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Joseph Bass
Computational Materials Engineer

Graphite Behavior Modeling

ART Advanced Reactor Technologies
GAS-COOLED REACTORS

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
- **ASME graphite assessment**
  - ASME Code application
  - ASME Code gaps

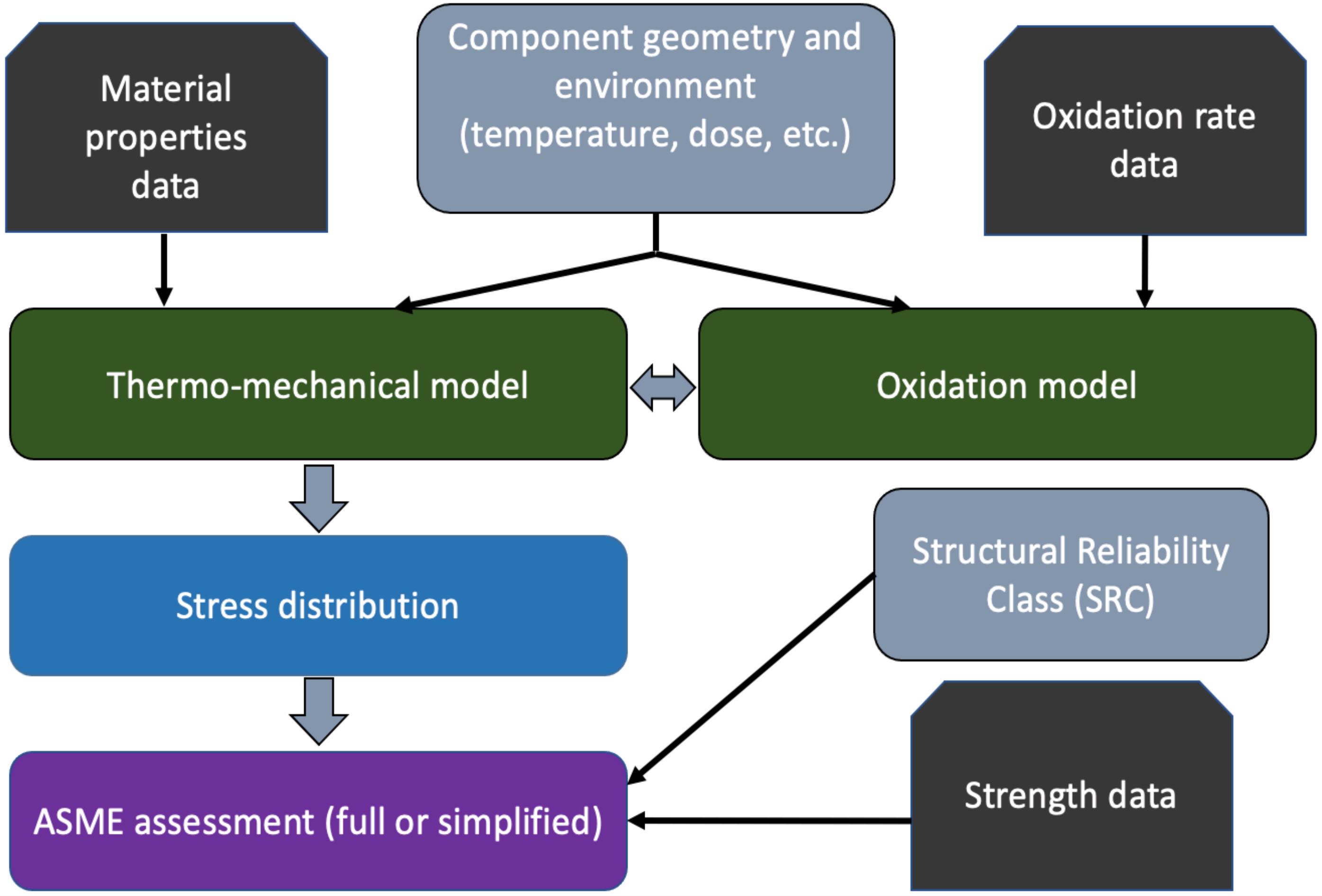
Background: Graphite Modeling as Required by ASME Section III, Div. 5

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

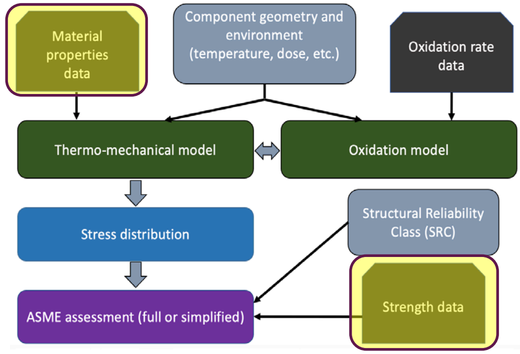
The ASME code required that an analysis account for the effects of oxidation and irradiation.

