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Graphite Modeling Overview

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Outline

- **Graphite modeling and assessment overview**
- **Stresses induced in graphite in a reactor environment**
  - Graphite properties and behavior
  - Graphite modeling stresses
- **Graphite oxidation**
  - Physics of oxidation
  - Oxidation modeling
- **MSR graphite modeling**
  - How could this be modeled
  - Needed experimental data

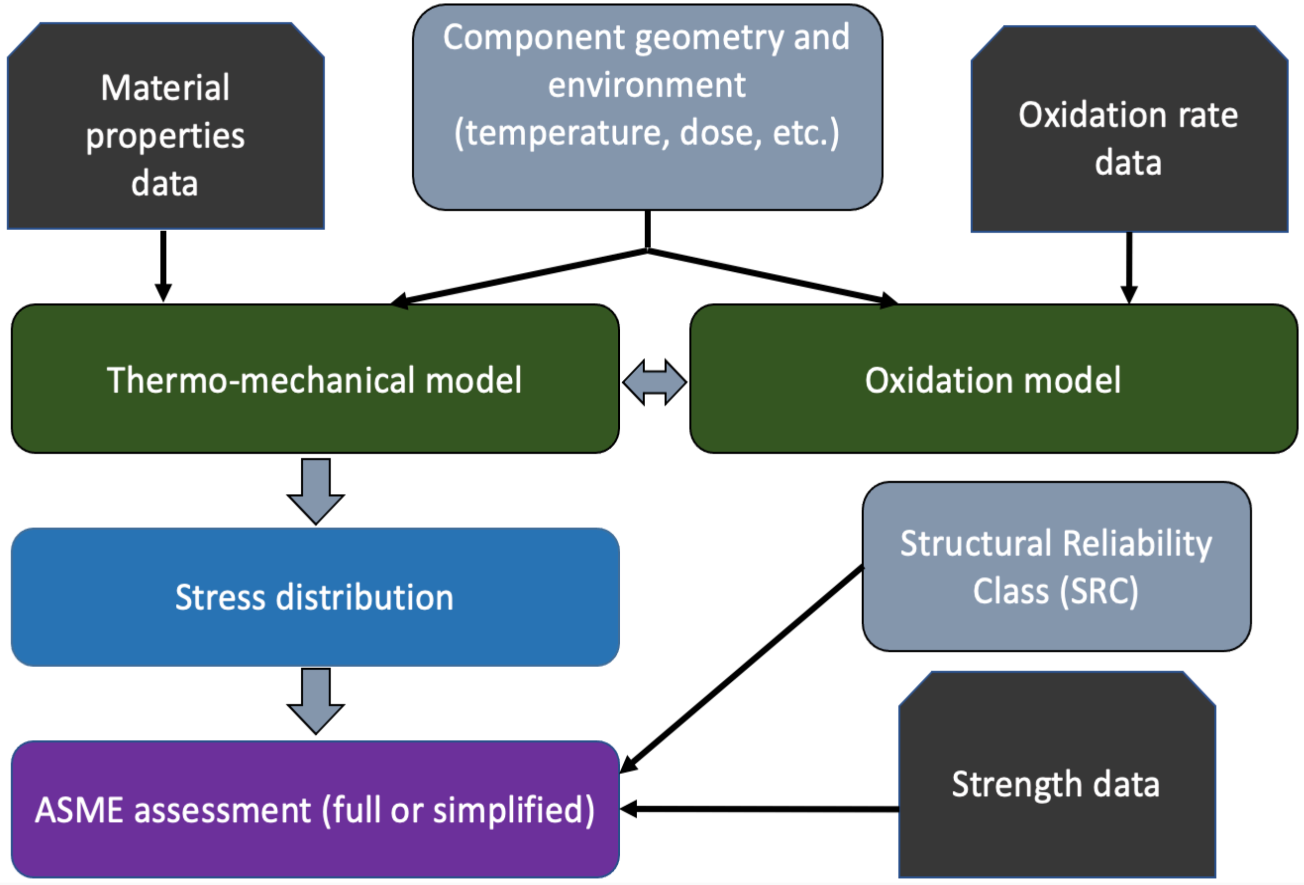
Background: Graphite Modeling as Required by ASME Section III, Div. 5

The ASME Code provides a methodology for assessing a graphite component intended for nuclear application.

