U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Advanced Reactor Stakeholder Public Meeting

December 15, 2022

Microsoft Teams Meeting
Bridgeline: 301-576-2978
Conference ID: 115 537 606#

Time	Agenda	Speaker
10:00 am – 10:10 am	Opening Remarks / Adv. Rx Integrated Schedule	NRC
10:10 am – 12:00 am	Graphite Component Modeling	NRC
12:00 pm –1:00 pm	Lunch Break	All
1:00 pm – 2:00 pm	MACCS Reports	NRC / Sandia
2:00 pm – 2:30 pm	Operator Cold License Training for Advanced Reactors	NEI
2:30 pm – 3:15 pm	NuScale DC Review Lessons Learned	NRC
3:15 pm – 3:25 pm	Break	
3:25 pm – 3:55 pm	Workshops on Licensing Review Framework for Advanced Reactors Instrumentation and Controls	NRC
3:55 pm – 4:00 pm	Future Meeting Planning and Concluding Remarks	NRC

Advanced Reactor Integrated Schedule of Activities

The updated Advanced Reactor Integrated Schedule

is publicly available on NRC Advanced Reactors website at:

https://www.nrc.gov/reactors/new-reactors/advanced/integrated-review-schedule.html

Advanced Reactor Integrated Schedule of Activities

Strategy 1	Knowledge, Skills, and Capability
Strategy 2	Computer Codes and Review Tools
Strategy 3	Guidance
Strategy 4	Consensus Codes and Standards
Strategy 5	Policy and Key Technical Issues
Strategy 6	Communication

Legend

Concurrence (Division/Interoffice)	• EDO Concurrence Period
Federal Register Publication	Commission Review Period**
Public Comment Period	▼ ACRS SC/FC (Scheduled or Planned)
Draft Issuance of Deliverable	External Stakeholder Interactions
Final Issuance of Deliverable	↓ Public Meeting (Scheduled or Planned)

Version 12/8/22

Present Day

Strategy	Regulatory Activity	Commission Papers	Guidance	Rulemaking	NEIMA	Complete	2022 Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	2023 Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
1	Development of non-Light Water Reactor (LWR) Training for Advanced Reactors (Adv. Rxs) (NEIMA Section 103(a)(5))					x																								
	FAST Reactor Technology				x	x																								
	High Temperature Gas-cooled Reactor (HTGR) Technology				x	x																								
	Molten Salt Reactor (MSR) Technology				x	x																								
	Competency Modeling to ensure adequate workforce skillset					x																								
	Identification and Assessment of Available Codes					x																								
	Development of Non-LWR Computer Models and Analytical Tools																													
	Reference plant model for Heat Pipe-Cooled Micro Reactor					x																								
	*Reference plant model for Sodium-Cooled Fast Reactor (update from version 1 to 2)****																													
	*Reference plant model for Molten-Salt-Cooled Pebble Bed Reactor (update from version 1 to 2)****					x																								
	Reference plant model for Monolith-type Micro-Reactor																													
	*Reference plant model for Gas-Cooled Pebble Bed Reactor (update from version 1 to 2)****																													
	*Reference plant model for Molten-Salt-Fueled Thermal Reactor (update from version 1 to 2)****																													
	Code Assessment Reports Volume 2 (Fuel Perf. Anaylsis)					x																								
	FAST code assessment for metallic fuel					x																								
	FAST code assessment for TRISO fuel					x																								
	Code Assessment Reports Volume 3 (Source Term Analysis)					x																								
	Non-LWR MELCOR (Source Term) Demonstration Project					x																								

https://www.nrc.gov/reactors/new-reactors/advanced/integrated-review-schedule.html

Graphite Aging and Degradation Tool

Christopher Ulmer and Joseph Bass
RES/DE/REB

Advanced Reactor Stakeholder Meeting
December 15, 2022

Outline

- Background on graphite aging and degradation tool development
- Graphite properties and behavior overview
- Graphite stress and oxidation modeling in MOOSE
- ASME assessment review and implementation

Background

- NRC staff are developing the regulatory framework and technical expertise to be able to regulate advanced non-light water reactors (ANLWRs)
- Specifically, NRC staff are interested in developing expertise and tools to model graphite behavior in ANLWRs
- Nonmetallic graphite and ceramic composite components for nuclear applications were added to the ASME Boiler Pressure and Vessel Code (BPVC)

Project Overview

- INL provided training to NRC staff on graphite degradation, aging, and failure mechanisms as applied to the use of graphite in ANLWRs
- INL developed a MOOSE-based tool that implements a graphite reliability model capable of performing component reliability and probability of failure (POF) analysis based on ASME BPVC III.5 graphite subsection HH subpart A requirements

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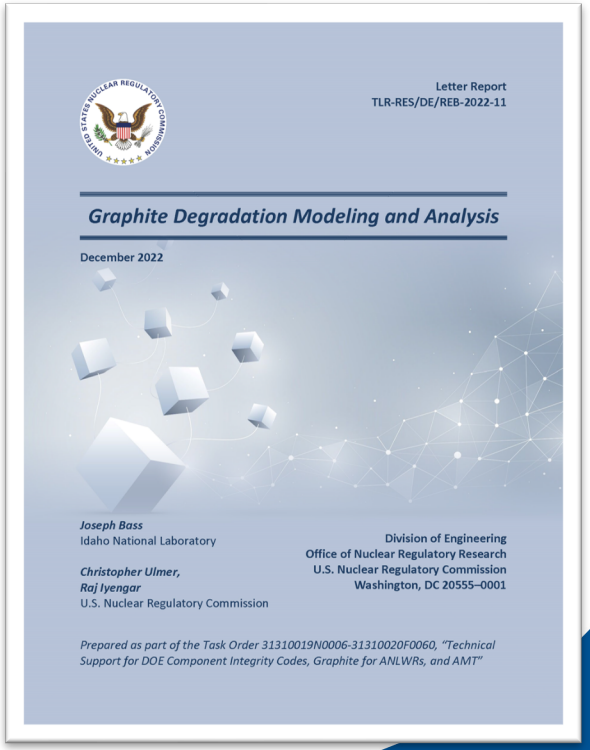
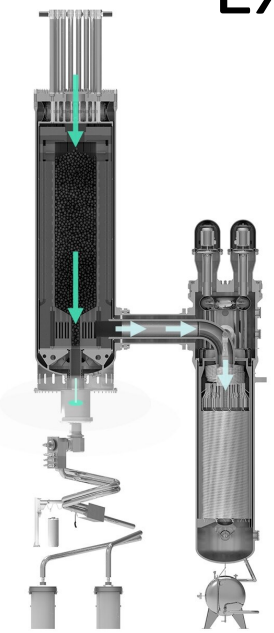


Graphite for ANLWRs

- Graphite materials may be used in thermal spectrum advanced reactors
- Graphite has excellent neutron moderation properties
- Graphite is also used for core support components

Examples:

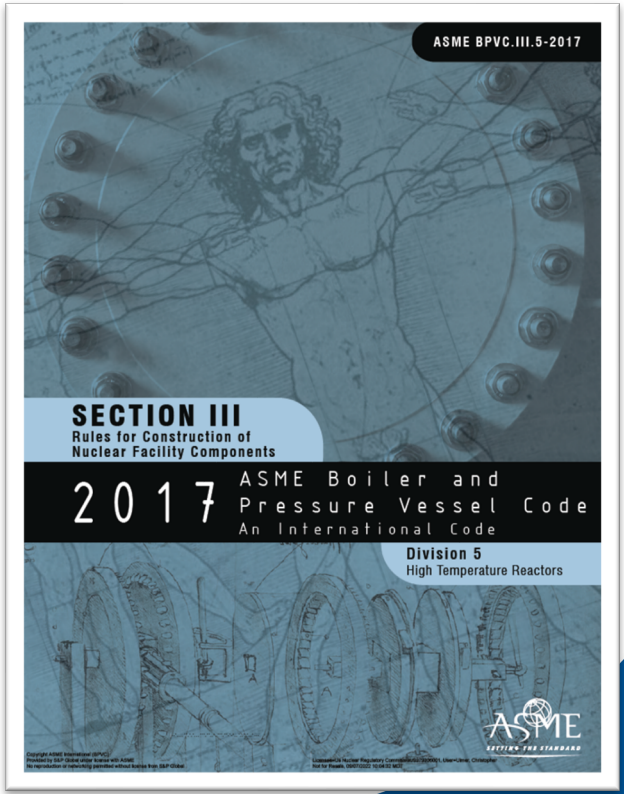


X-energy Xe-100

Terrestrial Energy IMSR

ASME Code

- Graphite assessment methodology was added to ASME BPVC Section III Division 5 in subsection HH subpart A
- Probability of failure in a graphite component is based on the inherent strength of a graphite grade and the applied stresses during operation
- Considerations include oxidation and irradiation
- NRC staff issued draft regulatory guide DG-1380 which endorses, with conditions, ASME BPVC III.5



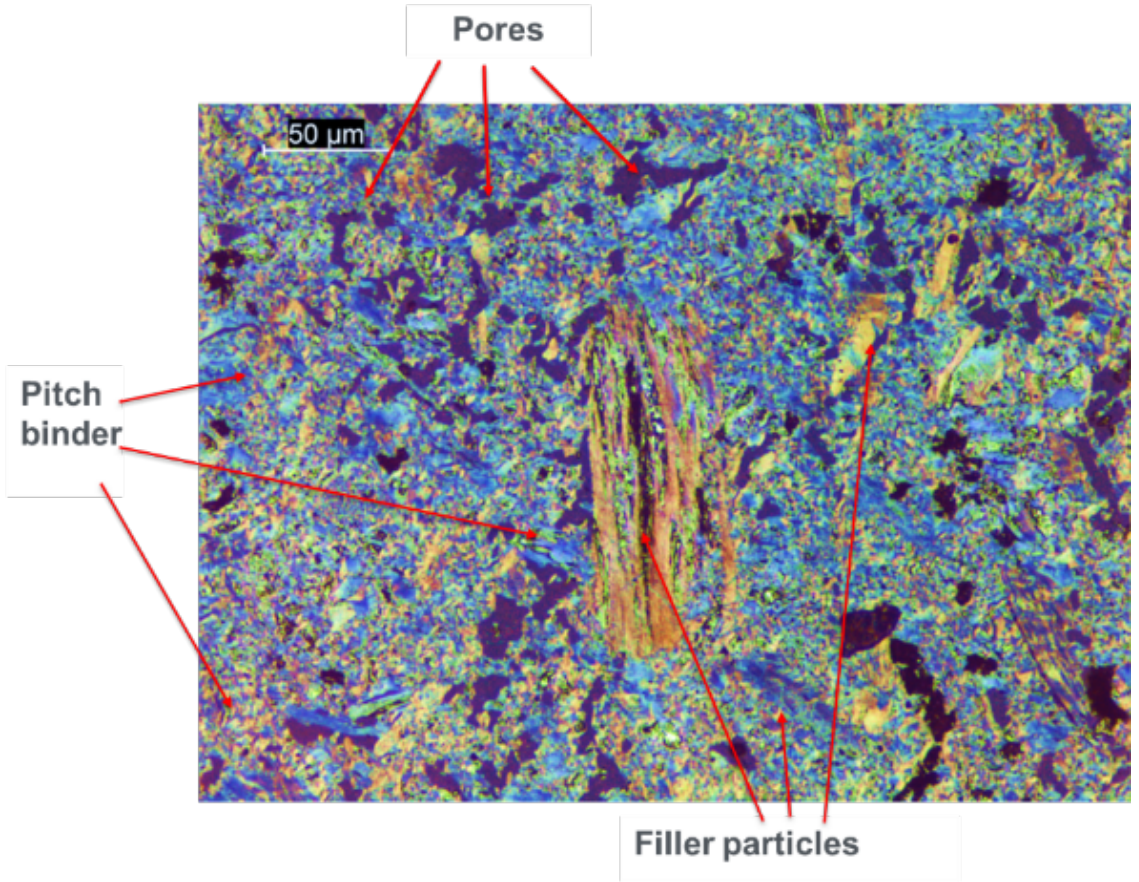
Material Properties

- Material isotropy is processing dependent
- High thermal stability > 3000°C
- High heat capacity (thermal sink)
- High thermal conductivity (better than metal)
- Density: 15% - 20% porosity
- Purified graphite: Low activation
- Molten salt interaction is an area of current research
- Neutron moderator (thermal designs)
- Easy machinability / cheap material
- High compressive / Low tensile strength
- Ceramic like material response
- Low fracture toughness (~ 1-2 MPa √m)
- Quasi-brittle cracking

From ASTM D7219

Property	Nominal Range
Density	1.7 - 1.9 g/cm^3
Thermal Conductivity (at Room Temperature)	> 90 W/m/K
Purity (Total Ash Content)	< 300 ppm
Tensile Strength	> 15 MPa
Compressive Strength	> 45 MPa
Flexural Strength	> 20 MPa
CTE (20°C to 500°C)	3.5 to 5.5 x 10^{-6} K^{-1}
CTE Isotropy Ratio	< 1.10
Dynamic Elastic Modulus	8 – 15 GPa

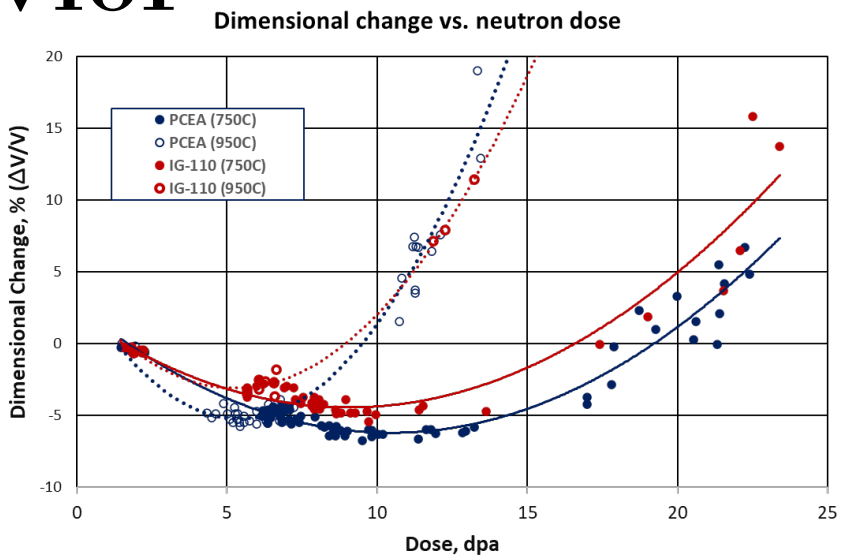
Graphite Microstructure



- Graphite microstructure has three phases: filler particles, binder phase, and pores (~20%)
- Pores and pore structure play an important role in graphite irradiation behavior
- Oxygen can penetrate the interior of the graphite pore microstructure

Irradiation Behavior

- Dimensional change is a life-limiting behavior
- Turnaround is a key parameter
- Affected by microstructure and temperature
- Internal stress build-up from dimensional changes
- Less predictable behavior and (micro)cracking after turnaround
- Irradiation creep can relieve internal stresses



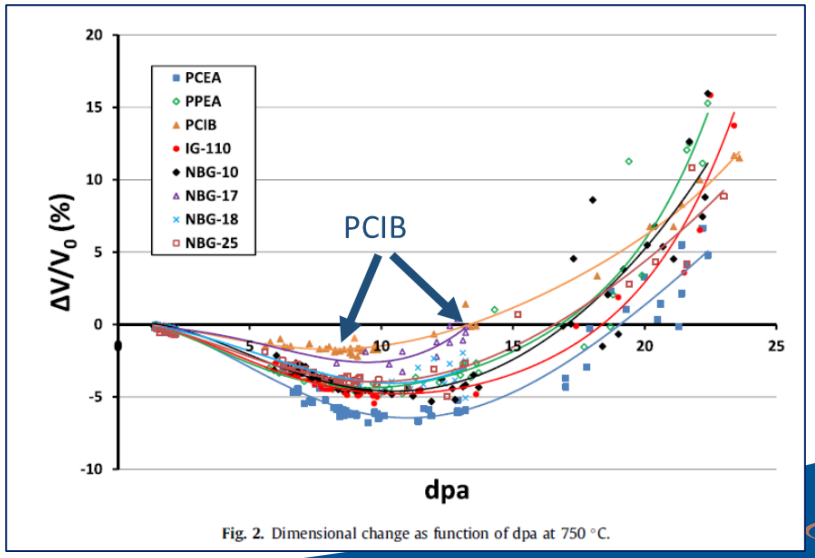


Fig. 2. Dimensional change as function of dpa at 750 °C.