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:

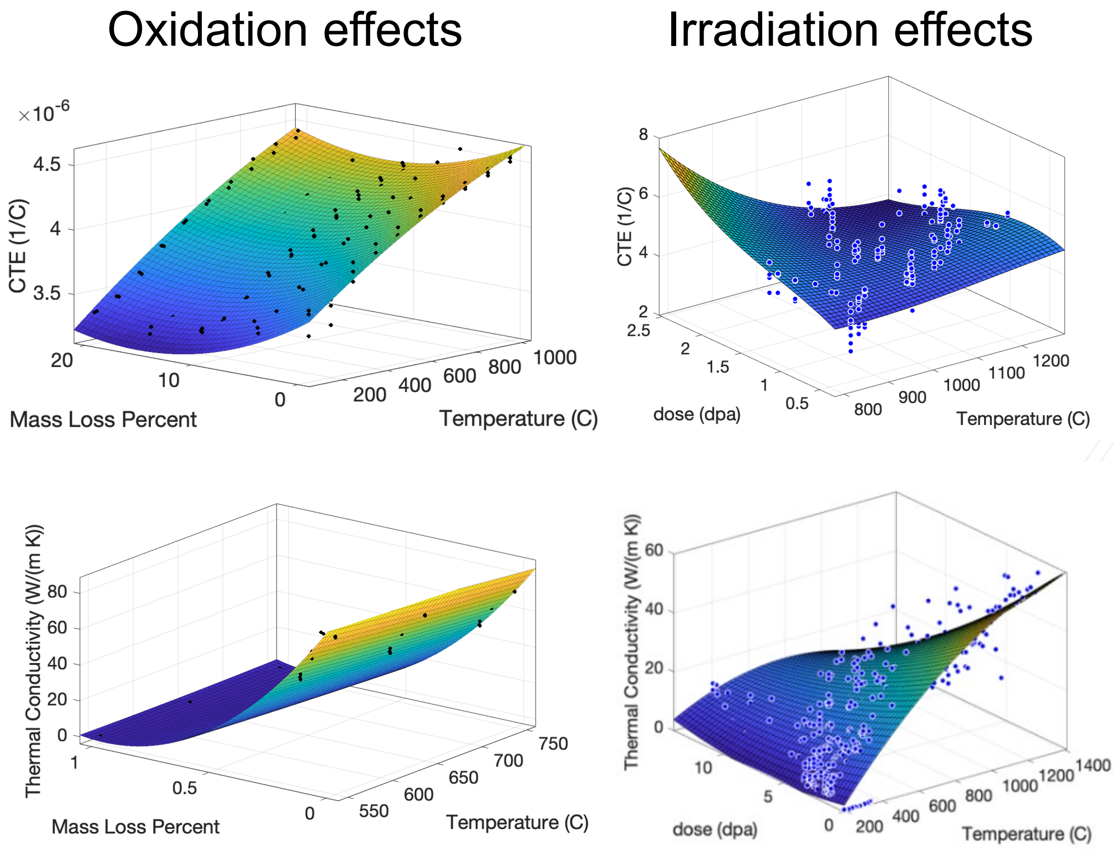
- As-manufactured properties graphite properties, like those determined in the base-line program, change as a function of the environment (temperature, oxidation, irradiation). This is exemplified in the plots on the right.

Eigenstrains:

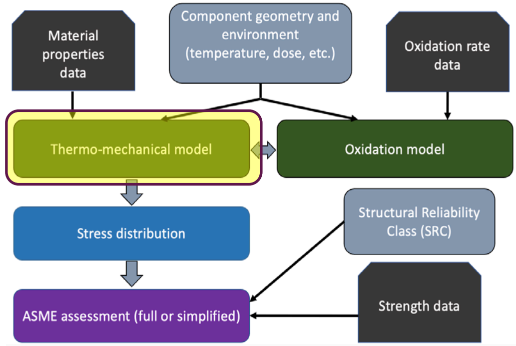
- The coefficient of thermal expansion is affected by dose as well as mass loss from oxidation.
- Irradiation induced swelling is a function of dose as well as irradiation temperature.