The ASME code required that an analysis account for the effects of oxidation and irradiation.

The inputs to the ASME Code for graphite are:

1) A computed stress distribution
2) Experimentally determined compressive and tensile strength (material properties)
3) SRC, which is based on the component's application/environment in the reactor



Background: Graphite Behavior

Properties:

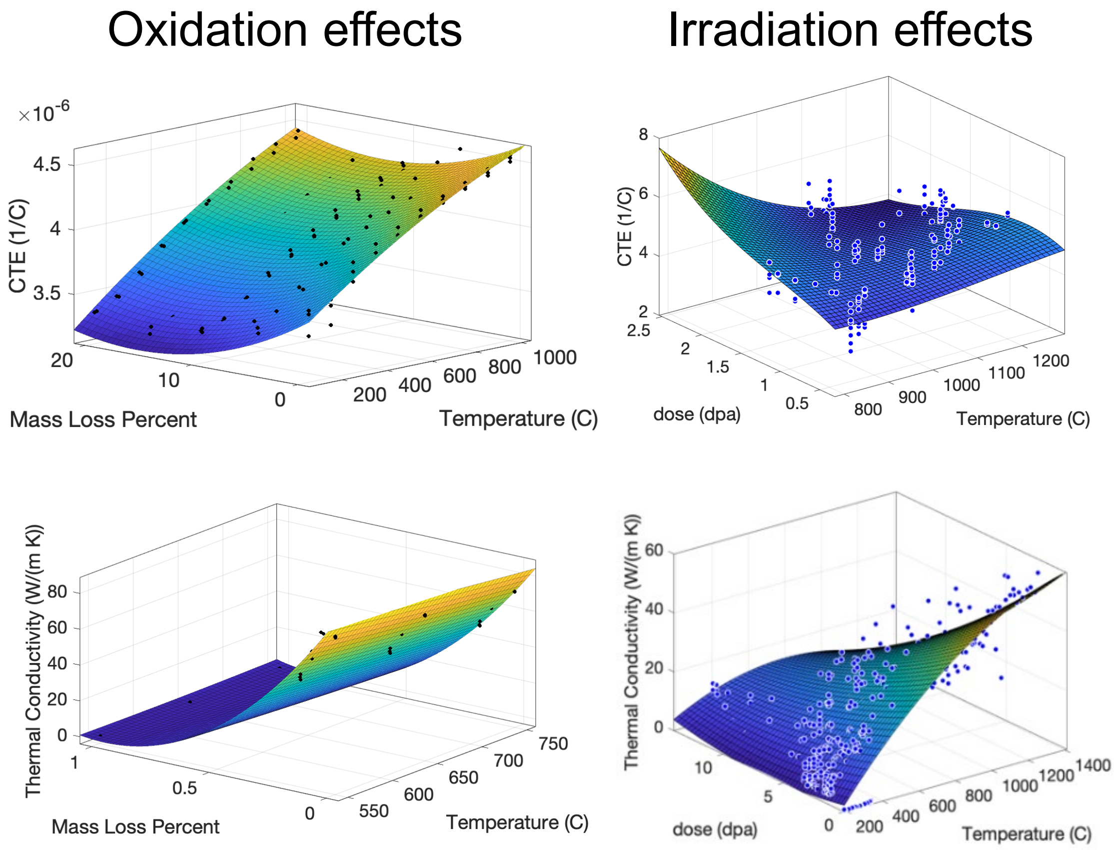
- As-manufactured properties graphite properties, like those determined in the base-line program at INL, change as a function of the environment (temperature, oxidation, irradiation). This is exemplified in the plots on the right.