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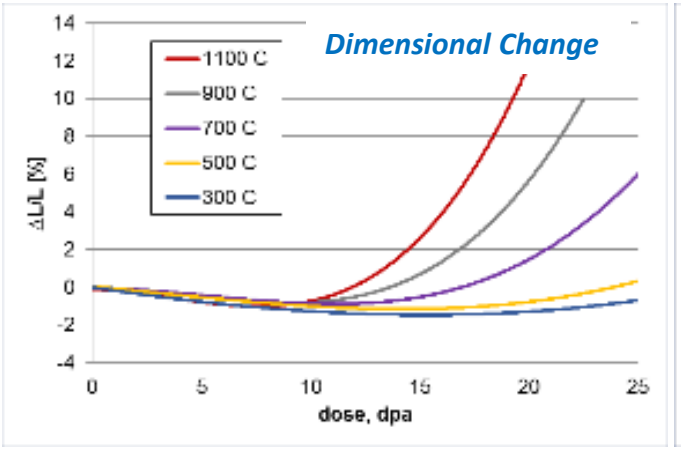
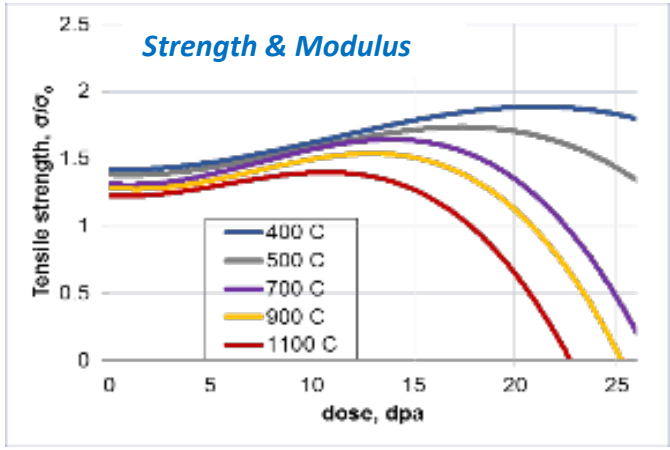
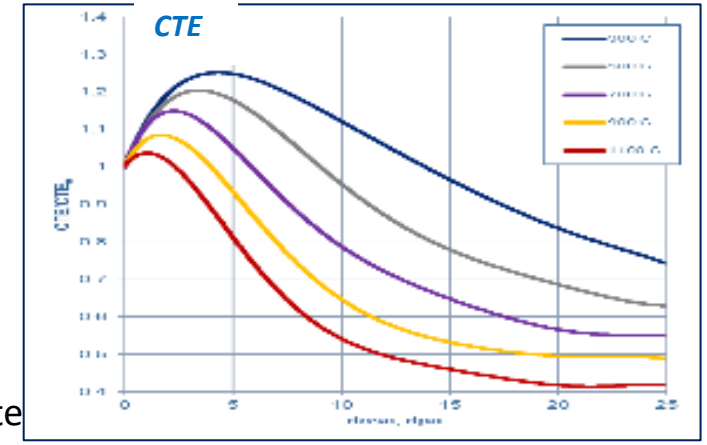
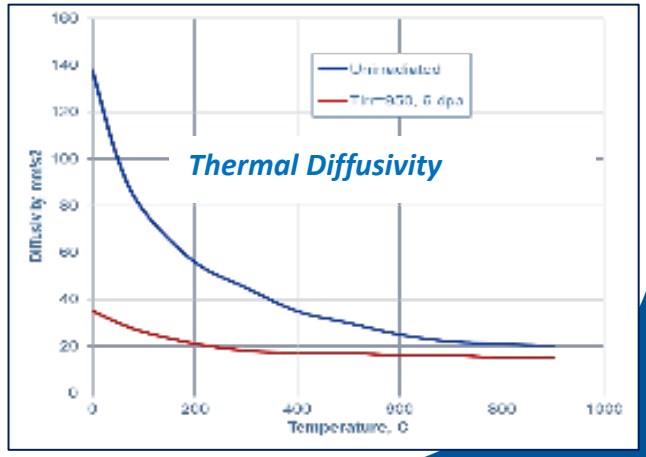
Irradiation Effects on Graphite Properties

- Dimensional change
  - Turnaround dose is key parameter
  - Highly temperature dependent
- Density
  - Graphite gets denser with irradiation until turnaround and then density decreases
  - Formation of microcracks (molten salt consideration)
- Strength and modulus
  - Strength increases until turnaround dose and then decreases
- Coefficient of thermal expansion
  - Initial increase but then decreases before turnaround
- Thermal conductivity
  - Decreases quickly to ~30% of unirradiated values
- Oxidation rate
  - Increases approximately 2-3 times over unirradiated rate



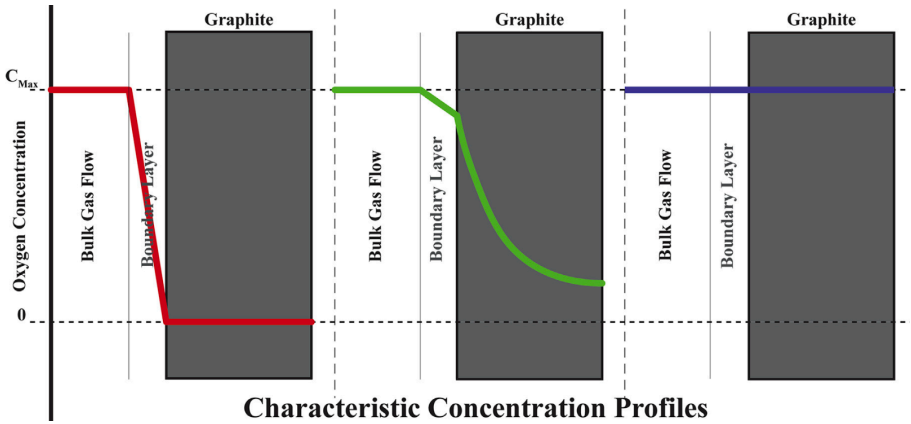




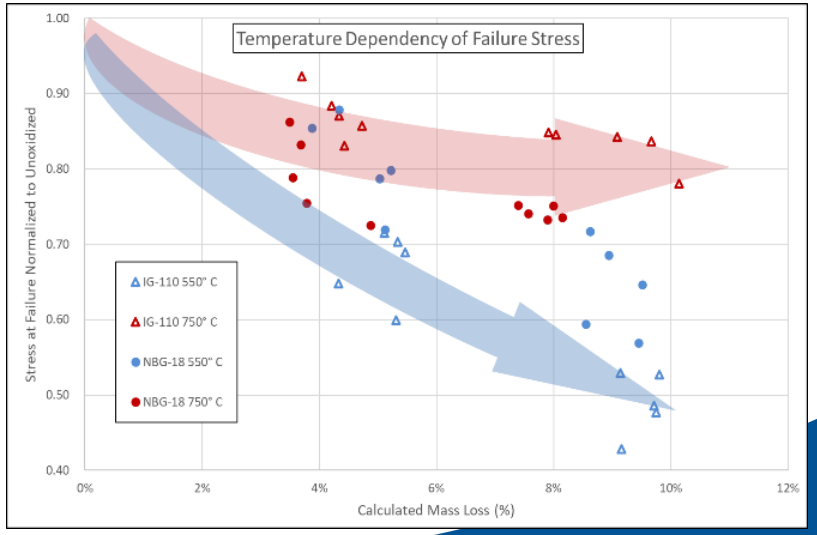


Graphite Oxidation

- Oxidation is a complex relationship between reactivity and diffusion of oxygen
- Reactive surface area is related to pore structure
- Oxidation kinetics and gas diffusion are affected by temperature
- It is important to know the strength remaining after oxidation
- Temperature and microstructure affect oxidation rate and the extent of component internal oxidation



Characteristic Concentration Profiles



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Graphite Modeling

Graphite Modeling Outline

- Summary of modeling goals
  - What can the model do?
  - What can't the model do?
- Modeling in MOOSE
  - What is MOOSE?
  - Introduction to using MOOSE
- Modeling stresses in graphite
  - Included physics, model formulation, and example problem
- Modeling degradation (oxidation) in graphite
  - Included physics, model formulation, and example problem
- Applying the ASME assessments for graphite components

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Summary of Modeling Goals

The primary modeling goal is to provide a tool to help in the assessment of graphite components.

How can we assess a component?

Section III Division 5, subsection HH subpart A, of the ASME BPVC provides guidance on assessing a graphite component.

Two topics which this tool addresses (which are required/discussed in the ASME Code) are:

1) Computing a stress distribution in the graphite component
   - Accounting for thermal and irradiation effects in the stress calculation
2) An analysis of the oxidation degradation
   - Computing temperature-dependent density profiles.

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Model Limitations

What can't the model do?

- Material properties as a function of the states (temp, dose, mass loss) must be known.
    - The combined effect of oxidation and irradiation has not been well explored, so well characterized properties do not currently exist.
    - Post-turnaround properties have increased scatter and much less data. Consequently, the model should only be used up to turn around.
    - All grades of graphite behave differently, so graphite specific parameterizations are necessary.

1. Not all loads from the ASME Code can be directly implemented in the model.
    - Excludes: Fatigue, erosion, earthquake.
2. This is model is not a neutronics model. The evolution of the dose in the graphite must be determined separately.

HHA-3122 Loadings

The loadings that shall be taken into account in designing the Graphite Core Components include, but are not limited to, those in (a) to (n) below. Note that some of the loadings below may be loadings on the Graphite Core Assembly that shall be reduced to loads on the individual Graphite Core Components.

(a) pressure differences due to coolant flow

(b) weight of the core components and fuel

(c) superimposed loads such as those due to other structures, the reactor core, flow distributors and baffles, thermal shields, and safety equipment

(d) earthquake loads or other loads that result from motion of the reactor vessel

(e) reactions from supports, restraints, or both

(f) loads due to temperature effects, thermal gradients and differential expansion of the Graphite Core Assembly, or any combination thereof

(g) loads resulting from the impingement or flow of reactor coolant, or other contained or surrounding fluids or gases

(h) transient pressure difference loads, such as those that result from rupture of the main coolant pipe

(i) vibratory loads

(j) loads resulting from operation of machinery such as snubbing of control rods

(k) handling loads experienced in preparation for or during refueling or inservice inspection

(l) internal loads such as those resulting from thermal stresses or irradiation-induced stresses resulting from temperature and flux/fluence distribution within a Graphite Core Component

(m) loading due to instabilities caused by component distortion (such as bowing of graphite columns)

(n) assembly loads and loading during construction

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What is MOOSE?

MOOSE is the framework where the graphite tool was developed.

Overview:

MOOSE (Multi-physics Object Oriented Simulation Environment) is an open-source, parallel finite element framework which has been under constant development at INL since 2008.

Purpose:

Designed to solve computational engineering problems and reduce the expense and time required to develop new applications.

Modules:

MOOSE contains modules which have been developed to simulate a variety of different physics and modeling methodologies including chemical reactions, contact, electromagnetics, heat conduction, phase-field, porous flow, tensor mechanics, XFEM and many others.

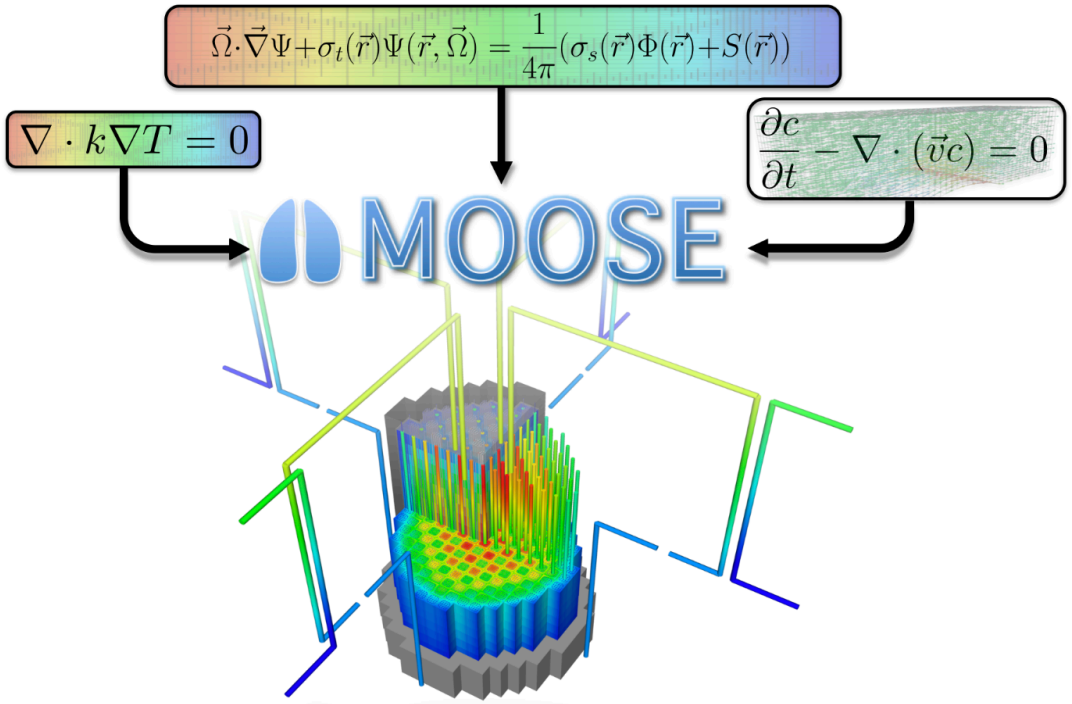

Image form: mooseframework.inl.gov

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MOOSE Organization

Applications which are built on the MOOSE framework are often given an animal name. Not all animals are open source, although anyone can request access.

The general organization of MOOSE including the physics modules and the more prominent animal is show in the figure below.

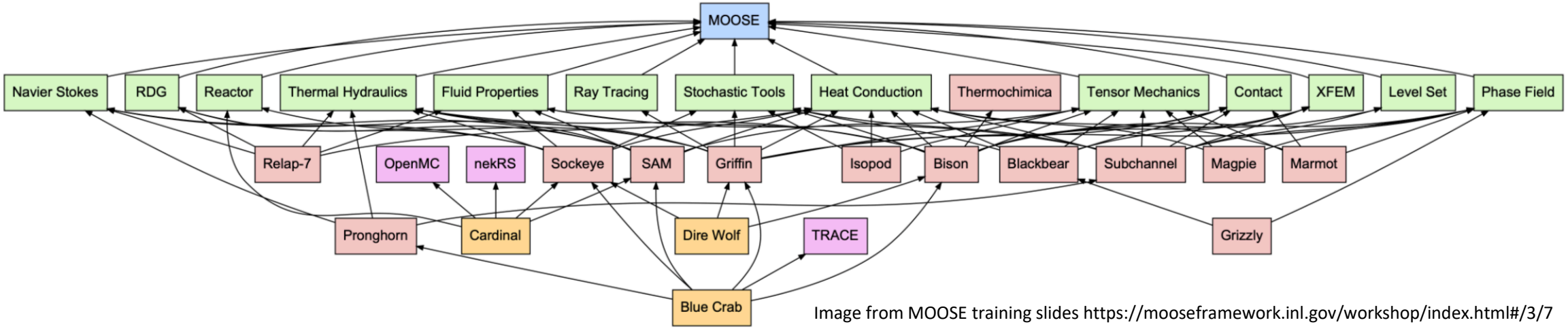

Image from MOOSE training slides https://mooseframework.inl.gov/workshop/index.html#/3/7

The graphite modeling capabilities discussed in this presentation are available in Grizzly. Everyone in the NRC has access to Grizzly through the Linux RESGC instances. External users must go through INL's Nuclear Computational Resource Center.

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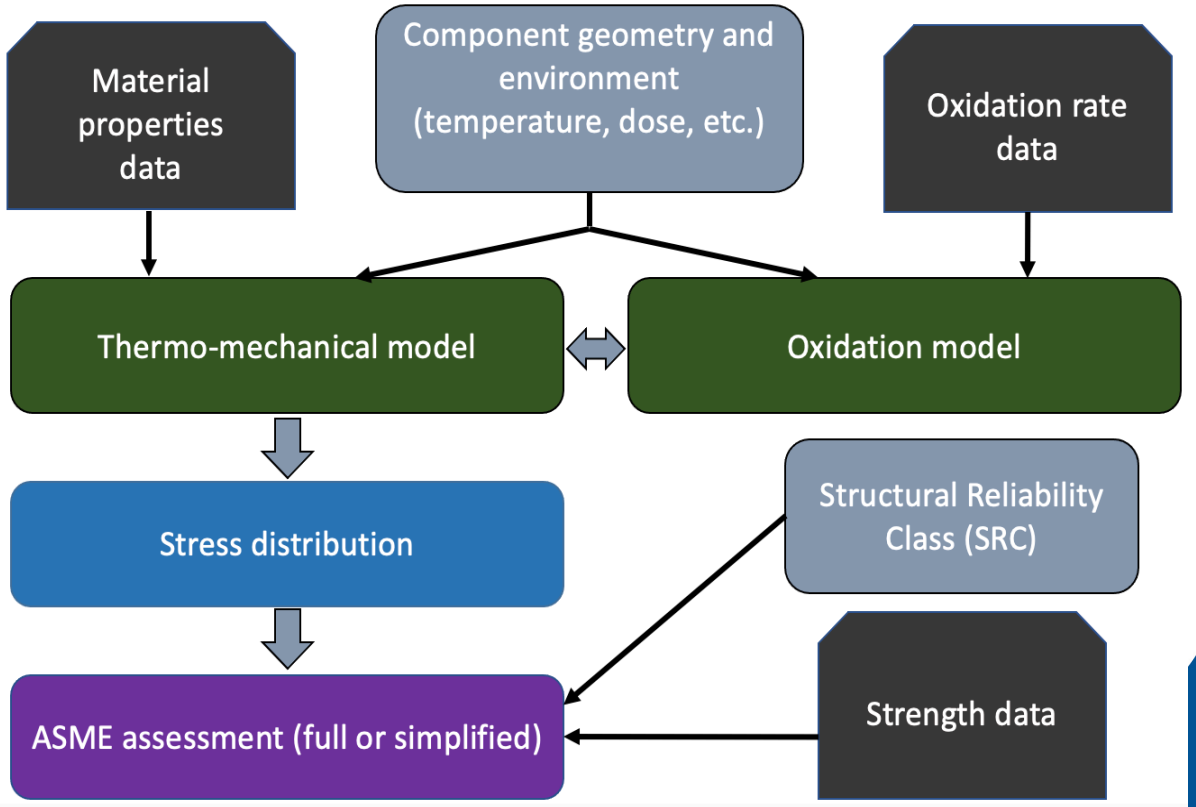
Graphite Assessment Overview

The flow chart on the right shows the various required pieces of performing a design by analysis assessment as outlined in the ASME code.

There are four distinct block types in the flow diagram

1. Required experimental data (brown blocks)
2. Parameters which are dependent on the design of the reactor (gray blocks)
3. Physics based models (green blocks)
4. ASME analysis methodology (purple block)



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Considerations when Modeling Stresses in Graphite

Properties:

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

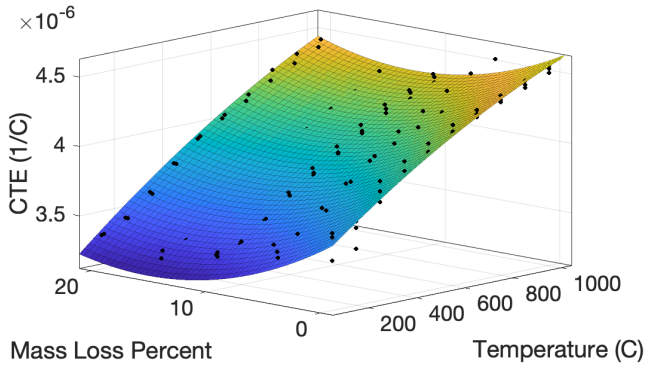
Eigenstrains:

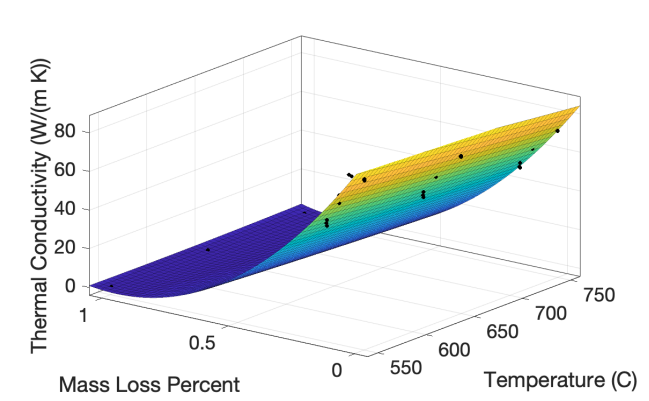
- The coefficient of thermal expansion is affected by dose as well as mass loss from oxidation.
- Irradiation induced swelling is a function of dose as well as irradiation temperature.