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

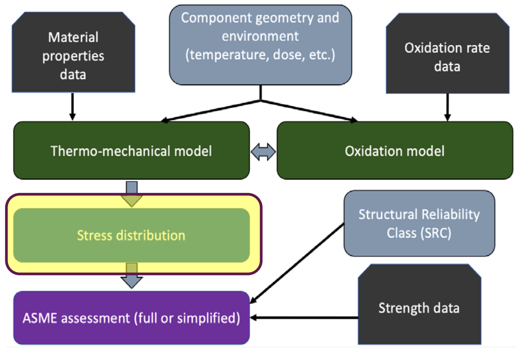
HHA-3214.11 Internal Stress. An internal stress may be a thermal stress or an irradiation-induced stress.

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.

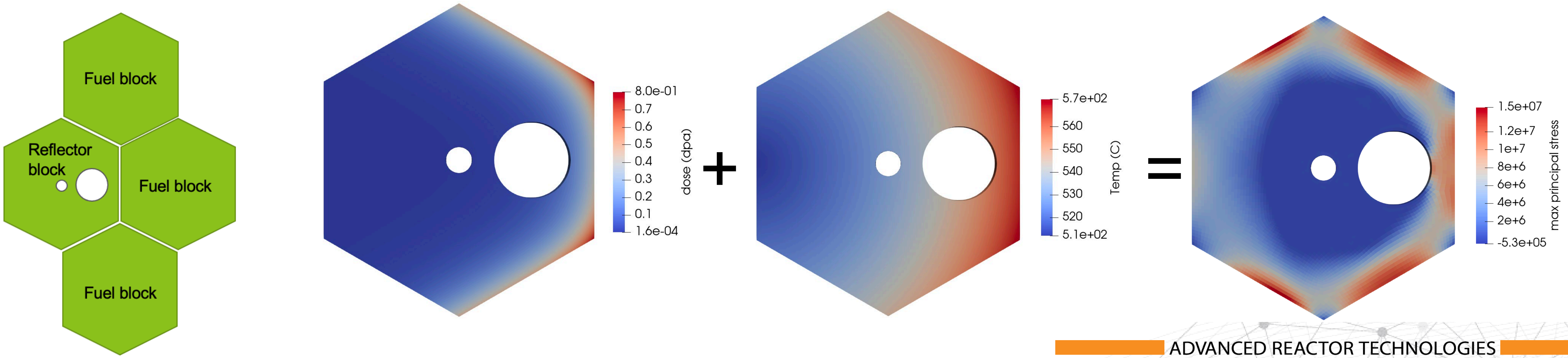
The following problem shows an approximate temperature and dose profile for the Ft. St. Vrain reactor and the computed stresses at 5 years.

Core Block Geometry

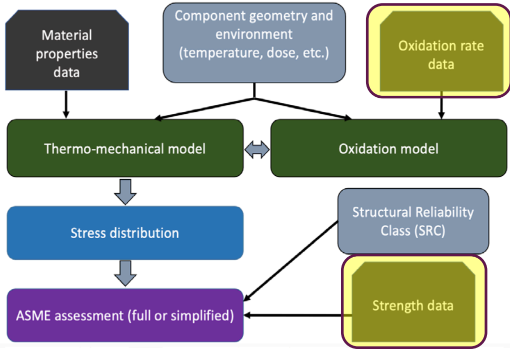
Dose Profile

Temperature Profile

Stress Distribution



Background: Oxidation Theory



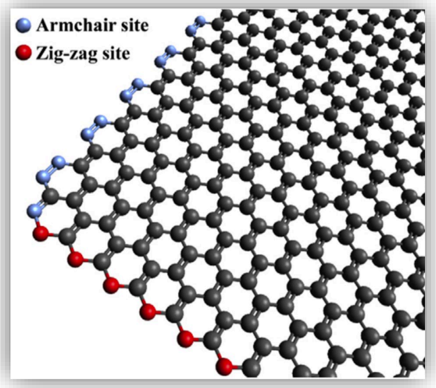
Overview

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.

