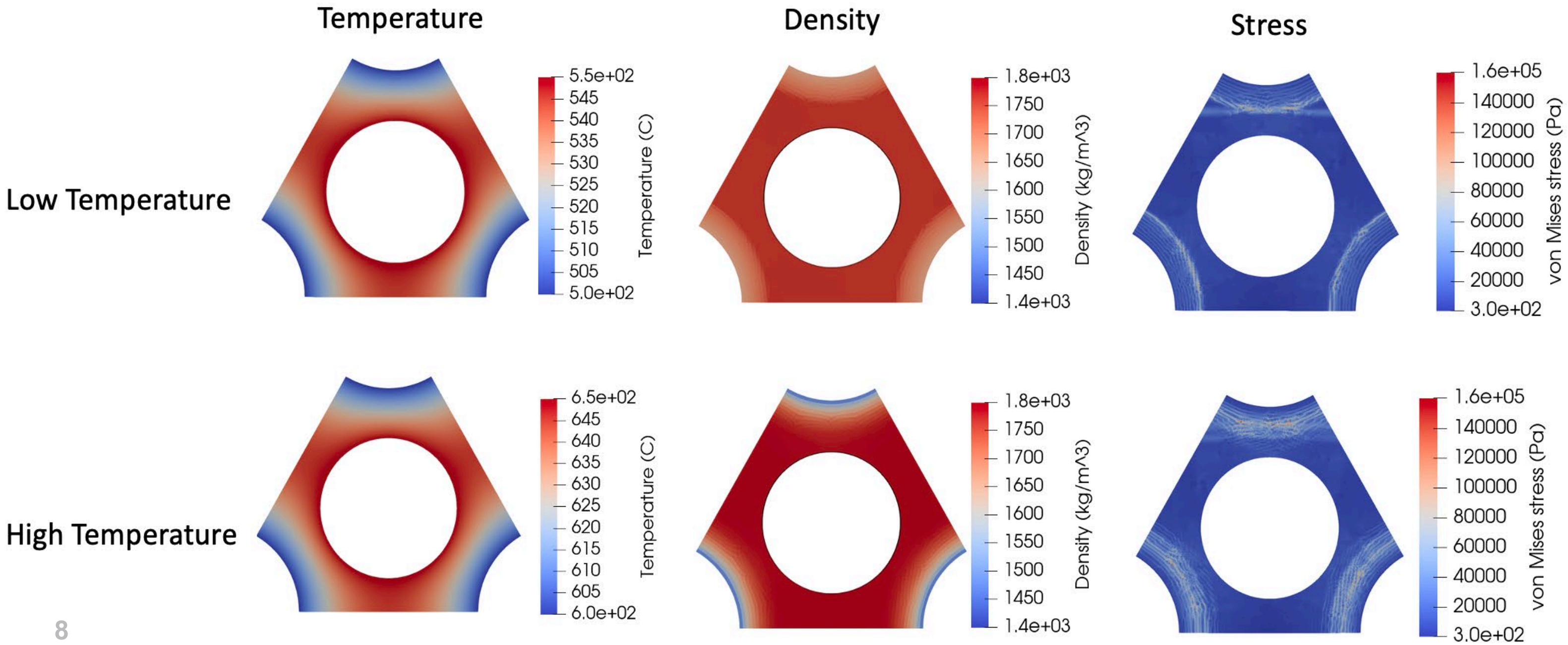
To compute the mass loss, the oxidation model, discussed previously, is incorporated.

Note that each of the properties (thermal conductivity, Young's Modulus, etc.) may be a function of the state variables.

MOOSE Modeling: Oxidized component stresses

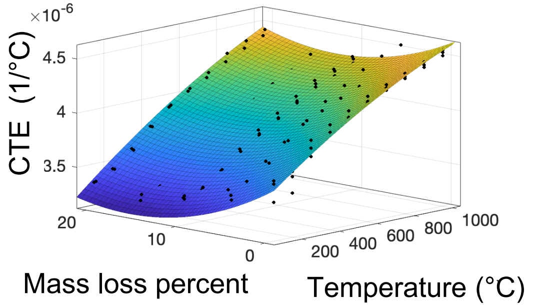
To compute stresses in an oxidized component, the mass loss profile as well as mass loss dependent properties must be known. Two example simulations were run, one at a higher temperature and one at a lower temperature. The temperature, density (at 5% mass loss), and resultant stress profiles are shown below. The magnitude of the stresses at the high and low temperature are similar. Although, it should be noted the regions with higher mass loss will have a more reduced strength.