Property Scatter:

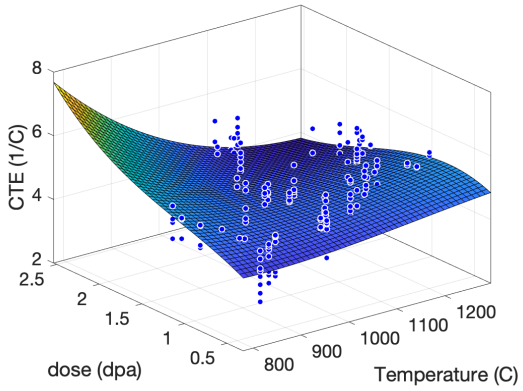
- Experimentally measured properties have more scatter post turn-around.
- Scatter in graphite strength has led to probabilistic failure assessment methodologies

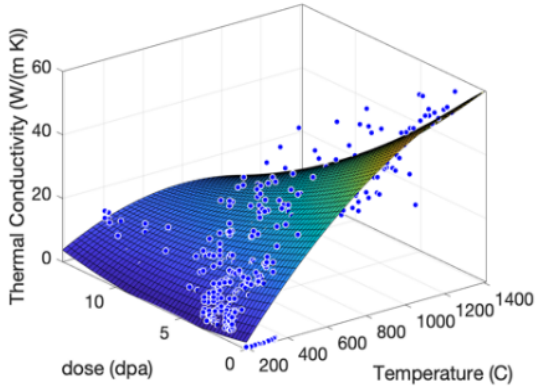
Oxidation effects





Irradiation effects





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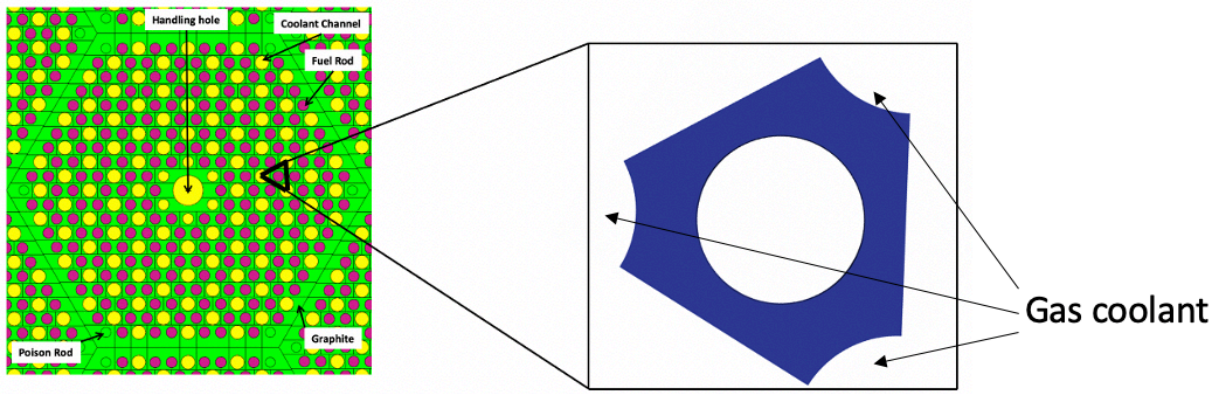
Thermo-mechanical Model: Overview (1/2)

Which type of problem is this model intended to solve?

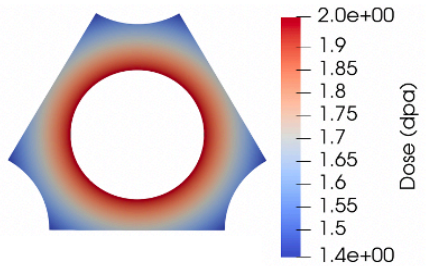
This portion of the model computes stress and temperature distribution at the engineering scale.



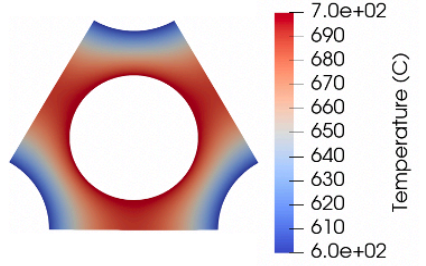
Included Physics:

1. Eigen strains generated from temperature and irradiation
2. Irradiation creep
3. Elastic strain
4. Heat Transfer (thermal conduction)
5. Material properties vary as a function of the states (temperature, dose, mass loss)

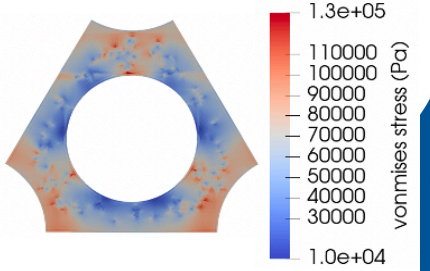
Temperature



Dose



Stress



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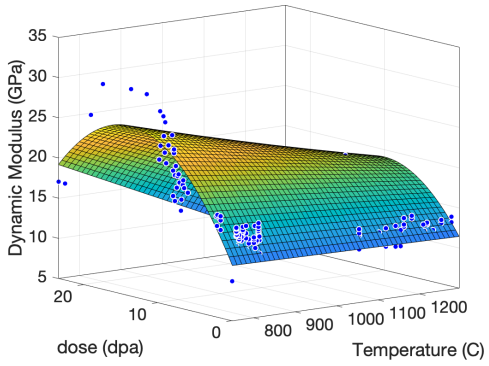
Thermo-mechanical Model: Overview (2/2)

Model Inputs and Outputs:

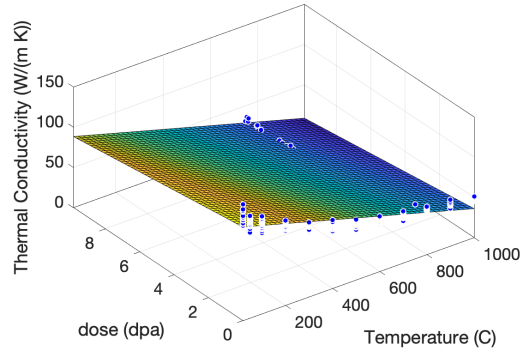
1. Material properties parameterized as a function of dose, temperature and mass loss.
2. Dose profile evolution (dose and dose time derivative)
3. Boundary conditions for variables.

Model Limitations

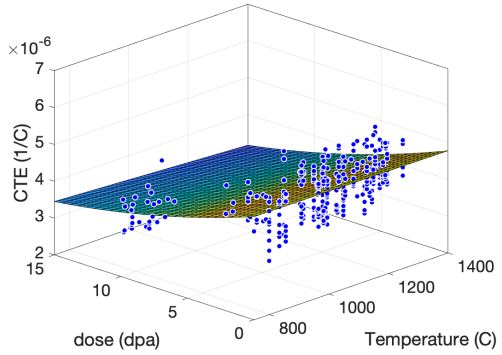
1. The model is parametrized for IG-110. To use the model for other grades a new parameterization should be implemented.
2. The model should only be used where experimental data exists (no combined irritation and oxidation, and the parameterization is not applicable past turn around)



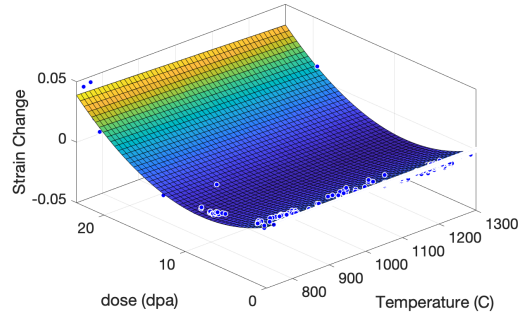
Elastic Modulus



Thermal Conductivity



CTE



Irradiation Strain

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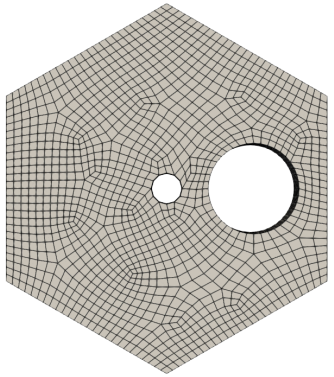
Thermo-mechanical Example Problem

The state variables in the thermo-mechanical model are **strain, temperature,** and **dose**. The model accounts for strain contributions from thermal, irradiation, and mechanical loads. In order to run an example problem, we must define the initial states in the system.

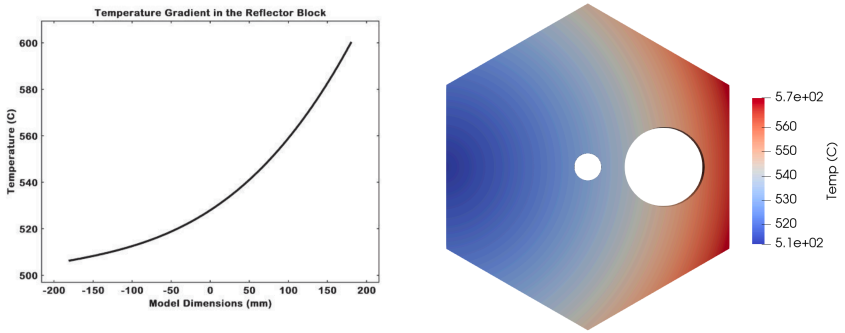
Problem Setup:

Assume we have the component geometry, temperature distribution, and dose evolution profile shown below:

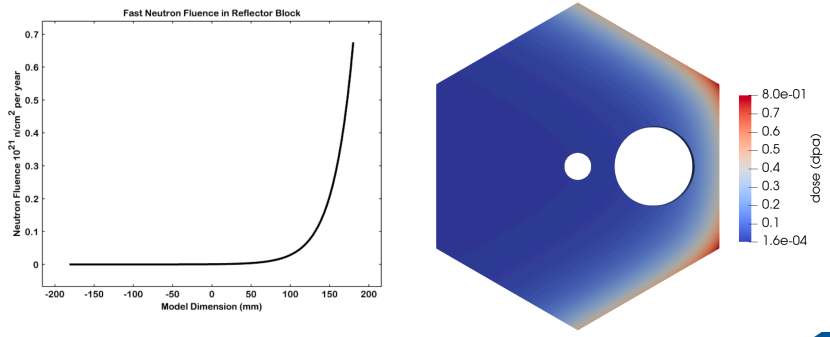
Geometry



Temperature Profile



Dose Profile Rate

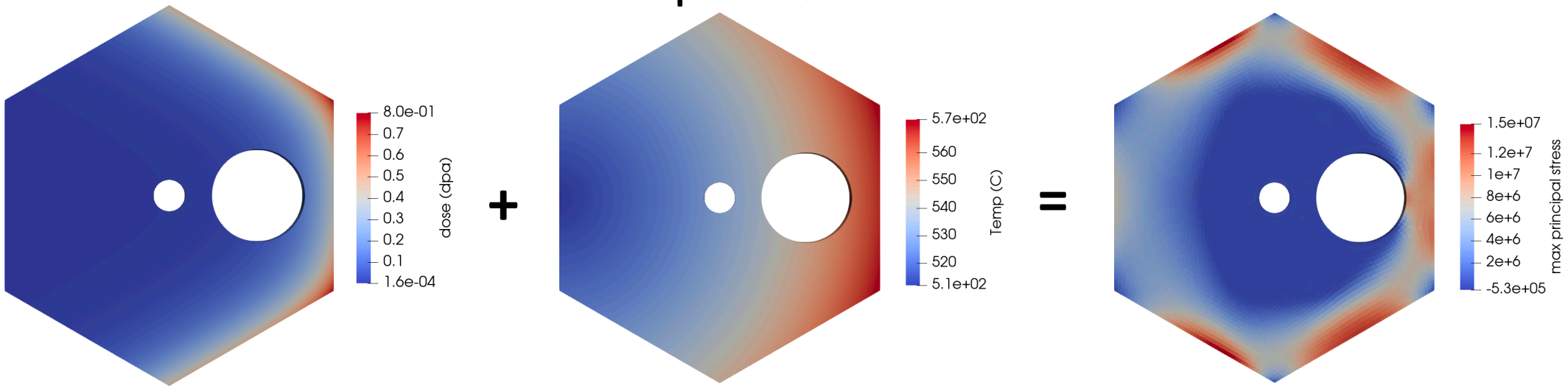


The output of interest from the thermo-mechanical model is the stress distribution. The stress distribution is used in the structural assessment in the ASME Code.

Simulation Results

The resultant stress distribution from the input temperature profiles, and irradiation effects are shown below. This results match well with previous studies which have simulated this problem.

Dose Profile **Temperature Profile** **Stress Distribution**



All variables and auxvariables can be output (including the outputs relevant the ASME code assessments)

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Oxidation Model Overview: Motivation for Model

Why is oxidation modeling important?

1. The strength and other properties of oxidized graphite are a function of mass loss.
2. The ASME requires that the effect of oxidation is accounted for in the analysis of a graphite component.

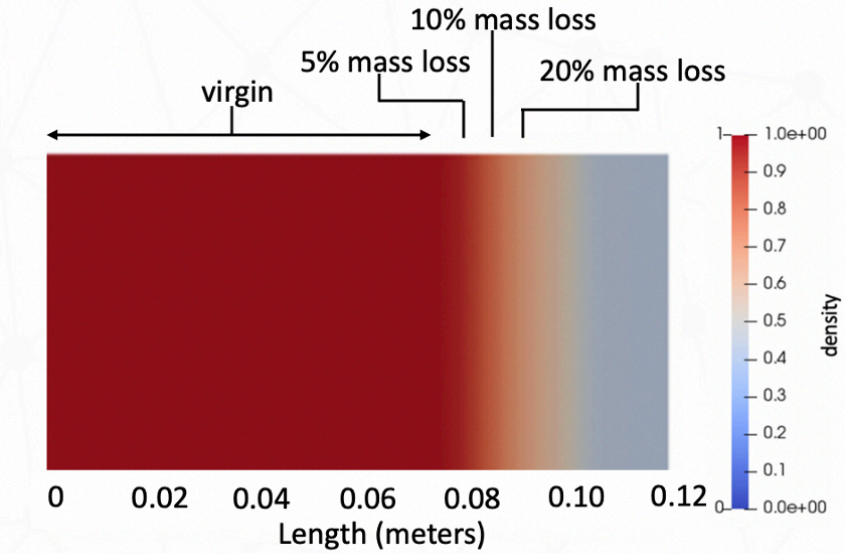
What does the oxidation model do?

1. The model computes mass loss (density profiles) in a graphite component.
2. Computes temperature change caused by heat generation from graphite – oxygen reaction.
3. The oxidation model can be coupled to thermo-mechanical model (stress calculations).

Local material properties need to be computed as a function of local mass loss.

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.



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Oxidation Model: Background

Graphite oxidation is a multiscale phenomena, but for analysis, **we are most interested in macroscale effects**.

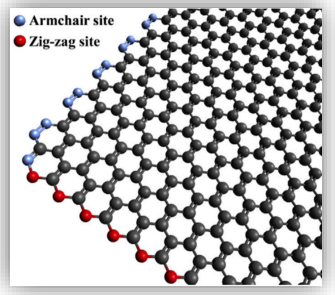
What physics is needed to model macroscale effects?

1. **Oxidant diffusion** through the graphite
    - Controlled by graphite microstructure
    - Is a combination of Knudsen and bulk contributions
    - Evolves with the microstructure as oxidation increases

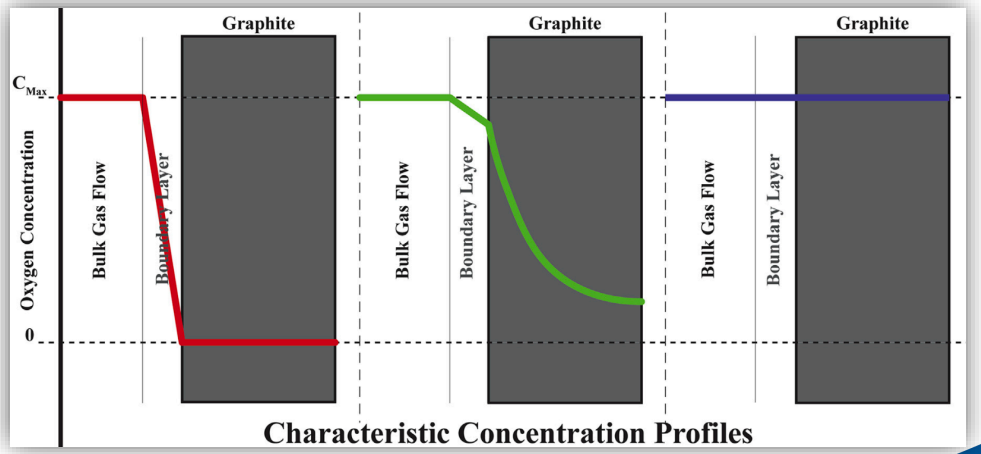
    This effect is modeled with a mass loss dependent effective diffusion coefficient (D_{eff})
2. **Reaction kinetics** of the graphite
    - Is a function of the graphite crystallites (ASA cites density)
    - Will evolve with mass loss

    This effect is modeled with a mass loss dependent parameters which is proportional to the ASA (S_A).
3. **Heat generation** from graphite-oxygen reaction
    - Thermal conductivity evolves with mass loss
    - Reaction products are temperature dependent

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



Walker Diagram



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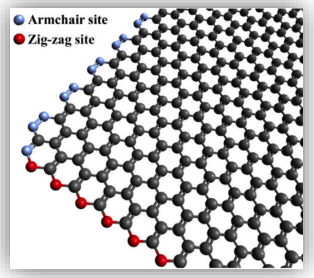
Oxidation Model: Assumptions

There are three primary assumptions used in the development of the oxidation model:

Assumption	Effects of Assumption
At the atomistic scale, the reaction between graphite and the oxidant does not differ across grades.	We can conclude that the observed oxidation rate is a function of the microstructure and can be described by parameters which are a function of the microstructure.
Oxidation occurs on the pore wall in the open porosity.	The observed oxidation rate is controlled by pore surface area density (typically proportional to active surface area) and oxidation diffusion through the pores.
Impurities in the graphite do not have an appreciable effect.	The model will not account for rate effects which can be caused by impurities.