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



Walker Diagram:

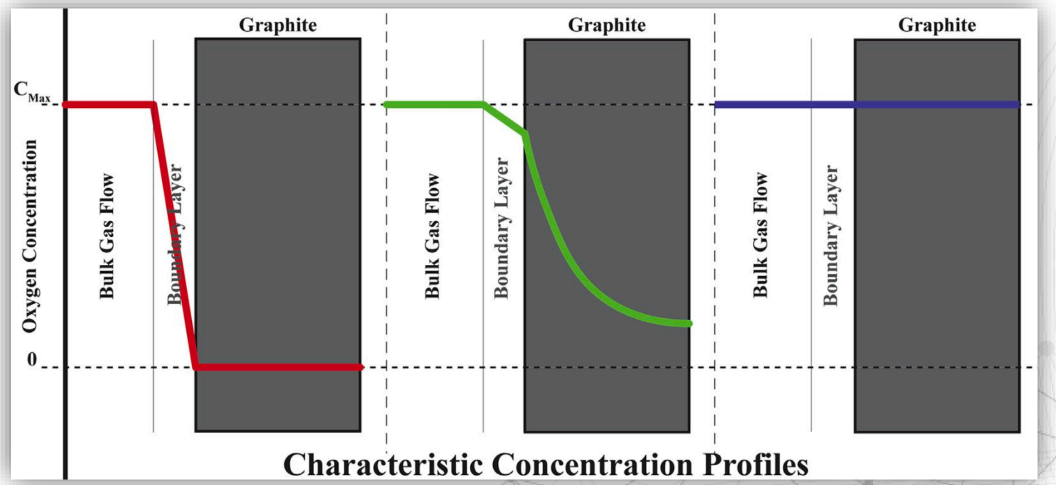
The Walker diagram shows the idealized behavior:

Low-temperature = kinetic controlled

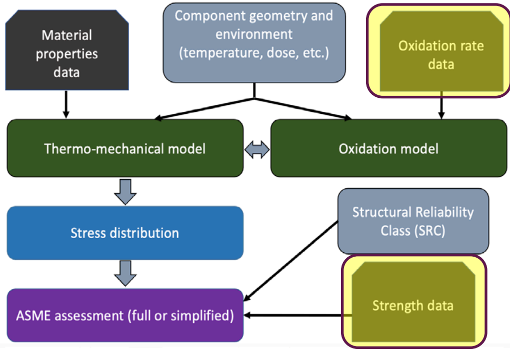
Moderate-temperature = diffusion controlled

High-temperature = boundary controlled

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.

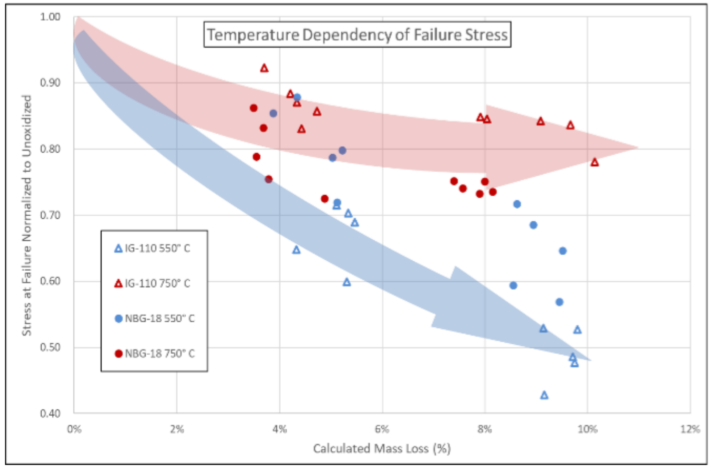


Background: Oxidized Component Behavior

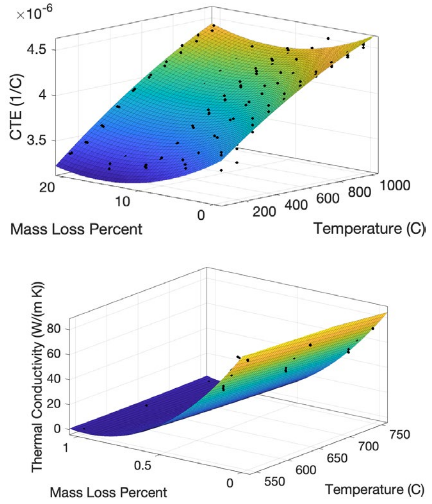
Oxidation causes property changes:

- 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



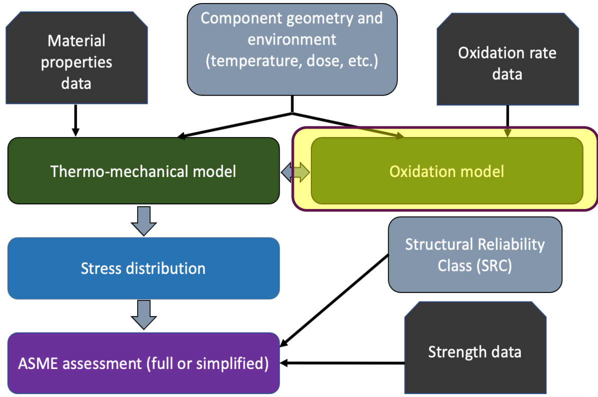
The oxidation profile strongly effects the overall behavior of a component.

- 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.

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

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

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

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

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

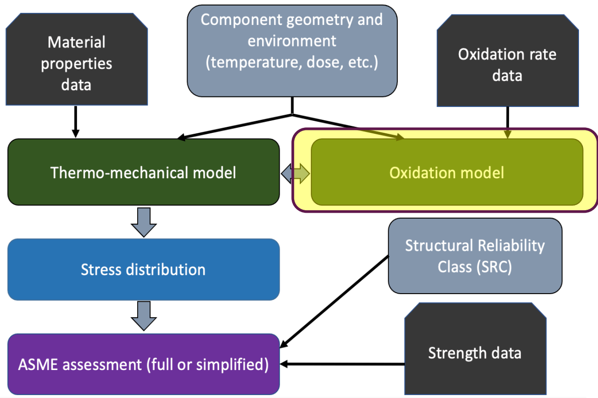
$$\frac{\partial \varepsilon[CO]}{\partial t} = -\nabla \boldsymbol{N_{CO}} + x\,k''_{eff}\boldsymbol{S_A}[O_2]$$

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:

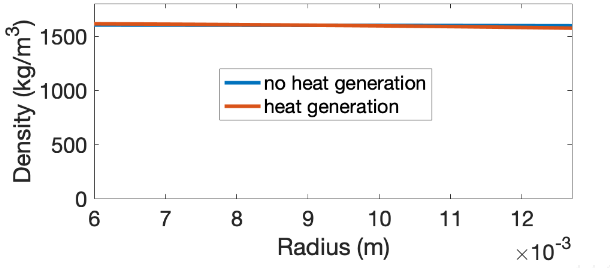
- The model can compute the evolution of the oxidation damage profile.
- The graphite model has been parameterized for IG-110 and NBG-18 from experiments performed at INL.
- Computes temperature effects caused by the reaction between graphite and oxygen.

Limitations:

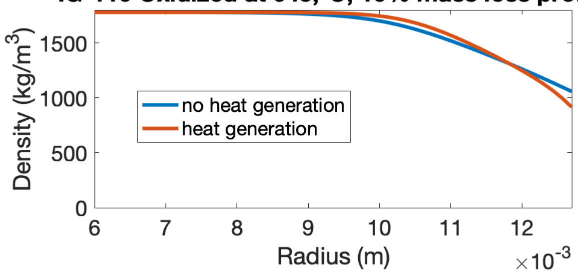
- Oxidation behavior varies between grades, so the model is limited to IG-110 and NBG-18
- The effect of irradiation and non-molecular-oxygen oxidants has not been included in the model
- Full scale validation is difficult

Example Problem

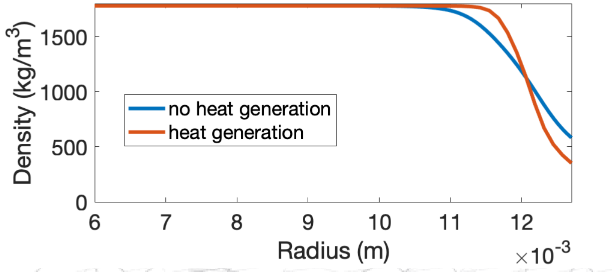
Low Temperature



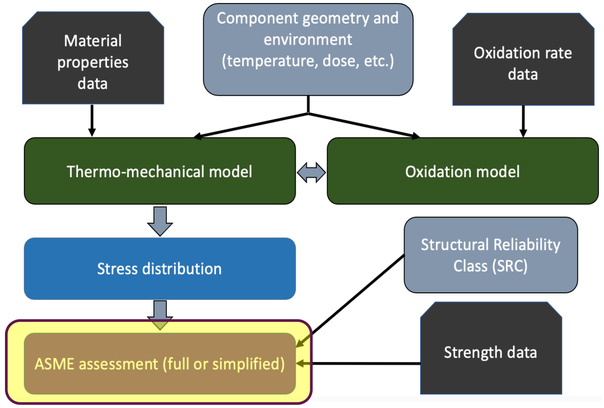
Moderate Temperature



High Temperature



Background: ASME Code (Sec. III Div. 5)