Results

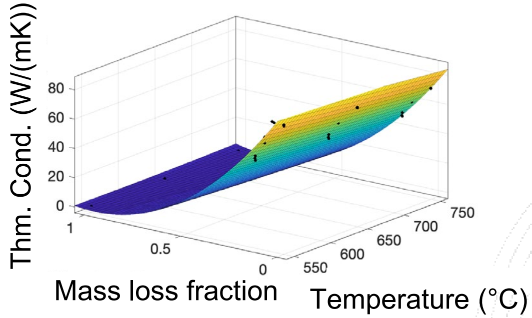


Property Trends

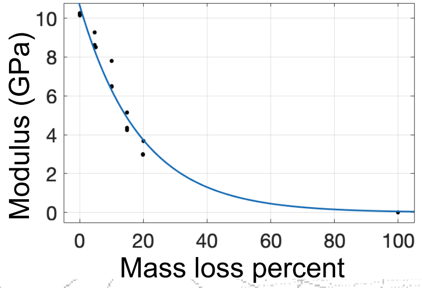
Coefficient of thermal expansion



Thermal conductivity



Elastic modulus



Irradiated Component Stresses

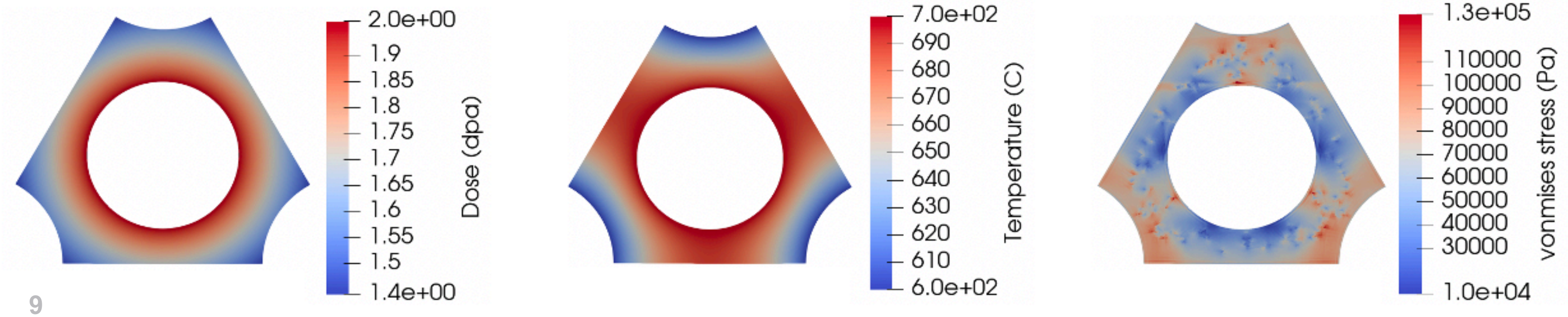
The stress in an irradiated component are a function of the temperature and fluence profiles. A preliminary example simulation was run with the following conditions:

1) The fluence profile was linearly increased with the simulation time.

2) The simulated runtime was 10,000 hours to allow for irradiation-creep effects to occur.

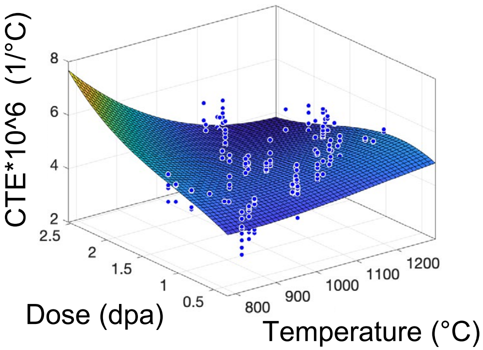
3) The temperature was fixed on the center hole and gas coolant surface.

Results at 10,000 hours

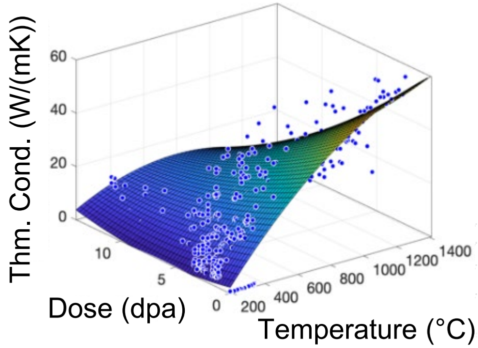


Property Trends

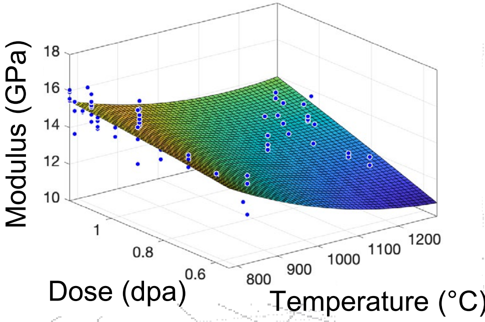
Coefficient of thermal expansion



Thermal conductivity



Elastic modulus



Future Work

Stress Modeling

- Additional verification and validation work are currently in progress. The ultimate step would be to validate against experimental results.
- The stress model will be coupled with the ASME code. This will allow for the Simplified or Full Assessments to be used to assess a graphite component.

Oxidation Modeling

- Plans have been made to parameterize the model for additional grades of graphite, likely including PCEA.
- The relationship between diffusivity and mass loss is not fully understood. Current experimental work at INL is investigating this relationship and these experimental results will be incorporated into the model.

Questions

Idaho National Laboratory