Note: Oxidation experiments on graphite powder were performed by Josh Kane in order to derive a generic oxygen-graphite reaction rate.
It is assumed that this derived reaction rate will be applicable to any graphite grade because the powdered graphite does not contain microstructural effects which would be present in a larger graphite specimen.

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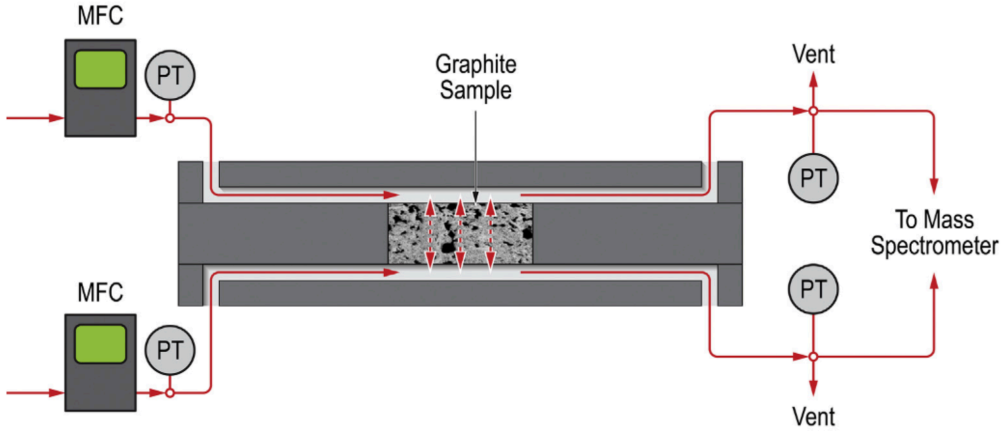
Oxidation Model: Formulation

The State variables in the oxidation model are the **temperature**, **chemical species concentrations**, and **graphite density**.

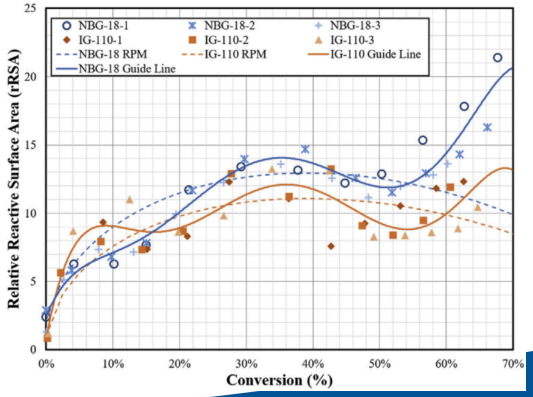
State variable evolution:
The species concentrations and graphite density evolve through gas diffusion and chemical reactions.
The temperature evolves through heat transfer and the exothermic reaction between graphite and oxygen.

Experimental testing is required to parameterize the model

Gas diffusivity experimental testing



Reactive surface area experimental testing



RSA evolution with mass loss

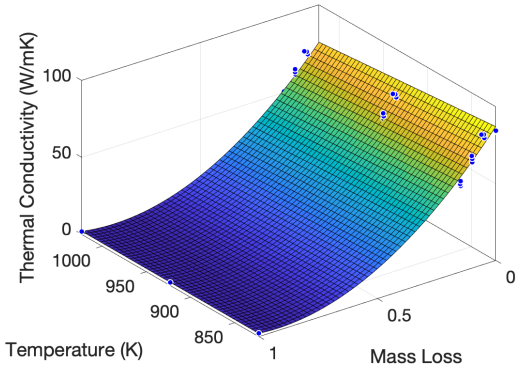
Modeling Oxidation Heating Generation

The reaction of oxygen and graphite is exothermic which may affect temperature which in turn may affect the oxidation rate.

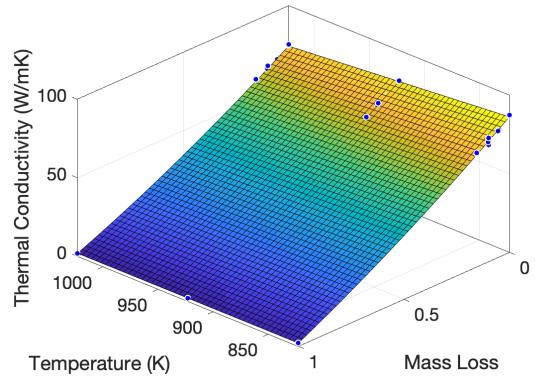
Several things need to be known to model the temperature effects of oxidation:

1. Thermal conductivity as a function of mass loss and temperature (experimental input)
2. Amount of heat generated
    - Reaction products
    - Reaction rate

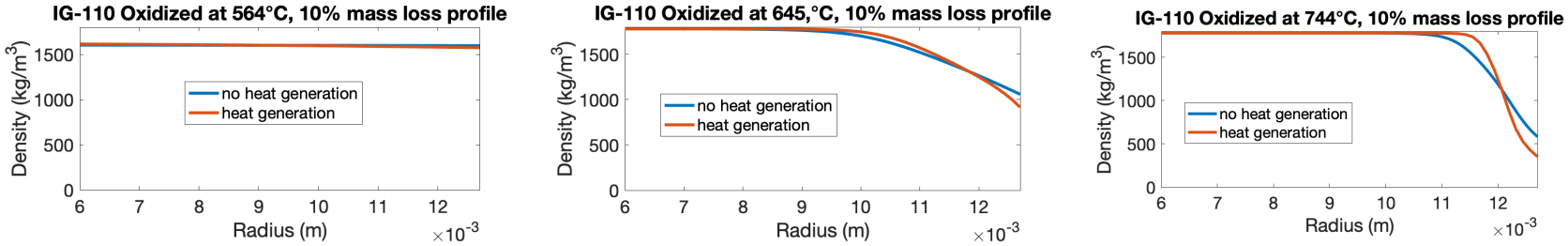
IG-110 Thermal Conductivity



NBG-18 Thermal Conductivity



Effect of heat generation on density profiles in oxidized cylinder



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Oxidation Example Problem: Introduction

This example problem investigates the temperature-dependent density profiles generated in a graphite cylinder (2-inch length, L, and 1-inch diameter, D).

Problem model setup:

Problem run to 10% mass loss in IG-110

BCs:

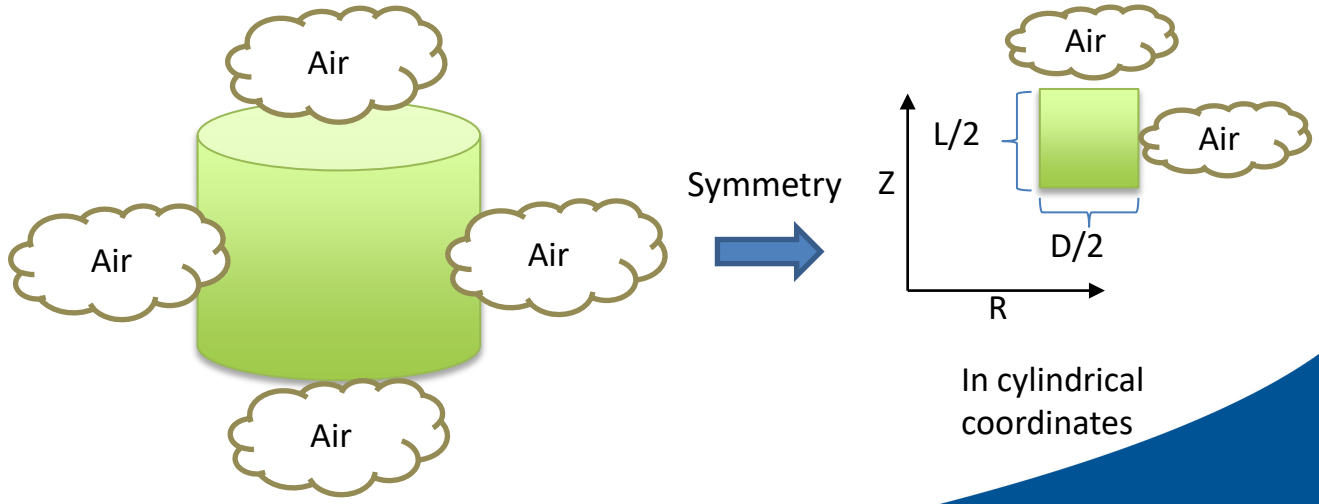
1) Air is on the outside of the cylinder

2) Temperature of 564, 645, and 744 °C

Wanted Result:

Density Profile

Problem Geometry:



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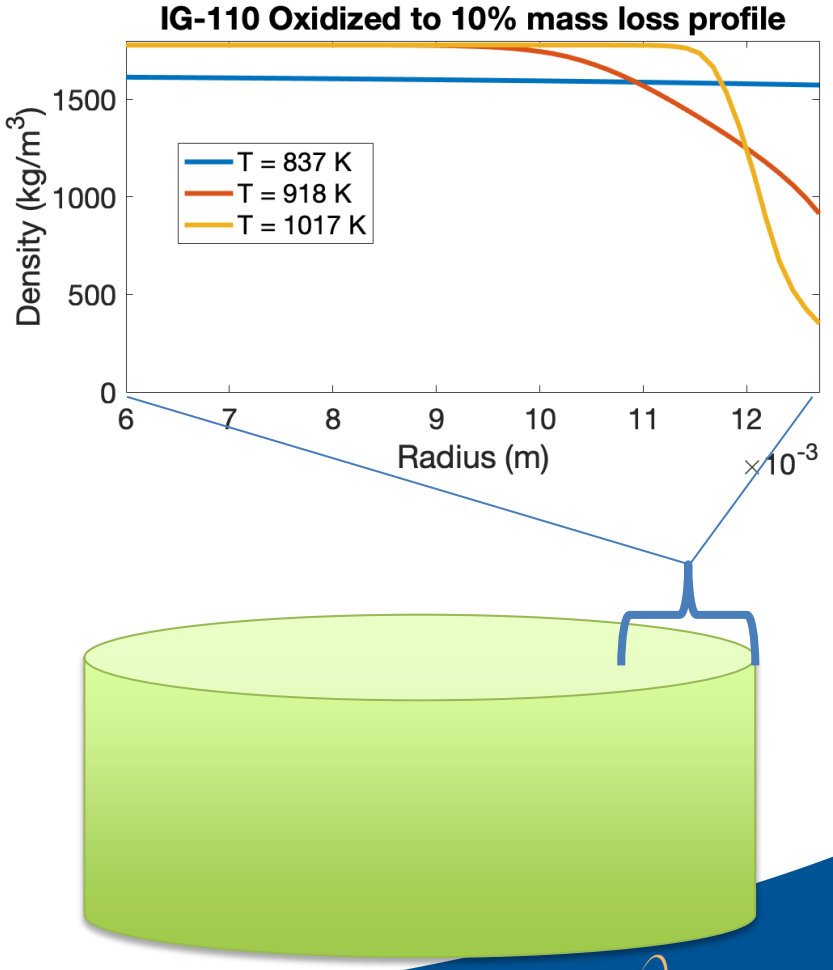
Example Problem: Results

To create the input file for this problem we must:

1. Generate a mesh
2. Specify boundary conditions (species concentrations and temperature)
3. Select a graphite grade (IG-110 or NBG-18)
4. Set a simulation run time



The plot on the right shows the resultant density profiles at three temperatures each of which are at 10% mass loss. The main takeaways from this plot are:

1. The slope of the density profile increases with an increase in temperature
2. This is the experimentally observed temperature-dependent density profile behavior

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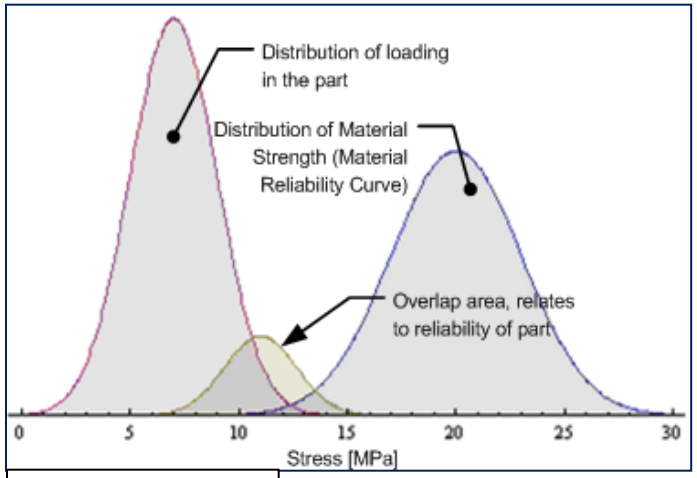
ASME Assessments for Graphite

The ASME Code provides guidance on what phenomena should be considered in an analysis of a graphite component subjected to a high temperature nuclear environment.

Three methods are provided for assessing structural integrity

1. Simple Assessment: Allowable stress
   - The computed peak equivalent stress is compared to an allowable value derived from Weibull theory and an allowable probability of failure (POF)
   - Conservative method based on Weibull derived ultimate strength
2. Full Assessment Method: Allowable Probability of Failure
   - Weibull statistics are used to predict failure probability over the stress distribution in a component. It gives a full statistical analysis of the entire stress distribution through the component volume.
   - Typically, less conservative than the simplified assessment
3. Qualification by Testing
   - Full-scale testing to demonstrate that failure probabilities meet all criteria of full-analysis method.



Dr. Mark Mitchell – PBMR Inc.

Applying the ASME Code

A python script has been written which uses the outputs from the thermo-mechanical model and applies the simplified or full assessment. The python code and user manual on available upon request.

Simplified Assessment

Inputs:
1) 2 parameter Weibull distribution of tensile strength
2) Compressive strength
3) Structural Reliability Class (SRC), which determined the allowable POF.
4) Principal stresses computed from FEA

Outputs:
1) Computed allowable peak equivalent stress
2) Pass or Fail

Full Assessment

Inputs:
1) 3 parameter Weibull distribution of tensile strength
2) Compressive strength
3) Structural Reliability Class (SRC), which determined the allowable POF.
4) Principal stresses computed from FEA

Outputs:
1) Computed probability of failure
2) Pass or Fail

The assessments currently determine the probability of crack formation. The nonmetallic ASME working group is currently looking into the best way to advance the definition of failure in graphite.

Summary

1. NRC staff are interested in developing expertise and tools to model graphite behavior in ANLWRs
2. INL developed a MOOSE-based tool to implement a graphite reliability model capable of performing component reliability analysis based upon ASME BPVC Section III Division 5, subsection HH subpart A requirements
   - Capabilities for modeling stresses in graphite were developed
   - Capabilities for modeling oxidation in graphite were developed
   - Python codes were written to implement the full and simplified assessments.
3. The graphite modeling capabilities discussed in this presentation are available in Grizzly. Everyone in the NRC has access to Grizzly through the Linux RESGC instances. External users must go through INL's Nuclear Computational Resource Center.
4. A report detailing this work titled "Graphite Degradation Modeling and Analysis" is available. Example problems on modeling graphite are available within Grizzly.

Questions?

Lunch Break

Meeting will resume at 1:00 pm EST

Microsoft Teams Meeting
Bridgeline: 301-576-2978
Conference ID: 115 537 606#

FY22 Advanced Reactor Code Development Updates for Consequence Analysis

Kyle Clavier, PhD, SNL

Dan Clayton, PhD, SNL

Keith Compton, PhD, US NRC

Advanced Reactor Stakeholder Meeting

December 15, 2022

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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Code Development Plan for Consequence Analysis

- Potential MACCS code technical issues identified in “Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis” (NRC, 2020)
- What have we accomplished in FY22?
- What is our path forward?

MACCS Technical Issues for Non-Light Water Reactors

- Near-Field Atmospheric Transport and Dispersion (Task CA1)
  - Based on the potential for non-LWRs to be located on sites with shorter site boundary distances than traditional LWR sites, improve MACCS near-field atmospheric transport and dispersion capability
- Radionuclide Screening (Task CA2)
  - Perform a screening analysis to identify which subset of radionuclides to include in MACCS calculations for each non-LWR type given the different mix of radionuclides that may be released in accidents from each type
- Chemical Form, Particle Size, and Shape Factor of Radionuclides and Impact on Atmospheric Transport and Dosimetry (Task CA3)
  - Evaluate potential differences in radionuclide releases from non-LWRs relative to LWRs including different aerosol size distributions, shape factors, and chemical forms. Based on the evaluation, improve MACCS capabilities for atmospheric transport and dosimetry to appropriately capture these issues for probabilistic consequence analysis. If necessary, consider a state-of practice resistance model for dry deposition.

MACCS Technical Issues for Non-Light Water Reactors (Continued)

- Tritium Modeling (Task CA4)
  - Develop MACCS model and/or dosimetry updates to better account for the unique behavior of tritium which is very mobile and can enter biological systems as part of water and organic molecules.
- Evolution of Radionuclide Properties in the Atmosphere (Task CA5)
  - Identify whether non-LWR accident releases may be more subject to evolution in the atmosphere relative to LWR releases based on differences in hygroscopic properties or potential for chemical reactions during transport.
- Impacts on Decontamination (Task CA6)
  - Based on the potential for non-LWRs to be sited in areas with different land use patterns than traditional LWR sites, develop updated decontamination cost models
- Chemical Hazards (Task CA7)
  - Examine issues associated with potential chemical releases to the environment. If appropriate, the staff will explore the use of the CHEM_MACCS tool for potential use with non-LWRs.