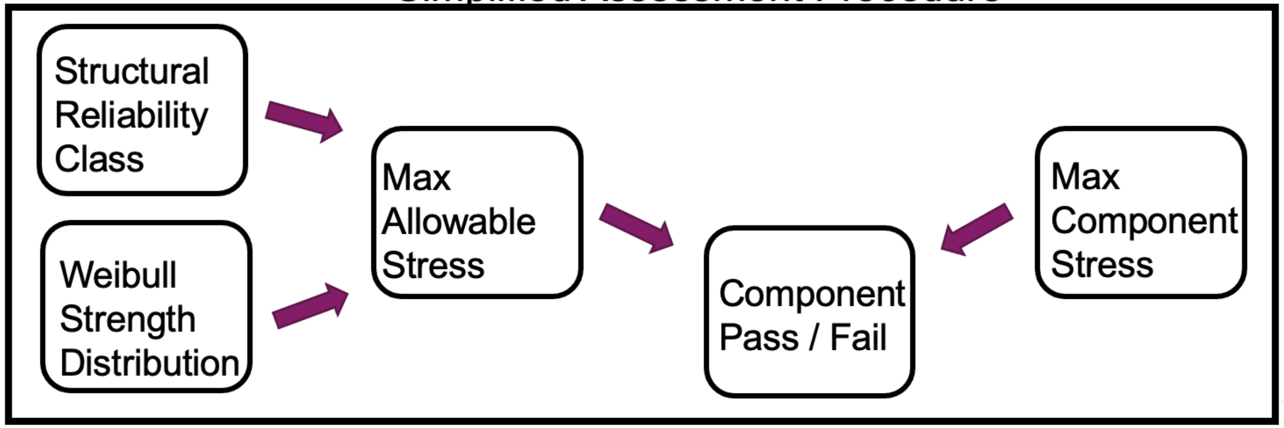
The Simplified and Full assessments are similar in that they both require:

1. Component stresses
2. A Weibull distribution of strength
3. A structural reliability class

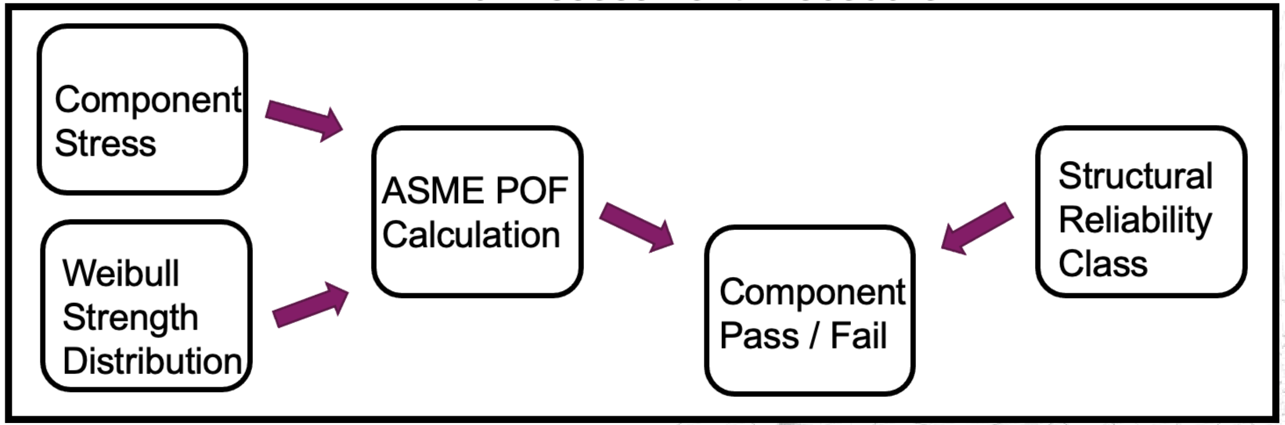
Both methods are aimed at determining if a crack will form in the component.

The main differences come from the fact that the full assessment considers the full stress distribution in a component, and the simple assessment only considers the maximum stress.