Eigenstrains:

- The coefficient of thermal expansion is affected by dose as well as mass loss from oxidation.
- Irradiation induced swelling is a function of dose as well as irradiation temperature.

Property Scatter

- Experimentally determined post-turn-around properties have more scatter prior to turn-around.
- Scatter is graphite strength has led to probabilistic failure assessment methodologies



Graphite Modeling: Thermo-mechanical

Model Overview:

The graphite model computes the evolution of stress and temperature profiles in a graphite components. The required inputs are received dose evolution and thermal inputs.

Model Formulation:

The state variables in the thermo-mechanical model are the **strain, temperature, dose**. The graphite model accounts for strain contributions from thermal, irradiation, and mechanical loads

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

Where ϵ_{total} is the total stain, ϵ_{therm} are eigen strains from thermal expansion, ϵ_{irr} are strains from irradiation induced dimensional change, ϵ_{creep} are strains from irradiation induced creep, and $\epsilon_{elastic}$ are elastic strains.

ASME Code on modeling Stress

HHA-3214.11 Internal Stress. An internal stress may be a thermal stress or an irradiation-induced stress.

HHA-3215.3 Stress Analysis of Irradiated Graphite Core Components. For irradiated Graphite Core Components [HHA-3142.1(c)], a viscoelastic analysis that takes into account the effects of irradiation damage on the properties of the graphite and on the development of stresses in the components shall be completed. This analysis shall account for irradiation-induced dimensional change and creep as well. The Designer is responsible for the accuracy and acceptability of the analysis methods used.

Model Limitations

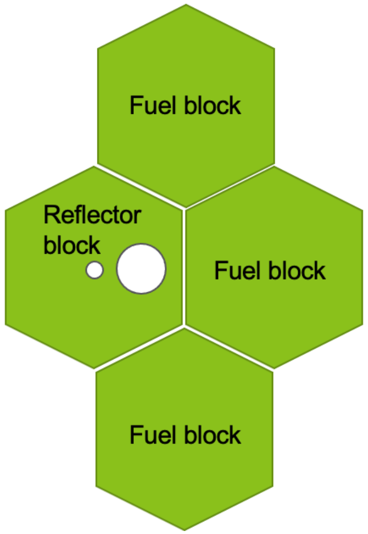
The model is parameterized for IG-110 prior to turn around. Each graphite grade behaves differently and requires its own parameterization.

Modeling Stress: Example Problem

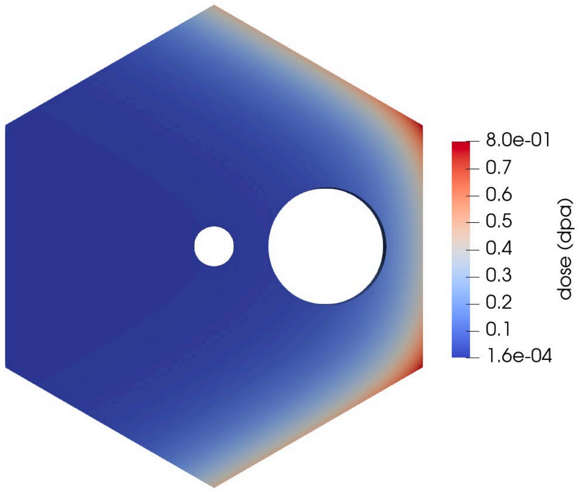
The most significant stresses which occur in graphite during normal reactor operation occur due to gradients in temperature and dose. These stresses are partially alleviated by irradiation creep.

The following problem shows an approximate temperature and dose profile for the Ft. St. Vrain reactor and the computed stresses at 5 years.