FY22 Tasks

- Radionuclide Screening (Task CA2)
- Chemical Form, Particle Size, and Shape Factor of Radionuclides and Impact on Atmospheric Transport and Dosimetry (Task CA3)
- Tritium Modeling (Task CA4)

Radionuclide Screening (Task CA2)

- Staff continued working on Task CA2 in FY22
- Section 3.3 and 8.2.1 of Appendix VI of WASH-1400 (NRC, 1975) identifies a subset of radionuclides to be included in a consequence analysis
- This methodology includes consideration of:
  - Radionuclide half-life
  - Emitted radiation type and energy
  - Inventory
  - Release fraction
  - Elemental chemistry

Alpert et al. (1986) updated the list of radionuclides identified in WASH-1400

- Estimation of release fractions was subject of considerable uncertainty at the time
- Alpert et al. developed a method to consider relative importance of individual elements to reactor accident consequences assuming equal release fractions
- Ultimately resulted in a list of 60 radionuclides
- This list was updated with the development of MACCS2
  - Explicitly includes 11 short lived decay progeny
  - 71 radionuclides in total identified for LWR consequence analysis

Table 1.

60 Nuclides Used for Offsite Consequence Assessment in MACCS

Element	Nuclides
Cobalt	58 60
Krypton	85 85m 87 88
Rubidium	86
Strontium	89 90 91 92
Yttrium	90 91 92 93
Zirconium	95 97
Niobium	95
Molybdenum	99
Technetium	99m
Ruthenium	103 105 106
Rhodium	105
Antimony	127 129
Tellurium	127 127m 129 129m 131m 132
Iodine	131 132 133 134 135
Xenon	133 135
Cesium	134 136 137
Barium	139 140
Lanthanum	140 141 142
Cerium	141 143 144
Praseodymium	143
Neodymium	147
Neptunium	239
Plutonium	238 239 240 241
Americium	241
Curium	242 244

* The 60 nuclides are the same as those examined in WASH-1400 [1] and in the CRAC2 computer code [9] except for the addition of six nuclides: Sr-92, Y-92, Y-93, Ba-139, La-141, and La-142.

Alpert et al., 1986

71 radionuclides were identified as important for LWRs based on inventory, half-life and potential biological hazard of radionuclides expected to be present in a large LWR

Chemical Group	Isotope	$T_{1/2}$
Noble Gas	Kr-85	10.72 yr
	Kr-85m	4.48 hr
	Kr-87	76.3 min
	Kr-88	2.84 hr
	Xe-133	5.25 d
	Xe-135	9.09 hr
	Xe-135m	15.3 min
Alkali Metals	Rb-86	18.7 d
	Rb-88	17.8 min
	Cs-134	2.062 yr
	Cs-136	13.1 d
	Cs-137	30.0 yr
Alkaline Earths	Sr-89	50.5 d
	Sr-90	29.1 yr
	Sr-91	9.5 hr
	Sr-92	2.71 hr
	Ba-137m	2.55 min
	Ba-139	82.7 min
	Ba-140	12.74 d
Halogens	I-131	8.04 d
	I-132	2.30 hr
	I-133	20.8 hr
	I-134	52.6 min
	I-135	6.61 hr
Chalcogens	Te-127	9.35 hr
	Te-127m	109 d
	Te-129	69.6 min
	Te-129m	33.6 d
	Te-131	25.0 min
	Te-131m	30.0 hr
	Te-132	78.2 hr
Platinoids	Ru-103	39.3 d
	Ru-105	4.44 hr
	Ru-106	368.2 d
	Rh-103m	56.1 min
	Rh-105	35.4 hr
	Rh-106	29.9 sec
Early Transition Elements	Co-58	70.8 d
	Co-60	5.271 yr
	Nb-95	35.1 d
Early Transition Elements	Nb-97	72.1 min
	Nb-97m	1.0 min
	Mo-99	66.0 hr
	Tc-99m	6.02 hr
Tetravalents	Zr-95	64.0 d
	Zr-97	16.9 hr
	Ce-141	32.5 d
	Ce-143	33.0 hr
	Ce-144	284.3 d
	Np-239	2.35 d
	Pu-238	87.74 yr
	Pu-239	2.41E4 yr
	Pu-240	6.54E3 yr
	Pu-241	14.4 yr
Trivalents	Y-90	64.0 d
	Y-91	58.5 d
	Y-91m	49.7 min
	Y-92	3.54 hr
	Y-93	10.1 hr
	La-140	40.3 hr
	La-141	3.9 hr
	La-142	92.5 min
	Pr-143	13.56 d
	Pr-144	17.3 min
	Pr-144m	7.2 min
	Nd-147	11.0 d
	Am-241	432.2 y
	Cm-242	162.8 d
	Cm-244	18.11 yr
Cadmium Group	Sb-127	3.85 d
	Sb-129	4.32 hr

Source: NUREG/CR-7270

Advancing reactor technology has motivated an investigation into developing a similar subset of radionuclides relevant to advanced non-LWRs

- High-temperature gas reactors (HTGR)
- Fluoride-salt-cooled high-temperature reactor (FHR)
- Molten-salt reactors (MSR)
- Sodium fast reactor (SFR)
- Liquid metal fast reactors (LMR)

The NRC Vision and Strategy Document (Vol. 3) outlines a radionuclide screening effort (Task CA2)

- Calls for the identification of a subset of radionuclides to be included in MACCS calculations for non-LWRs
- Radionuclide selection should be based upon factors such as:
  - Core inventory
  - Nature of radioactivity
  - Specific organ effects
- FY22 work expands upon previous qualitative efforts to screen advanced reactor radionuclides in *Preliminary Radioisotope Screening for Off-site Consequence Assessment of Advanced Non-LWR Systems* (Andrews et al., 2021)
  - Developed a preliminary, qualitative list of radionuclides for these reactors (57 radionuclides)
  - Identified knowledge gaps that still exist regarding reactor chemistry and system behavior

57 radionuclides identified in preliminary qualitative screening assessment (Andrews et al., 2021)

Chemical Group	Isotope	$T_{1/2}$	Reactor Type
New Proposed Group	H-3	12.3 y	HTGR, FHR, MSR, SFR
	C-14	5,730 y	HTGR, FHR
Alkali Metals	Na-22	2.6 y	SFR
	Na-24	15 h	SFR
Alkaline Earths	Ra-224	3.66 d	MSR
Noble Gas	Ar-41	110 m	SFR
	Kr-83m	1.83 hr	MSR
	Xe-131m	11.9 d	MSR
	Xe-133m	2.2 d	MSR
Early Transition Elements	Cr-51	27.7 d	SFR
	Mn-54	312.3 d	SFR
	Fe-59	44.5 d	SFR
	Nb-93m	16.13 yr	MSR
	Ta-182	114.4 d	SFR
Cadmium Group	As-77	38.5 hr	MSR
	Cd-113m	14.1 yr	MSR
	Cd-115m	44.5 d	MSR
	Sb-125	2.8 y	HTGR, FHR
	Sb-126	12.3 d	MSR
	Sb-128	9.01 hr	MSR
Chalcogens	Se-81	18.4 m	MSR
	Se-81m	57.3 m	MSR
	Se-83	22.3 m	MSR
	Te-125m	57.5 d	MSR
	Te-133m	55.4 min	MSR
	Te-134	41.8 min	MSR
Halogens	Br-83	2.4 hr	MSR
	Br-84	31.8 min	MSR
Platinoids	Pd-109	13.7 h	MSR
	Pd-112	21.0 hr	MSR
Tin Group	Ag-110m	250 d	HTGR, FHR
	Ag-111	7.45 d	MSR
	Sn-117m	13.7 d	MSR
	Sn-119m	293 d	MSR
	Sn-121m	43.9 yr	MSR
	Sn-123	129 d	MSR
Trivalents	Pr-146	24.2 hr	MSR
	Pm-147	2.6 y	HTGR, FHR, MSR
	Pm-148m	41.3 d	MSR
	Pm-149	53.1 hr	MSR
	Pm-151	28.4 hr	MSR
	Sm-151	88.8 y	HTGR, FHR, MSR
	Sm-153	46.3 hr	MSR
	Eu-154	8.6 y	HTGR, FHR, MSR
	Eu-155	4.8 y	HTGR, FHR, MSR
	Eu-156	15.2 d	MSR
	Eu-157	15.2 hr	MSR
	Cm-243	29 y	MSR, LMR
	Cm-245	8,500 y	HTGR, FHR, MSR, LMR
	Cm-246	4700 y	MSR, LMR
	Am-242m	150 y	MSR, LMR
	Am-243	7400 y	MSR, LMR
Tetravalents	Th-228	1.91 y	MSR
	Pa-233	27.0 d	MSR, MSR, LMR
	Pu-242	373,300 y	HTGR, FHR, MSR, LMR
Uranium Group	U-232	68.9 y	MSR
	U-237	6.75 d	MSR, LMR

Source: Andrews et al., 2021. *Preliminary Radioisotope Screening for Off-site Consequence Assessment of Advanced Non-LWR Systems*, SAND2021-11703

Advanced reactor research is still underway, but some preliminary information does exist

- Information on half-life and potential biological hazard for 825 radionuclides in MACCS is available
- Still need reliable information for advanced reactors:
  - Inventories
  - Transport pathways
  - Chemistries
- Some preliminary inventories are available
  - INL Heat Pipe Reactor Design
  - See Walker et al. (2022) *SCALE Modeling of the Fast-Spectrum Heat Pipe Reactor*
- Available inventories allow us to illustrate a method that can be applied to identify a list of radionuclides for any advanced reactor technology, provided that a quantitative inventory is available
  - Method analogous to Alpert et al. to estimate relative importance assuming equal release fraction
  - Identify “most important” contributors based on relative importance
  - Consider doses to multiple organs, scaled to that of I-131 (early phase) and Cs-137 (long-term phase)

MACCS 4.1 was used to assess the relative importance of advanced reactor radionuclide suite

- **Step 1**: calculate an activity-normalized dose of combined list of 57 preliminary radionuclides and heat pipe reactor suite
  - Screen heat pipe reactor by eliminating radionuclides with short half-lives (<1 hour) and low contribution to the total inventory (<0.0001%)
    - > 1200 radionuclides reduced to 108
  - EARLY and CHRONC doses from a unit 1-Ci release were modeled for each of these radionuclides and normalized to equivalent releases of I-131 and Cs-137, respectively
  - In this manner, a relative biological hazard list was developed
- **Step 2**: illustrate using a heat pipe reactor inventory to scale these “hazard rankings” by the inventory (relative to I-131 or Cs-137 as appropriate)
  - Identify radionuclides that, if released in sufficient quantities, may be important to early or long-term dose
- **Step 3**: additionally screen this list by eliminating radionuclides with effective and organ doses less than 1% of those of I-131 (early phase) and Cs-137 (late phase doses)

The MACCS assumptions used for this analysis mirrored those in Alpert et al. (1986)

- L-ICRP60ED dosimetric quantity used as surrogate for potential latent health effects from both EARLY and CHRONC phase doses. A-RED MARR and A-LUNG used for surrogates of early health effects from early phase doses
- Constant, “typical” weather conditions – D stability, 4 m/s windspeed, no rain
- Release occurs outside of the growing season
- Doses from elements/isotopes include the effect of radioactive decay and in-growth or decay progeny during transport.
- Nonbuoyant release from a single plume at 40 m elevation. Uniform 1-hour release immediately after accident initiation
- 0.002 m/sec dry dep. velocity, radiation protection factors of 0.75, 0.22, and 0.46 for cloudshine, groundshine, and inhalation and skin, respectively
- Uniform population distribution of approximate CONUS average
- No emergency protective actions, exposure duration of 7 days for EARLY, CHRONC duration of 1 year, no intermediate phase

Analysis suggests that 69 heat pipe reactor radionuclides may be of importance if released in sufficient quantities

- 48 of these radionuclides are already considered for LWR analyses
- 21 new radionuclides listed here
- Note: decay progeny not listed here

Isotope	EARLY Relative ICRP60 Effective Dose	EARLY Relative Red Marrow Dose	EARLY Relative Lung Dose	CHRONC Relative ICRP60 Effective Dose	CHRONC Relative Red Marrow Dose	CHRONC Relative Lung Dose
Ag-111			0.04			
Ag-112			0.01			
Cd-115			0.03			
Eu-155			0.017			
Eu-156		0.031	0.063			
Nb-95m			0.06			
Nd-149		0.014	0.22			
Pd-109			0.09			
Pm-147	0.34		1.57			0.03
Pm-148m			0.015			
Pm-149	0.035		0.97			
Pm-151	0.012	0.043	0.396			
Pr-145	0.03		1.58			
Sb-125		0.02	0.017	0.04	0.04	0.04
Sm-153			0.173			
Sn-121			0.011			
Sn-125			0.0301			
Sn-127			0.028			
Te-125m			0.0107			
U-234	0.40		0.663			0.03
U-237	0.035	0.041	0.663			

Summary and Limitations – Radionuclide Screening

- A method for the identification of radionuclides of potential for advanced reactors – based on half-life, biological hazard, and relative abundance in a core – is provided and illustrated using a radiological inventory developed for a heat pipe reactor
- Radionuclides were progressively screened, first based on half-life and relative inventory, and then further based upon relative biological hazard to develop a list of 69 radionuclides (48 of which are already considered for LWR analyses and 21 of which are not currently considered) to include in the heat pipe reactor consequence analyses
- Method provides a traceable and transparent basis for selecting radionuclides for inclusion in advanced reactor consequence analysis
- In theory, this method can be applied to any advanced reactor inventory as they become available
- NRC staff considers work on Task CA2 to be completed based on the development of a quantitative methodology that can be applied to the diverse radiological inventories that may be present in advanced reactor design (see Clavier et al 2022a for summary report).
- Further work may be undertaken in future years to continue refining the methodology.
  - Some radionuclides did not have dose coefficients in MACCS
  - Complexities of H-3 and C-14 are generally unaccounted for in MACCS
  - Food ingestion ignored
  - Normalizing to doses of volatile isotopes of iodine and cesium means that large releases not associated with high elemental volatility may need to be reassessed
  - Other thresholds for half-life, relative abundance, or relative biological hazard may be used

Chemical Form, Particle Size, and Shape Factor of Radionuclides and Impact on Atmospheric Transport and Dosimetry (Task CA3)

- Staff began working on Task CA3 in FY22
- In a nuclear accident scenario, it is possible that there are multiple chemical and physical forms of a given radionuclide released
- NRC non-LWR Vision and Strategy (NRC, 2020) calls for an investigation into how MACCS handles radionuclide size, shape and chemical form in atmospheric and dosimetry calculations
  - Inform potential improvements to MACCS capabilities for atmospheric transport and dosimetry
- MACCS has robust, flexible modeling capabilities that are generally well-suited to accommodate diverse forms of a given isotope
  - Understanding existing capabilities will help to inform improvements
- It is pertinent to investigate MACCS variables relevant to chemical and physical form modeling and how MACCS functionality facilitates the analysis of accident consequences from varying forms of a given isotope
  - Look into dosimetry and transport assumptions relative to state of practice
  - Technology neutral fashion

The MACCS dosimetry model

- EARLY: cloudshine, groundshine, direct/resuspension inhalation and skin deposition
  - Difference dose coefficients for each pathway read from the DC file supplied with MACCS
  - Generally, dose is a product of exposure and dose coefficient
- CHRONC: MACCS additionally considers food and water ingestion (in addition to groundshine and resuspension inhalation doses)
  - Indirect late-phase doses from ingestion may occur in different spatial elements than where the deposition processes occurred
  - Food ingestion doses will depend on farmable land area and ground concentration
  - Water ingestion will depend on direct deposition and washoff to freshwater bodies (simple secondary transport equation)
- MACCS currently does not allow for multiple chemical forms for the same isotope
  - Each isotope of a given element is attributed the same dose coefficient (for a given organ/pathway)

The MACCS deposition model

- MACCS allows user to assign radionuclides to various high-level chemical groups based on physical and chemical properties that are assumed to be identical
  - Typically defined to be consistent with accident progression codes like MELCOR
- Assuming every isotope in a group behaves the same ignores the unique physical/chemical properties of radioactive molecules
  - Particle size
  - Transformation in the environment
  - Hygroscopicity
  - Agglomeration
  - Density
- Aerosol size distribution is used to assign a dry deposition velocity
  - Dry deposition a function of ground level air concentration and dry deposition velocity
  - Particle size distribution are binned and each assigned dry deposition velocity
- Wet deposition functions independently of particle size

Other summary observations regarding the MACCS conceptual models

- The dose calculation for a given radioisotope in MACCS assumes chemical form does not change following release to the atmosphere
- No secondary environmental transport is assumed after deposition
- Risk coefficient uncertainty can vary considerably across applications
  - E.g., inhalation risk may depend strongly on availability of information on the chemical/physical form inhaled
- FGR 13: “the biokinetic, dosimetric, and radiation risk models generally have been derived from much less detailed and sometimes inconsistent databases (with) substantial uncertainties”
- Default absorption types are recommended, but information regarding this selection is often limited and, in many cases, reflects occupational rather than environmental experience
- An analyst should consider the timescale in which chemical transformations are expected to happen
  - Environmental transformation processes happen slowly
  - E.g., is a given radionuclide expected to oxidize before substantially decaying?