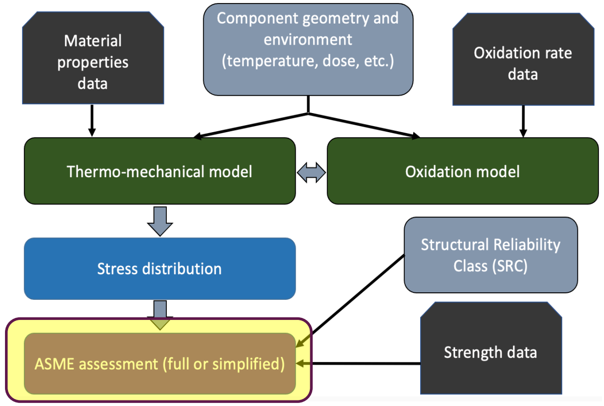
Simplified Assessment Procedure



Full Assessment Procedure



ASME Code Application

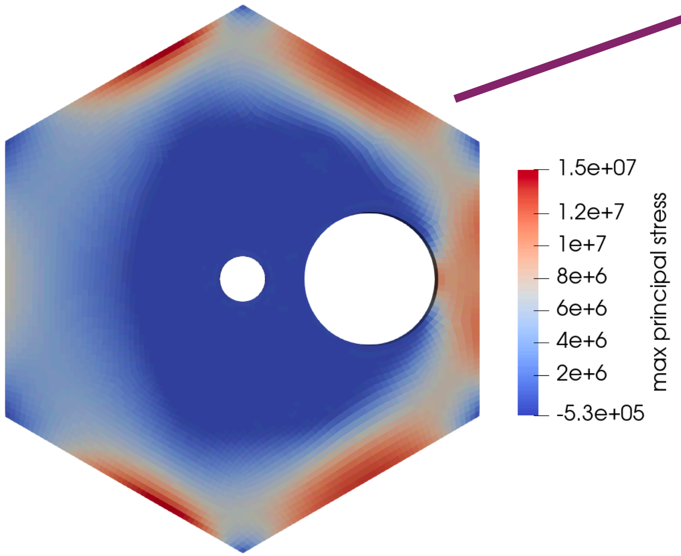


Work Done

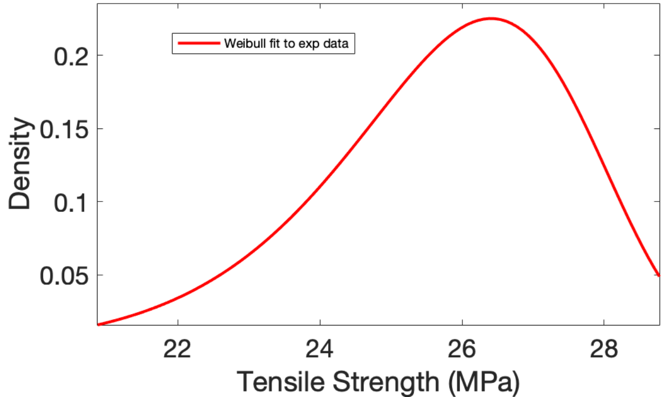
A post-processor was written in Python which can implement the simplified and full assessment as they appear in the ASME 2021.

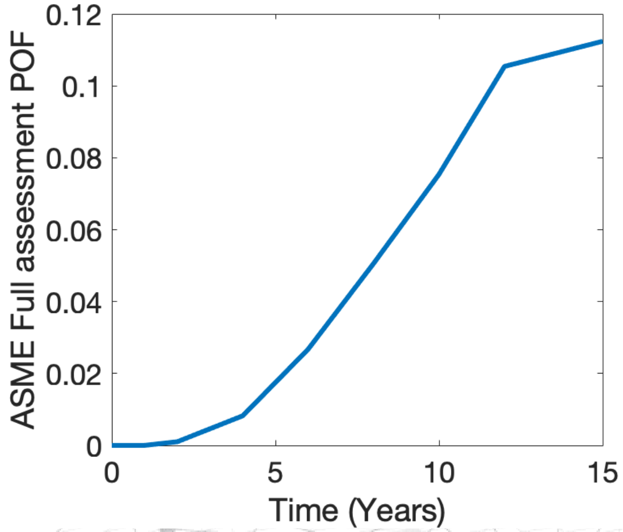
Sensitivity analysis of various parameters in the ASME code have been performed. Andrea Mack has been leading these sensitivity studies.