Core Block Geometry



Dose Profile



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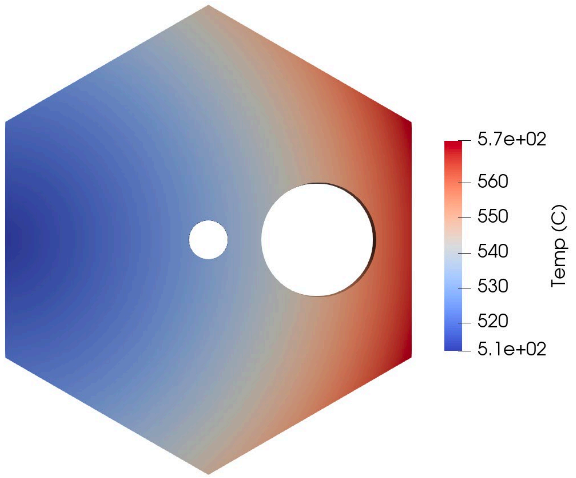
Temperature Profile



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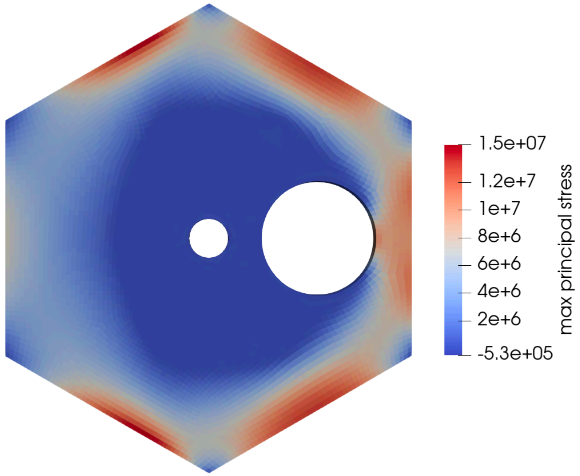
Stress Distribution



Background: Oxidation Theory

Overview

Oxygen will readily react with graphite to produce carbon monoxide and carbon dioxide at high temperature.

When, where to, and how much oxidation occurs is controlled by a combination of the diffusion of the oxidant and the reaction kinetics.

The over oxidation behavior will be strongly tied to the temperature at which oxidation occurs.

Walker Diagram:

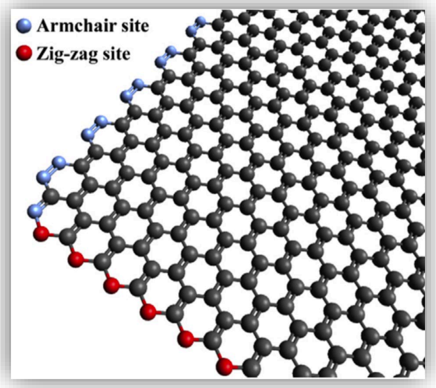
The Walker diagram shows the idealized behavior:

Low-temperature = kinetic controlled

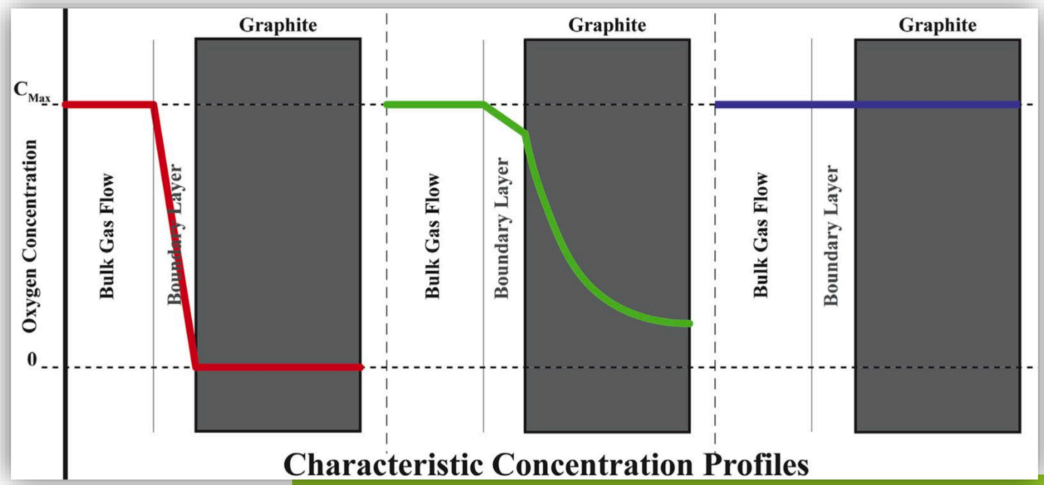
Moderate-temperature = diffusion controlled