Conceptual accounting for alternate physical/chemical forms in dose coefficient development

- EPA regularly publishes federal guidance reports to assist with radiation protection programs
  - Federal Guidance Report (FGR) 13 (Eckerman et al., 1999) provides technical accounting for risk coefficients, dependent on age, gender, metabolism, dosimetry, radiogenic risk, and competing causes of death
  - A supplement to FGR 13 provides the basis for current dose coefficients in MACCS
  - Effective dose coefficients based on ICRP60 recommendations for tissue weighting
- Absorption type/clearance class in MACCS consistent with Runkle and Ostmeyer (1985), a study discussing dosimetric data for accidental radionuclide release from nuclear reactors
  - Runkle and Ostmeyer (1985): “the most probable chemical forms of the inhaled radionuclides are used to assign clearance classes…except for Cs and I isotopes, most of the important inhaled radionuclides will be in the form of insoluble compounds (principally oxides and hydroxides)”

More on the MACCS dosimetry lineage

- FGR 12 and ICRP 72 informed external and internal dose coefficients, respectively, included in FGR 13
  - External considered radionuclides with a half-life of at least 10 minutes or occurring in the decay chain of a radionuclide that does
  - Internal excluded radionuclides with half-life less than 10 minutes and isotopes of noble gases
  - No practical differences between ICRP 72 dose coefficients and those used to develop FGR 13 for isotopes of interest for consequence analysis

Clearance class and f_1 development dates back to the 1950s

- ICRP 2 (1959) – provided a foundational, single compartment model for the lung to predict deposition, retention and clearance of inhaled aerosols
- ICRP 30 (1979) – supersedes ICRP 2, improved estimations of deposition in and clearance from the respiratory tract
  - 3 anatomical compartments were used: nasopharyngeal, tracheobronchial and pulmonary
  - Introduced the “D, W, Y” shorthand
- ICRP 66 (1994) – further revises ICRP 30 model and includes morphometry, respiratory physiology, radiation biology, deposition, clearance, and dosimetry
  - Changed the “D,W,Y” clearance class convention to “F,M,S”
  - Broad nature of clearance class timelines means the risk associated with some radionuclides may be over/underestimated (actual clearance times are on lower/upper end of clearance time bin)

Other relevant, newer documentation exists for dosimetry but are often associated with occupational intakes

- ICRP 68 supersedes ICRP 61 and provides dose coefficients for occupational intake of radionuclides
  - Used the lung model from ICRP 66
  - Tabulates effective dose coefficients for inhalation for varying isotopes, clearance classes, and particle sizes
  - Provides recommendations for clearance types and f_1 values for various chemical compounds
- Beginning in 2015, Occupational Intakes of Radionuclides (OIR) reports published by ICRP to replace the ICRP 30 series, ICRP 54, 68, and 78
  - Contains more up-to-date and detailed information than ICRP 68
  - Detailed information on chemical forms commonly encountered in an occupational setting and associated clearance class and f_1 values
  - An update to FGR 13 may logically include a reference to the OIR series

Other deposition models exist, but MACCS is consistent with state-of-practice specifically for modeling variable chemical/physical forms

- EPA AERMOD model (see, e.g., Wesely et al. 2002) includes algorithms for both dry and wet deposition for particulates and gaseous emissions and relies on the resistance model
  - Particulate deposition calculation method based on particle size
  - Wet deposition depends on washout coefficient and precipitation rates
- NOAA HYSPLIT (see, e.g., Stein et al. 2015) uses either a user-specified velocity or calculated using a known particle diameter, air density and particle density
  - Users can optionally select the resistance model
  - Wet deposition model assumes a scavenging ratio to account for rainout and washout (removal constant)
- Generally, the impact of chemical form on wet and dry particulate deposition is not currently account for in state-of-practice models for deposition, including MACCS

Additional work may be warranted to produce data necessary to inform model improvements

- Identify whether non-LWR accident releases contain chemical forms other than insoluble oxide or hydroxide forms, and what those forms are
- Conduct a sensitivity analysis for dose coefficients for variable chemical forms
- Expand the dose coefficient file and allow the user to define which chemical form should be used
- Enhance MACCS to allow a user to specify release fractions for different chemical forms of the same isotope
- Review non-LWR accident progression analyses to determine whether significant gaseous releases are likely
- Benchmark the MACCS dry and wet deposition models against alternate state of practice models

Summary and Limitations – Effects of Alternate Physical/Chemical Forms on Deposition and Dosimetry

- NRC staff considers Task CA3 to be completed based on identifying methodological issues that would need to be addressed in specific analyses (see Clavier and Clayton 2022b for summary report).
- However, further work may be undertaken in future years, subject to the availability of information on reactor-specific chemical forms as well as the availability of staff and contractor resources. Such work may include:
  - Review non-LWR accident progression analyses to determine whether significant gaseous releases are likely
  - Benchmark the MACCS dry and wet deposition models against alternate state of practice models
  - Conducting sensitivity analyses of the effect on dose coefficients of alternate inhalation clearance classes to understand the uncertainty associated with alternate chemical forms
  - Identifying which non-LWR accident releases may contain chemical forms other than the insoluble oxide or hydroxide forms characteristic of LWR releases.
  - Expanding the MACCS dose coefficient file to include dose coefficients for all chemical forms available in FGR-13 (and FGR-11 if computing TEDE) and allow the user to define which chemical form should be used
  - Enhancing MACCS to allow a MACCS user to specify release fractions for different chemical forms of the same isotope.

Tritium Modeling (Task CA4)

- Staff began working on Task CA4 in FY22
- Tritium has highly unique chemical behavior in the environment and may become important for advanced reactor consequence analyses
- If released in large enough quantities, it may be warranted to update MACCS capabilities to model tritium fate and transport more effectively in an accident scenario
- Updates may be informed by existing modeling capabilities from other tritium models
- MACCS has been used in previous studies to model tritium releases

Tritium behaves similarly to hydrogen in the environment and biological processes

- Weak beta emitter – primary radiological hazard is through ingestion of tritiated organic molecules
- Chemical form can heavily influence radiological risk posed by tritium
  - Inhaling gaseous tritium poses relatively limited radiological risk (low absorption, significant exhale). Dermal contact also limited
  - Ingestion and dermal contact with HTO poses a comparatively larger risk (high biological uptake)
  - Meaningful concentrations of HTO can also be absorbed through the skin at a rate approximately half that of inhalation
  - Can also bind to carbon through photosynthetic processes and create OBT

Tritium Form	Dose Coefficient (Sv/Bq)
Organically Bound Tritium (Ingestion)	4.2 E-11
Tritiated Water (Ingestion)	1.8 E-11
Tritium Gas (Inhalation, Moderate Absorption)	1.8E-15
Organically Bound Tritium (Inhalation)	4.1E-11
Tritiated Water (Inhalation)	1.8E-11

Existing tritium models

- UFOTRI – the most comprehensive model regarding tritium releases, dispersion, deposition and the subsequent movement and transformation through the environment
  - Similar Gaussian dispersion model to MACCS
  - Differentiates between different forms of tritium in the environment, has a detailed reemission physics model, accounts for the conversion of tritium to HTO, uptake by plants, and conversion into OBT
- GENII – well documented dose and risk assessment model developed by EPA
  - Utilizes special tritium models for acute and chronic exposures
  - Chronic module depends on hydrogen content of plant/animal being contaminated
  - Also accounts for OBT generation
- RSAC – Radiological Safety Analysis Computer program
  - Uses different equations for calculating ingestion doses from tritium
  - Assumed ratios of plant water and tritium concentration in plant water vs atmospheric water
- Other less documented/research models

Multiple pathways may exist for updates to MACCS to accommodate acute tritium releases

- The atmospheric transport processes are largely similar, but MACCS may benefit from updates to longer-term environmental process models
- Multiple pathways for updates:
  - Simply continue to use the most conservative dose coefficient for HTO in the existing MACCS code with no changes to the atmospheric transport or longer-term processes. Reduces the need to have an exact accounting of the chemical form of tritium releases
  - Develop the capabilities for MACCS to identify multiple different chemical forms of tritium and associated transformation. Variable tiers of complexity for which this might be accomplished (e.g., incorporating a simple transfer rate model)
  - Introduce tritium accounting capabilities like those in UFOTRI and the more complex capabilities of other models. This would require substantial effort but would provide more detailed estimations of tritium in an accident scenario
- NRC staff considers this task to be active (see Clavier and Clayton 2022c for current status) and expects efforts to evaluate MACCS capabilities for assessing tritium release consequences to continue beyond FY23.
- In FY23, staff plans to
  - conduct a model intercomparison study involving alternate state-of-practice tritium models (e.g., UFOTRI and GENII codes), coupled with a review of documented cases of tritium releases, to understand the degree to which differences in tritium modeling capabilities may impact severe accident dose assessments.
  - better understand the magnitude of tritium release necessary to yield significant doses at various distances. This will allow staff to understand which advanced reactor technologies may contain tritium inventories capable of resulting in significant doses.

Summary

- NRC staff considers Tasks CA1 to CA3 to be completed:
  - The MACCS code has been updated to improve modeling capability in the nearfield region (Task CA1)
  - A methodology has been developed to identify radionuclides for inclusion in consequence analyses for non-LWR cores (Task CA2)
  - MACCS code capabilities are consistent with state of practice for modeling effect of alternate chemical forms on dosimetry (Task CA3)
  - MACCS is consistent with the current state of practice for modeling deposition of particulate releases (Task CA3)
  - If significant gaseous releases are expected from advanced reactor technologies, MACCS may require updates to improve capability for modeling gaseous deposition (Task CA3)
- Although Tasks CA2 and CA3 are considered complete insofar as the existing MACCS code capabilities are likely adequate, coordination is needed to determine whether the necessary information on the chemical and physical form of released radioactivity will be available to implement the recommendations for modeling impacts on aerosol dosimetry and deposition.

Path Forward

- In FY23, staff plans to
  - Continue work on evaluating MACCS capabilities for assessing the consequences of severe accident tritium releases (Task CA4)
  - Begin work on the evolution of radionuclide properties in the atmosphere (Task CA5), including a limited literature review to understand what types of chemical and physical transformations are possible and how these transformations are modeled in other state-of-practice codes for atmospheric transport, diffusion, and deposition.
  - The initial Task CA5 evaluation will be documented in a contractor report to be issued in September 2023, which will identify a more detailed plan for implementation in future years.
- In FY25 and beyond, staff intends to begin work on Task CA6 to examine the impact of siting decisions on decontamination cost estimation, and on Task CA7 to examine issues associated with potential chemical releases to the environment.

Thank you!

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NEI 23-01 Cold License Training Plan for Advanced Nuclear Reactors (DRAFT)

Rick Stadtlander
Sr. Project Manager, NEI

December 15, 2022

NUCLEAR ENERGY INSTITUTE

Background

- Prior to operation, plant experience requirements specified in regulatory and industry guidance cannot be met.
  - There is a need to provide a method to acquire the knowledge and experience required for licensed operator duties during new plant construction & initial operations

- Focused on creating guidance for all Advanced Nuclear Reactors
  - Not specific to any technology
  - Includes LWR SMRs and non-LWRs

Background

- NEI 06-13A, Appendix A
  - Current NRC endorsed Cold License Training Plan
    - Used with Vogtle's AP1000
  - Does not allow for technology updates in the Advanced Nuclear Reactors being designed & licensed today

Background

- New guidance document
  - NEI 23-01, Cold License Training Plan for Advanced Nuclear Reactors
    - Drafted by Industry Team
  - Takes into consideration:
    - Shorter construction times
    - Smaller licensed operator staff
- Incorporates OE & lessons learned from Vogtle

NEI 23-01 vs NEI 06-13A

- Focuses only on Cold License Training
- Like NEI 06-13A
  - Provided paths for 3 positions
    - RO
    - Direct SRO
    - SRO with previous experience
- Utilizing similar methodology for experience credit
- Enhancements:
  - Includes definition section for commonly used terms
  - Provide flow charts to add clarity to the written descriptions

Program Updates

- Reduced crew cumulative experience
  - Based on smaller crew size
  - Taking advantage of inherent and/or passive safety features
  - Reduction in the number of Operator actions

- Associate degree or higher for direct SRO path
  - Must be in science or applied science
  - Degrees in communication, natural sciences, humanities, or social sciences are not credited

Program Updates

- Scheduling for initial license test
  - No specified time frame in NEI 23-01
  - Discussed during pre-application meetings

- Licensed Operator Continuing Training
  - Required within 90 days of passing initial license exam
  - Maintain program until licenses issued and requalification training begins
  - Systematically determined training to maintain operator knowledge of plant operation

Path forward for NEI 23-01

- Part 53
  - General Licensed Operators
    - Will be incorporated as the rule solidifies
- Update NEI 23-01 based on input from today's discussion
- Submit draft guidance to NRC around year end
- Schedule public meeting for about 1 month after submittal
- Plan to submit final guidance around mid March of 2023 for NRC review and endorsement

Questions & Comments

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Using Lessons Learned to Optimize Advanced Reactor Licensing Activities

December 15, 2022

Periodic Advanced Reactor Stakeholder Meeting

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Background

- NuScale Lessons Learned Team established in November 2020 following August 2020 issuance of Final Safety Evaluation Report for NuScale Design Certification (DC)
- February 19, 2021, letter from NuScale outlining its lessons learned from the DC Application (DCA) review process along with five recommendations for NRC staff consideration
- April 15, 2021, NRC staff acknowledgement of NuScale lessons learned letter
- March 30, 2022, NRC staff letter to A. Veil (NRR) documenting lessons learned from NuScale DCA review along with four recommendations and responses to NuScale and NEI recommendations
- **November 14, 2022, NRC staff letter to R. Taylor (NRR) outlining how four recommendations are being addressed**

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Staff Responses to Recommendations

- Recommendation 1: Design Finalization at Application and Changes During Licensing
  - Guidance on pre-application engagement with NRC staff addresses impacts of substantive design changes
  - Pre-application readiness assessment audits provide insights into design uncertainties and potential schedule impacts
- Recommendation 2: Application of a Holistic, Risk-Informed Review Strategy
  - Early establishment of multidisciplinary core review teams
  - Pre-application review activities include reviews of draft PRA
  - Guidance development and rulemaking activities underway

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Staff Responses to Recommendations

- Recommendation 3: Enhancements to the Requests for Additional Information and Audit Processes
  - Increased use of audits and requests for confirmation of information (RCIs) to ensure appropriate information is docketed in a timely manner
  - Implementation of revised office instruction on RAIs (LIC-115)
- Recommendation 4: Establishment and Management of Review Schedule and Resource Estimates
  - Development of standardized dashboards
  - Enhanced project controls established for accountability and to improve management of changes during project

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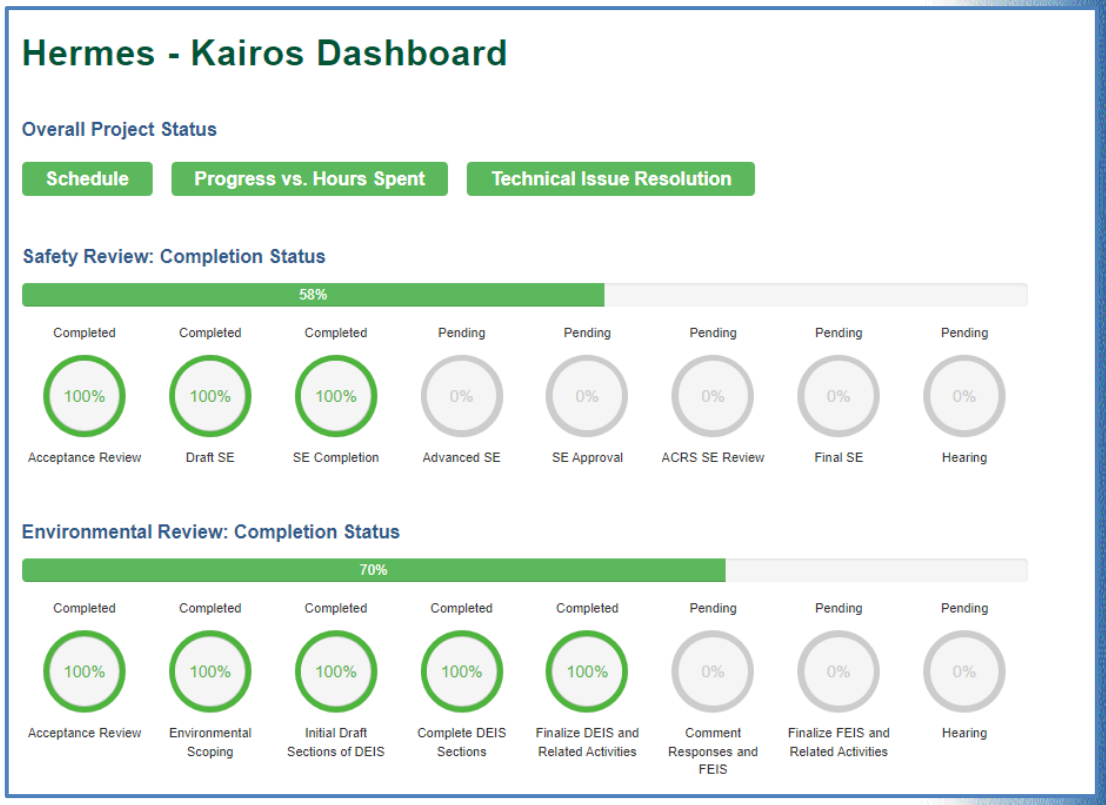
Optimizing and Applying Lessons Learned

- Kairos Hermes Test Reactor
  - Established 21-month review schedule based on robust preapplication engagement and a high-quality application
  - Internal and external dashboards developed to provide stakeholders with up-to-date information on review status
  - Use of a multidisciplinary core review team to ensure risk-informed review of the CP application
  - Increased use of audits and RCIs to optimize the use of RAIs
  - Leveraging collaborative tools to support more efficient concurrence process