Multiple example problems have been run using the ASME code methodologies. The computed POF for the Ft. St. Vrain example problem is shown below.

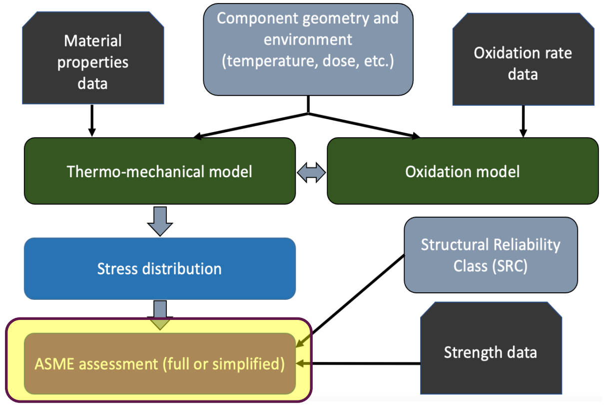


ASME Full Assessment





Example Problem: ASME Limitations



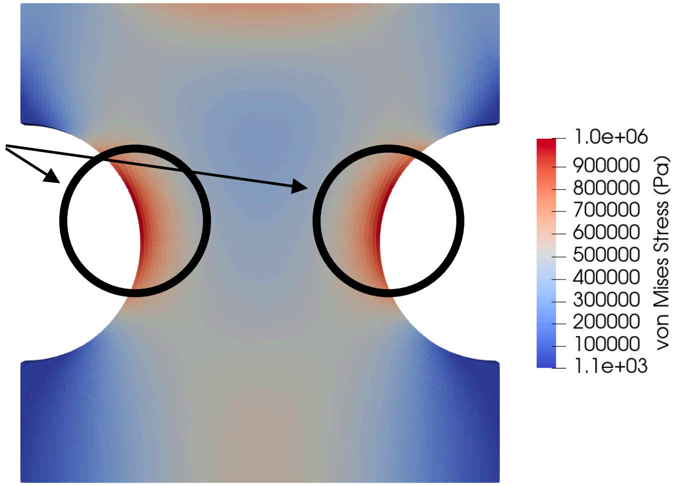
Application of the ASME code has identified some limitations in the methodology in the Full assessment.

The Full assessment does not account for location. This causes:

1. Volume grouping is location independent.
2. Property gradients are not appropriately accounted for.
3. Crack formation in a non-critical location is the same a critical location

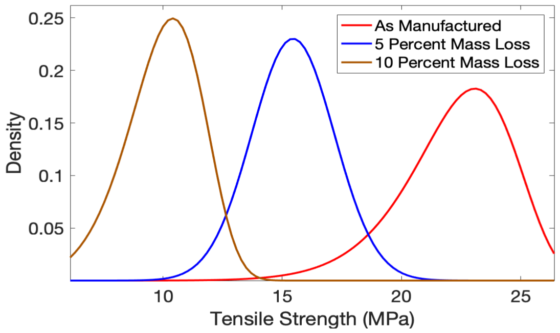
Grouping is done by stress magnitude so multiple location can be put in one group.

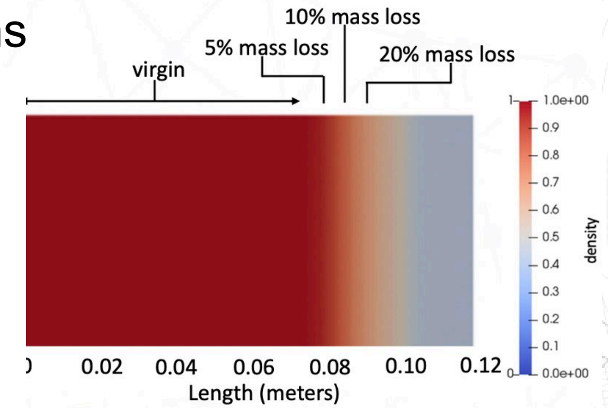
The first group will include elements from multiple locations



Accounting for degradation gradients is not considered in the full assessment

Oxidation Strength Distributions





Future Work

Modeling Graphite Future Work:

Future work in modeling efforts have three focuses:

1) Modeling degradation in molten salt reactors
   - Erosion/abrasion
   - Hot spot issues
   - Chemical interaction
2) ASME assessment incorporation of heterogenous material properties
   - POF calculation inclusion of oxidation and irradiation effects
3) Non-ASME failure (crack modeling)

Questions