High-temperature = boundary controlled

Graphite basal plane showing the carbon atoms available for oxidation (zig-zag and arm-chair.)



Walker Diagram



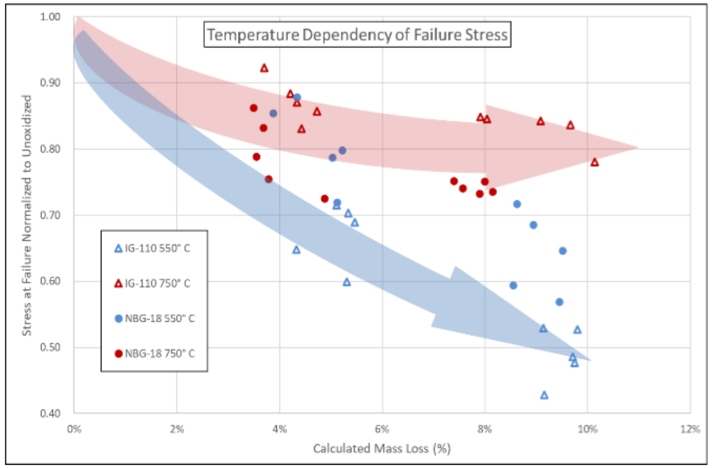
[1] J. Kane et al. (2017). Understanding the reaction of nuclear graphite with molecular oxygen: Kinetics, transport, and structural evolution. *Journal of Nuclear Materials,* Volume (493), pp. 343-367.

Background: Oxidized Component Behavior

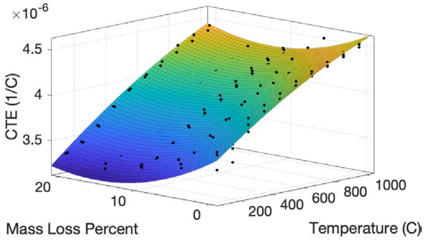
Oxidation causes property changes:

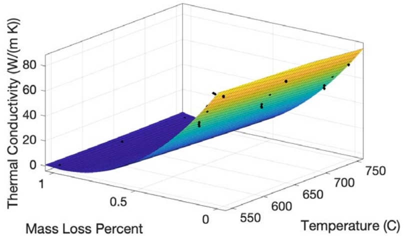
- Strength degradation
- Thermal property changes can lead to variation in temperature profiles which may result in increased stresses
- Dimensional changes
- Irradiated graphite has shown to increase oxidation rates

Strength Change



Various Material Property Changes





The oxidation profile strongly effects the overall behavior of a component.

- This fact is recognized by the ASME as shown in the excerpt to the right.
- Low temperature testing is essential for determining material properties from homogeneously oxidized graphite.

HHA-3141 Oxidation

Oxidation analysis shall be carried out in detail to estimate the weight loss profiles of graphite structures, since reaction rates depend on the temperature, reactants, and graphite grade.

Modeling: Oxidation Formulation

Oxidation Modeling formulation:

The primary physical considerations in the model are the **diffusivity** of the chemical species and local **reaction kinetics.**

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

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

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

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

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

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

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

Microstructural evolutions effect:

As the graphite is oxidized the microstructure changes. Therefore, the effective diffusivity, D_{eff}, thermal conductivity, k_T, and active surface area, $\boldsymbol{S_A}$, are a function of the mass loss.