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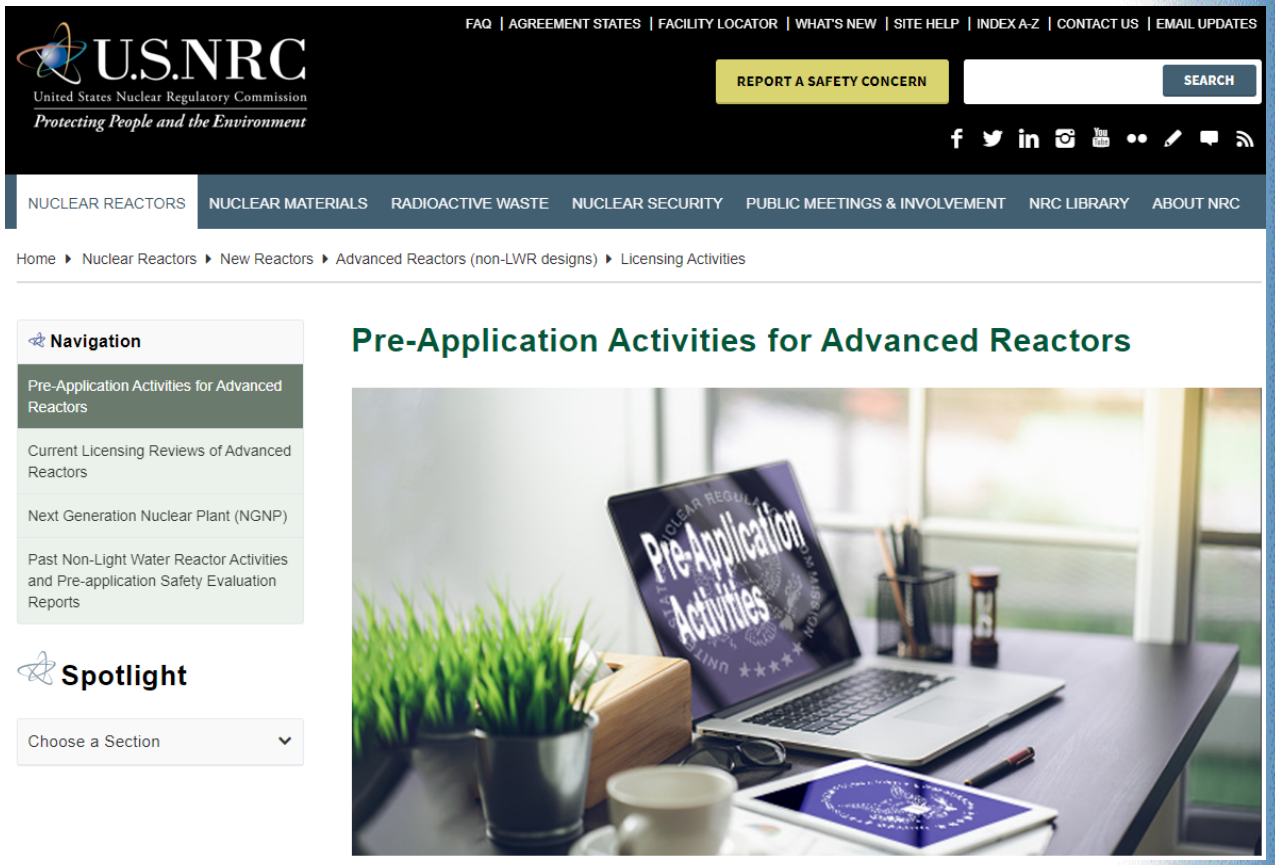
Optimizing and Applying Lessons Learned

- SHINE Technologies Medical Isotope Facility
  - Enhanced organizational engagement, including use of routine management meetings for enhanced project controls
  - Expanded use of audits to resolve key issues (e.g., Technical Specifications)
  - Centralized decision-making functions for the review
  - Enhanced internal and external communications on project schedule
- Abilene Christian University Molten Salt Research Reactor
  - ACU review is building off of the lessons learned from Kairos and Shine reviews (e.g., use of dashboards, maximizing the use of audits, internal project controls)
  - Early engagement on key technical issues ensures that review is risk-informed and minimizes the potential for downstream schedule risk
    - Five key issues discussed conveyed in acceptance review letter
    - Public meeting to discuss these issues held in December 2022
  - Enhanced communication with applicant on resource estimates and schedule

Pre-Application Activities by the Numbers

- NRC staff are currently engaged with 15+ entities in pre-application activities
- 13+ current and potential applications by 2027
- 6+ potential operating licenses by 2027
- 51 topical reports and white paper reviews completed for 7 vendors
- 28 topical reports and white papers under review from 8 vendors



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Questions?

Break

Meeting will resume at 2:55 pm EST

Microsoft Teams Meeting
Bridgeline: 301-576-2978
Conference ID: 115 537 606#

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Workshops on Licensing Review Framework for Advanced Reactors Instrumentation and Controls

Introduction to Proposed Future Workshops

December 15, 2022

Requests for Workshop on Instrumentation and Control (I&C) Design Review Guide (DRG) Implementation

- Final I&C DRG issued in February 2021 (ML21011A140) for non-LWR I&C design reviews by NRC staff
- NRC staff reviews / pre-application engagements underway for a variety of potential LWR and non-LWR I&C designs
- NRC staff engaged by industry interested in the background and details on the DRG—and relationship to NEI documents
  - Initial workshop planning ongoing and being coordinated with NEI
  - Additional workshops on other I&C-related topics are intended to benefit all designers

Workshop #1 Proposed Topics

- Overview of recent and ongoing initiatives:
  - Licensing Modernization Project (LMP) and RG 1.233
  - Technology-Inclusive Content of Application Project (TICAP)
  - Advanced Reactor Content of Application Project (ARCAP)
- Overview of I&C DRG
  - Focus on safety-significant SSCs; Use of reliability / capability targets
  - Developed for non-LWRs, but can be used for all reactor designs
  - Specific industry challenges or questions

Workshop #2 Proposed Topics

- Codes and Standards
  - How performance-based concepts can be applied to prescriptive requirements of endorsed codes and standards
  - Applicability of IEEE 603 and related standards
  - Use of international codes and standards
- NRC staff review expectations
  - I&C-specific Principal Design Criteria
  - Fundamental I&C design principles
  - I&C architecture and safety classification of I&C platforms

Workshop #3 Proposed Topics

- Content of Applications
  - Clarity on applicability of Part 50/52 requirements
  - Expectation for construction permit applications
  - Non-power vs. power reactor applications
    - Use of NUREG-1537; Path forward for future power reactors

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Questions?

For more information, contact:

Jordan.Hoellman2@nrc.gov

Future Meeting Planning

- The next periodic stakeholder meeting will be scheduled for late January or February 2023.

- If you have suggested topics, please reach out to Steve Lynch at Steven.Lynch@nrc.gov

How Did We Do?

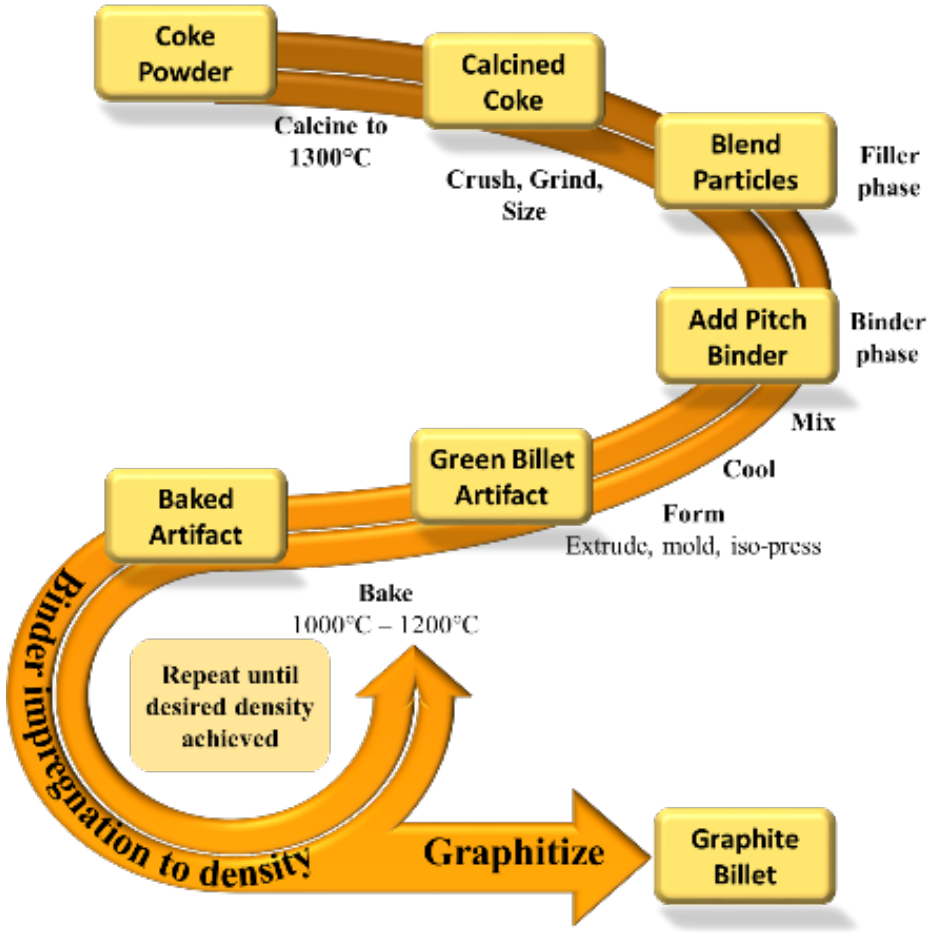
- Link to NRC public meeting feedback form:

https://www.nrc.gov/pmns/mtg?do=details&Code=20221170

Backup Slides

Graphite Background

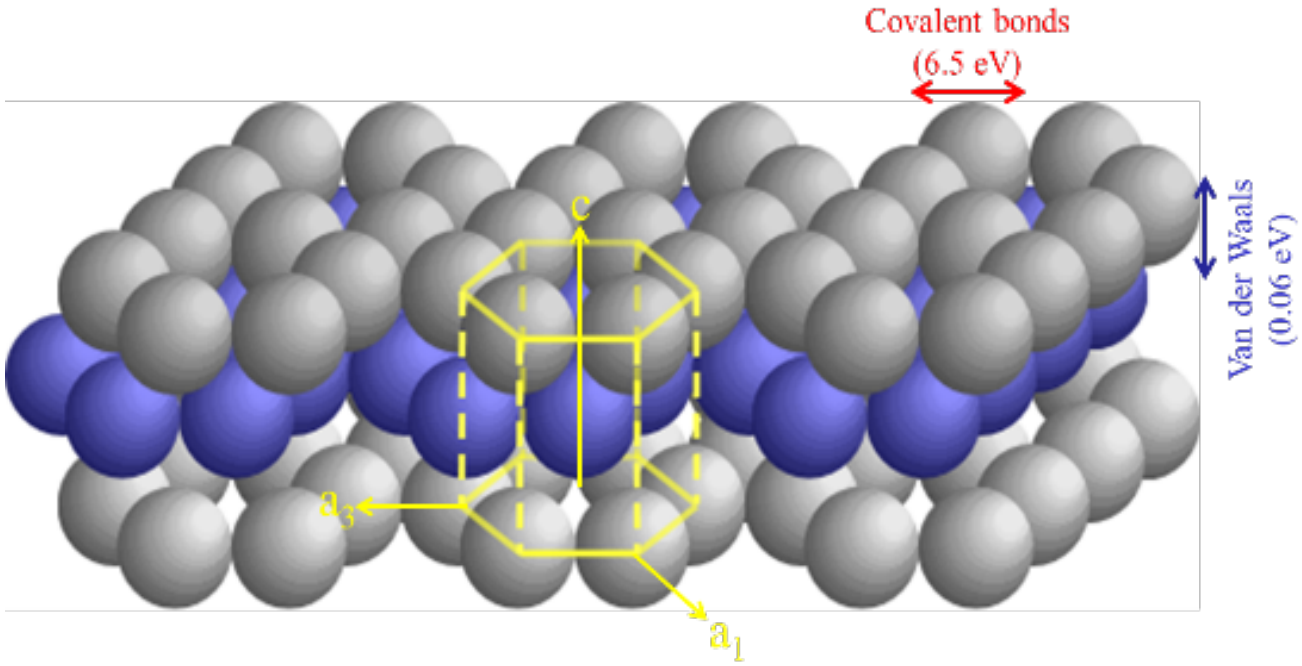
Graphite Manufacturing

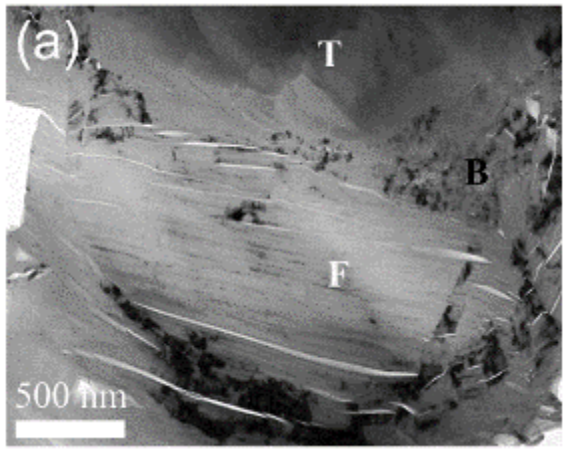


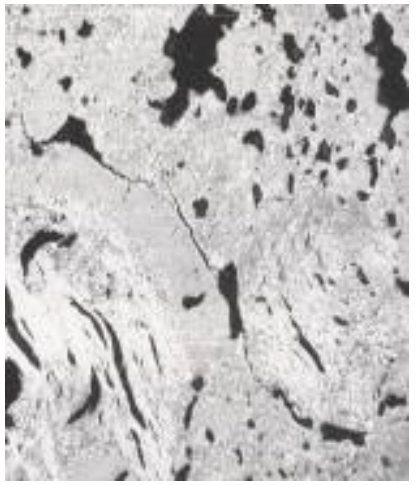
- Graphite properties depend on the manufacturing process
- Graphite is made using filler particles (coke) and a binder phase (pitch)
- Billets are formed by extrusion, vibration molding, or isostatic molding

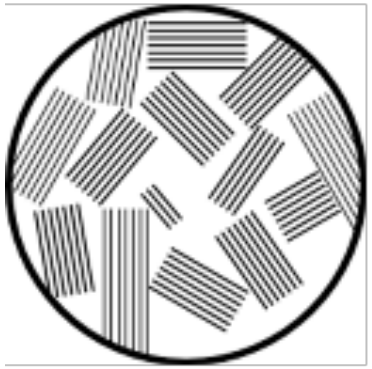
Graphite Microstructure

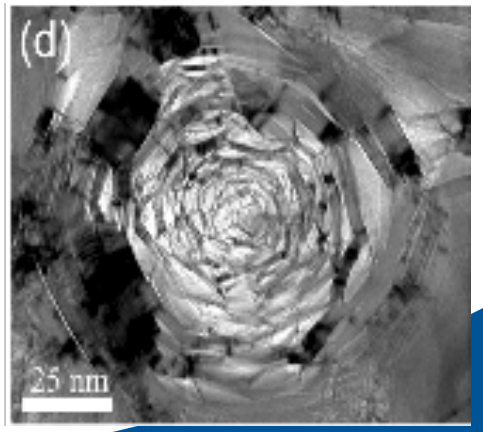
Graphite sheets, Mrozowski cracks, crystallites, and pores…











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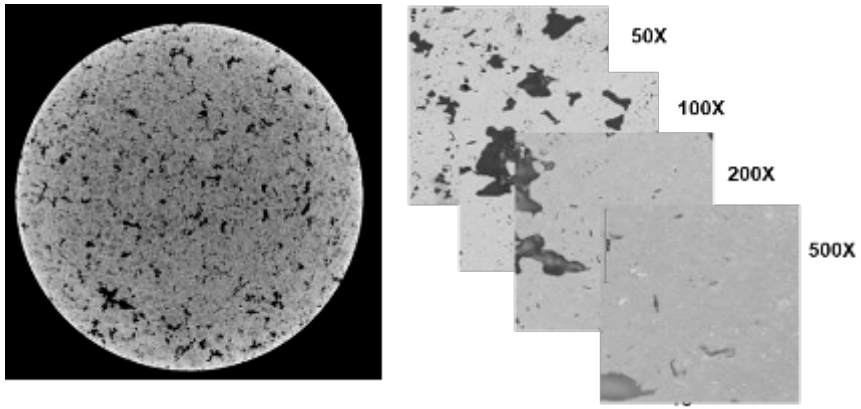
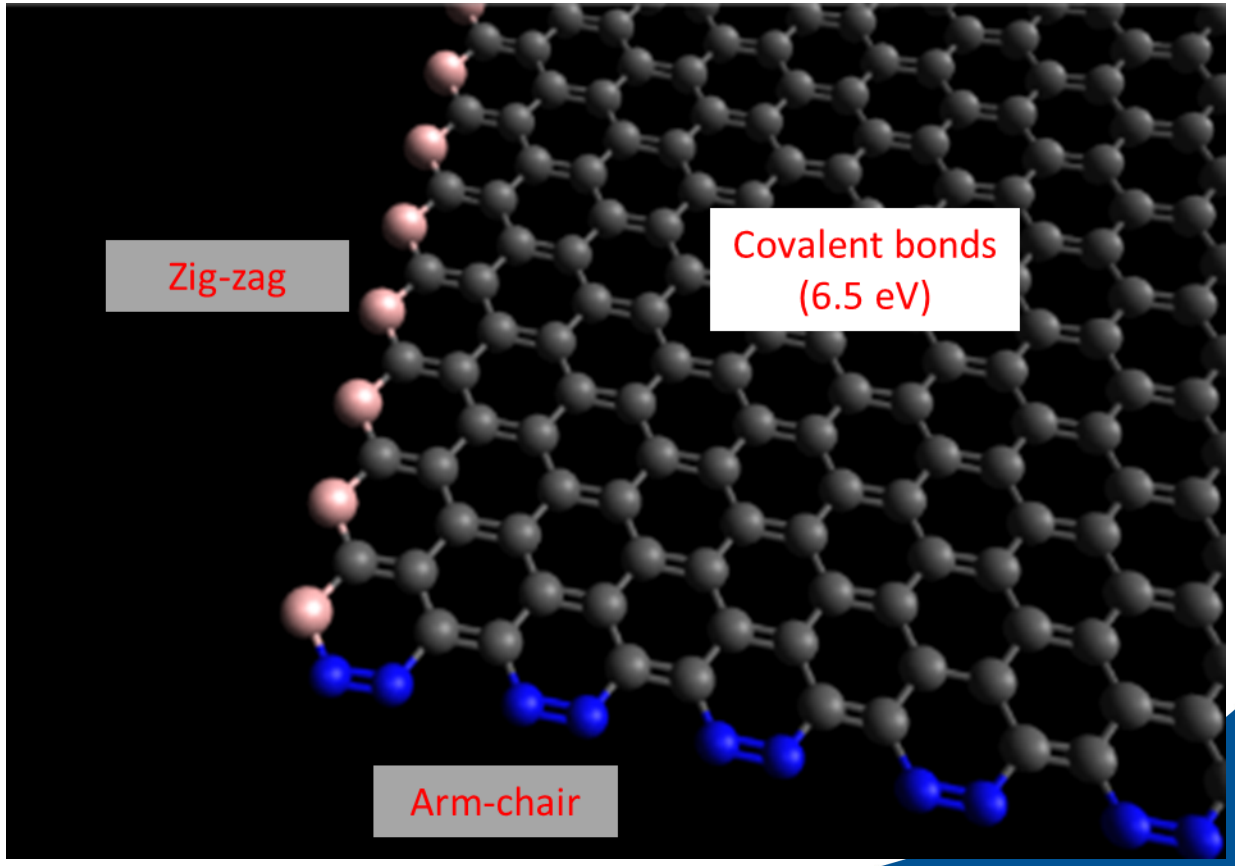
Graphite Oxidation