[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.

Modeling: Oxidation Example

Capabilities:

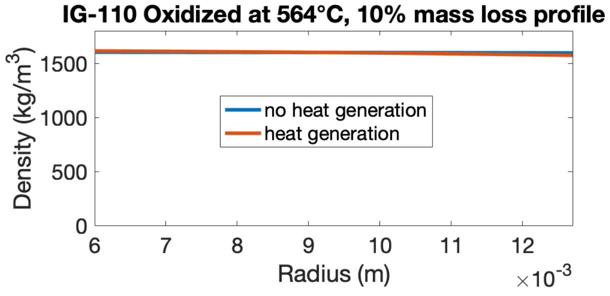
- The model can compute the evolution of the oxidation damage profile.
- The graphite model has been parameterized for IG-110 and NBG-18 from experiments performed at INL.
- Computes temperature effects caused by the reaction between graphite and oxygen.

Limitations:

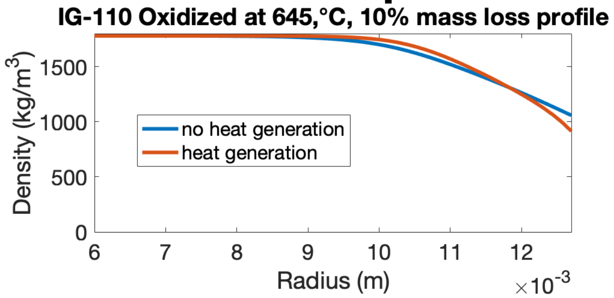
- Oxidation behavior varies between grades, so the model is limited to IG-110 and NBG-18
- The effect of irradiation and non-molecular-oxygen oxidants has not been included in the model
- Full scale validation is difficult

Example Problem

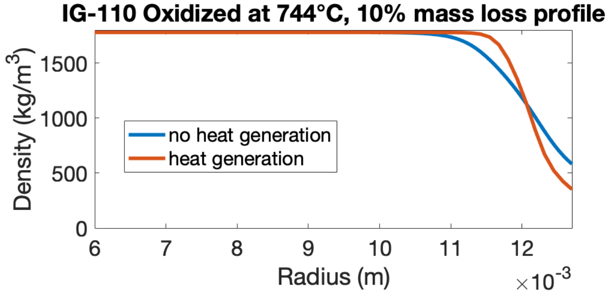
Low Temperature



Moderate Temperature



High Temperature



MSR modeling

Where and how much are the thermo-mechanical properties being altered?

We need the properties as a function of the state (temp, dose, salt concentration).

1. Salt penetration depth needs to be determined
2. How are the properties effected by salt interaction
   - Thermal conductivity
   - Strength
   - Turn around dose
   - CTE
   - Elastic Modulus

Modeling erosion and abrasion

Erosion and abrasion rates are needed. This can be treated the same was as regime 3 oxidation.

How are eigen strains effected?

Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program Molten Salt/Graphite Modeling

- The NEAMS program is developing multiphysics simulation codes for LWR and advanced reactor systems, primarily based on the MOOSE platform
- Structural Materials & Chemistry area of NEAMS program is developing an integrated set of codes for modeling integrity of alloy structural components and MSR chemistry
  - Grizzly: Structural component integrity. Models for creep, creep-fracture in high temperature alloys
  - Mole/Pronghorn/MOSCATO: Species tracking, corrosion, depletion & plating of species in flow channels in MSRs at various levels of fidelity
  - MSTDB: Thermophysical and thermochemical databases for molten salt systems
  - Yellowjacket: Phase-field models for corrosion in salt-facing alloys at grain scale
- Structural graphite is of interest in this effort, and there are preliminary plans for capability development by NEAMS to complement ongoing efforts by other programs
  - Many possibilities for leveraging already existing capabilities to graphite, e.g., fracture mechanics, integration with system-level species tracking/corrosion codes

Questions