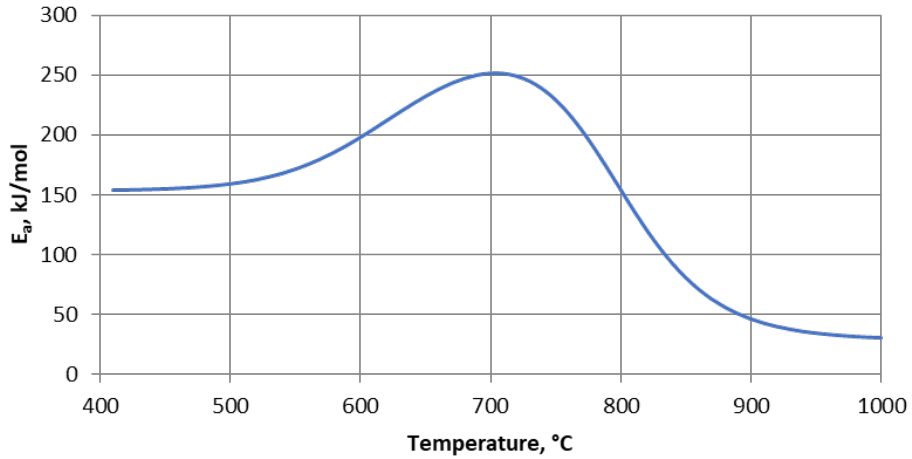
- Oxidation occurs along the outer edges of the basal planes ("zig-zag" and "arm-chair" sites)
- Oxygen can penetrate the interior of the graphite pore microstructure

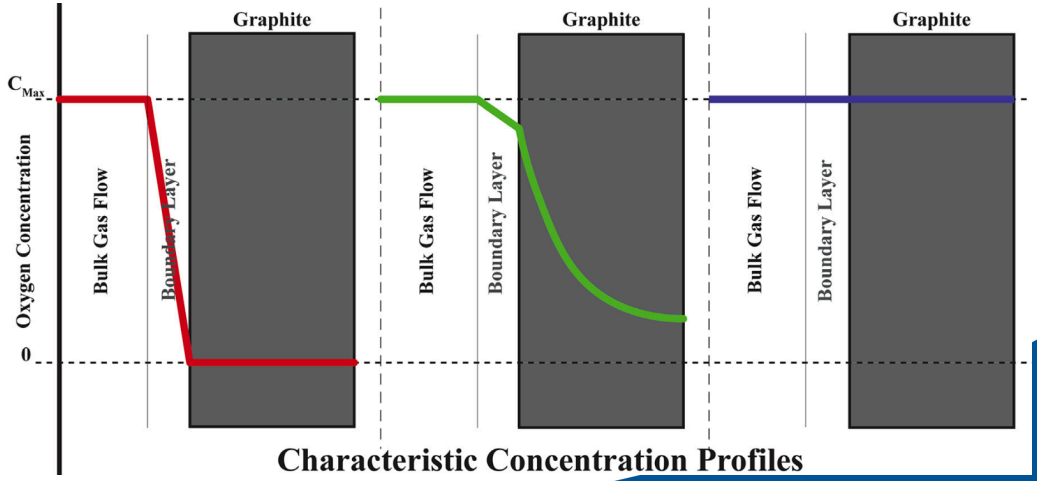




Temperature Effect on Oxidation

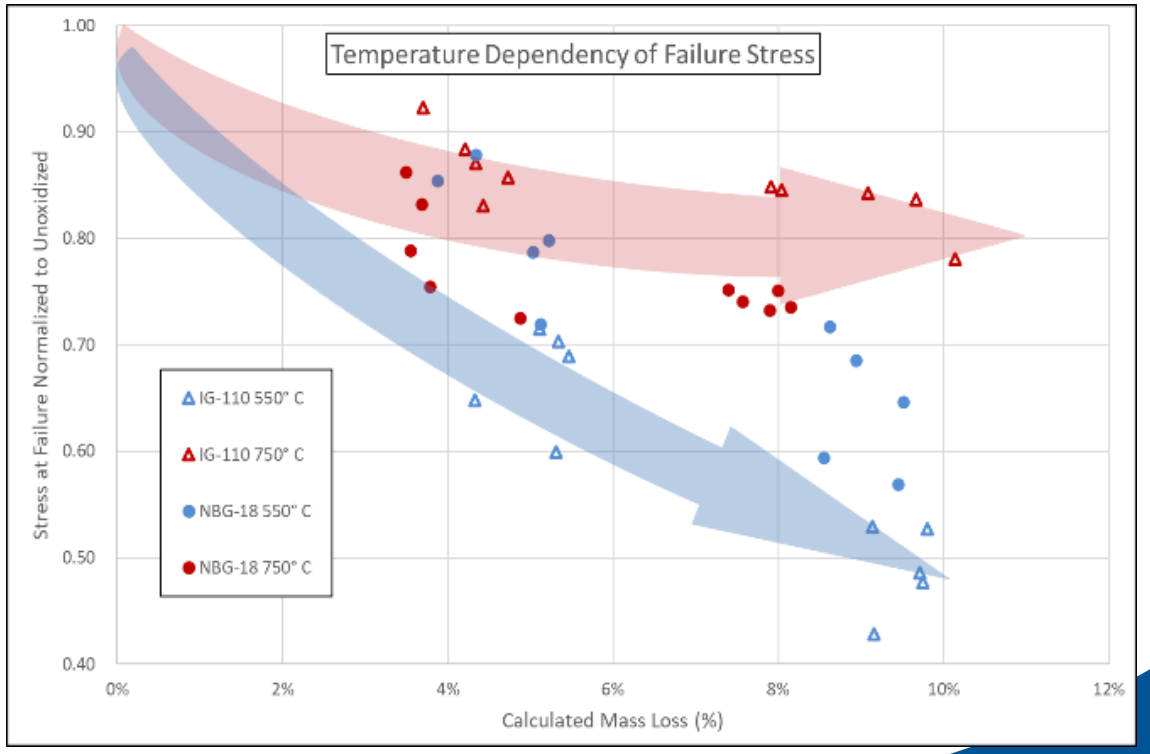
- Oxidation is a complex relationship between reactivity and diffusion of oxygen
- Reactive surface area is related to pore structure
- Oxidation kinetics and gas diffusion are affected by temperature





Oxidation Effects

- It is important to know the strength remaining after oxidation
- Temperature and microstructure affect oxidation rate and the extent of component internal oxidation



MOOSE Background

MOOSE Summary

MOOSE Overview

1. MOOSE is a finite element framework which can be used with a few or many processors to solve engineering problems.
2. MOOSE is broken into many systems which provides a modular approach which allows for coupling of previous code and simple application of new physics.
3. MOOSE has been under development at INL for over a decade and has had multiple modeling methodologies and physical behavior already implemented.

Getting Started with MOOSE:

1. Downloading a text editor with MOOSE plugins is a good first step
2. Instructions for downloading and getting started with MOOSE can be found on https://mooseframework.inl.gov/
3. The website also has training slides on MOOSE, a video of the last MOOSE training, as well as several other helpful features.

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MOOSE Modularity and Pluggable Systems

MOOSE beaks up FEMs into multiple pluggable "systems". This method has multiple advantages:

1. Promotes the reuse of objects
2. Allow for decoupling of code
3. Simplified addition of physics
4. Objects can be mixed and matched to achieve simulation goals

There are multiple pluggable systems within MOOSE:

Actions, AuxKernels, Base, BCs, Constraints, Controls, Dampers, DGKernels, DiracKernels, Distributions, Executioners, Functions, Geomsearch, ICs, Indicators Interface Kernels, Kernels, LineSearches, Markers, Materials, Mesh, MeshGenerators, MeshModifiers, Multiapps, NodalKernels, Outputs, Parser, Partitioner, Postprocessors, Preconditioners, Predictors, Problems, RelationshipManagers, Samplers, Splits, TimeIntegrators, TimeSteppers, Transfers, UserObject, Utils, Variables, VectorPostprocessors

These pluggable systems correspond to different aspects which make up an FEM simulation

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How to use MOOSE

What inputs are needed for MOOSE?

A text file which include the following blocks (systems):

- **Mesh**: Defines the geometry of the domain
- **Variables**: Defines the variables to be solved
- **Kernels**: Defines the equation(s) to solve
- **BCs**: Defines the boundary condition(s) of the problem
- **Executioner**: Defines how the problem will be solved
- **Outputs**: Defines how to output the results

The mesh will often be generated external to MOOSE.

Example "Variables" Block

```
[Variables]
  [./temp]
    order = FIRST
    family = LAGRANGE
    initial_condition = 925
  [../]
[]
```

Choosing a text editor:

Any text editor will technically work, but some editors are better than others.

The current recommended editor is VSCode. Instructions on getting started with this editor can be found on the MOOSE framework website at: https://mooseframework.inl.gov/help/development/VSCode.html

Generating Meshes

Generating a mesh is required as part of running a problem in MOOSE.

There are multiple way to get a mesh in MOOSE:

1) Generate the mesh internally to MOOSE using the mesh block below. These can be ideal when performing simple tests

```
[Mesh]
  # mesh information:
  type = GeneratedMesh
  dim = 2
  nx = 100
  ny = 20
  xmax = 0.0127
  ymax = 0.0254
[]
```

2) Generating meshes in other tools like CUBIT

- Other tools are needed to create more complex meshes

```
[Mesh]
  file = mesh.e
[]
```

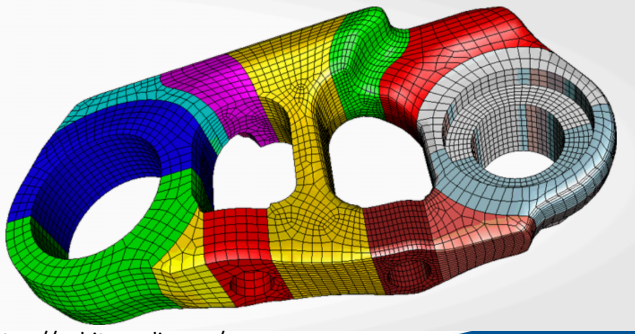


Image from https://cubit.sandia.gov/

Thermo-mechanical

Model Formulation

The state variables in the thermo-mechanical model are **strain, temperature,** and **dose**. The 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.

Thermal Strain	Irradiation Strain	Irradiation Creep	Elastic Strain
$\epsilon_{therm} = CTE(T - T_o)$	$\epsilon_{irr} = f(T, \gamma)$	$\epsilon_{creep} = A\sigma\left(1 - exp(-b\gamma)\right)/E + K\sigma$	$\sigma = E\epsilon_{elastic}$
CTE is an average between T and T_0	f is an experimentally determined function	A, b, and K are experimentally determined coefficients	Stress is computed based on elastic strain

Irradiation Creep Implementation

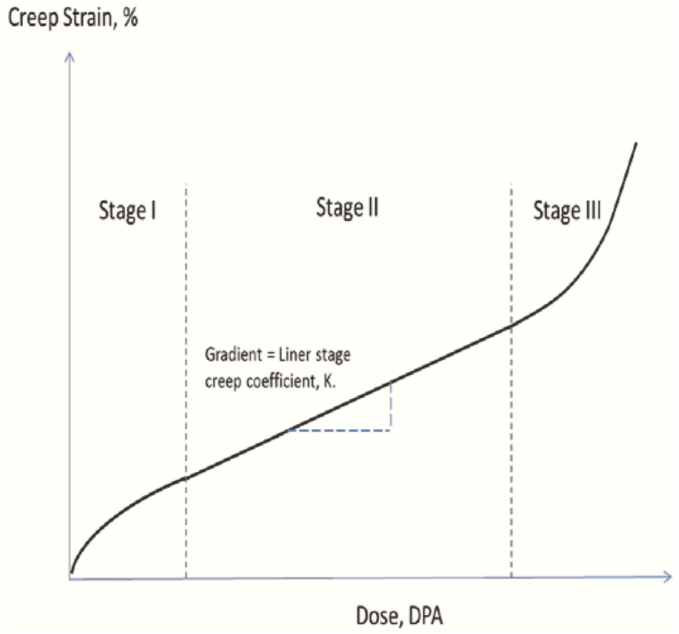
Two graphite creep models are currently available. If the secondary creep is the primary mechanism of concern, the creep can be modeled.

Material Block

```
[./radial_return_stress]
  type = ComputeMultipleInelasticStress
  inelastic_models = 'graphite_creep'
  tangent_operator = elastic
[../]

[./graphite_creep]
  type = GraphiteIrradiationCreep
  coefficient = 1.6714e-10
  temperature = temp_aux
  fluence_dT = df_dt
[../]
```

In general, the secondary creep will dominate the creep behavior for any significant doses (prior to turn around)



From:
INL/JOU-17-41026

This model assumes that the secondary creep coefficient is a constant.

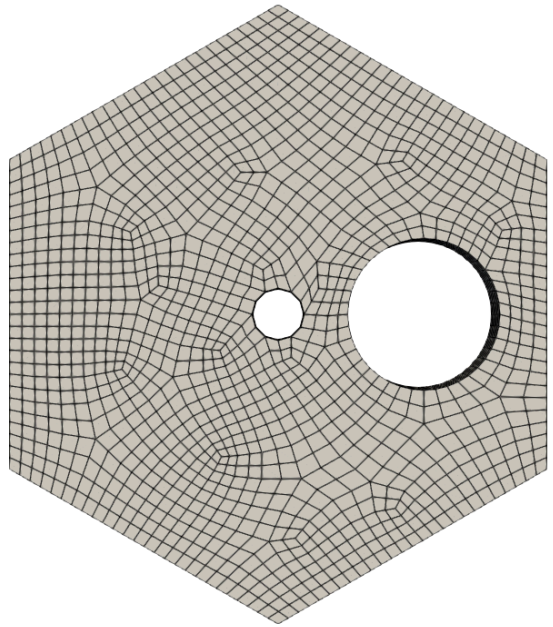
How do we set up this problem?

What inputs are needed for this problem?

A text file which include the following blocks (systems):

- **Mesh**: Defines the geometry of the domain
- **Variables**: Defines the variables to be solved
- **Functions**: For inputting functions
- **Auxvariables**: Auxvariables to be solved
- **Materials**: Defines material behavior
- **Kernels**: Defines the equation(s) to solve
- **AuxKernels**: Define AuxVariable equations
- **BCs**: Defines the boundary condition(s) of the problem
- **Executioner**: Defines how the problem will be solved
- **Outputs**: Defines how to output the results

Mesh Generated in Cubit



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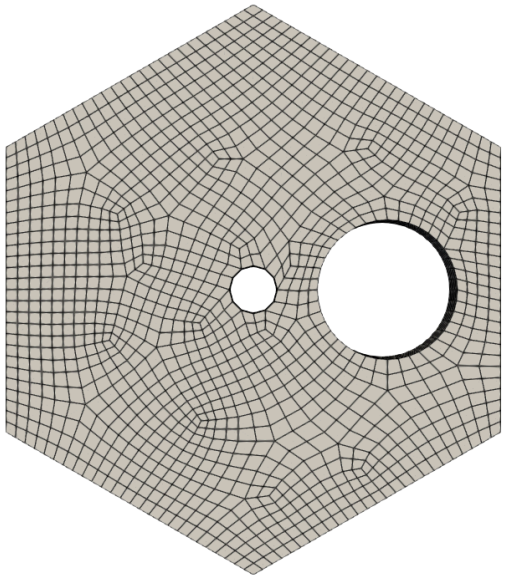
Thermo-mechanical Example Problem

The output of interest is the stress distribution.

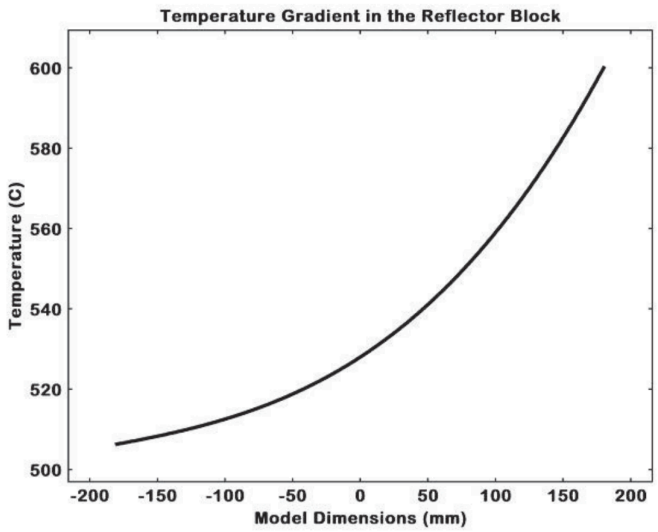
Problem setup:

We have a known geometry, temperature profile, time dependent irradiation profile as shown below

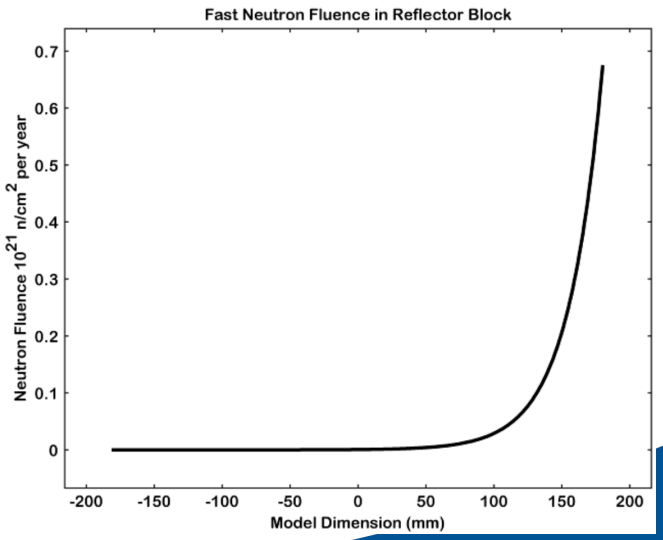
Geometry



Temperature Profile

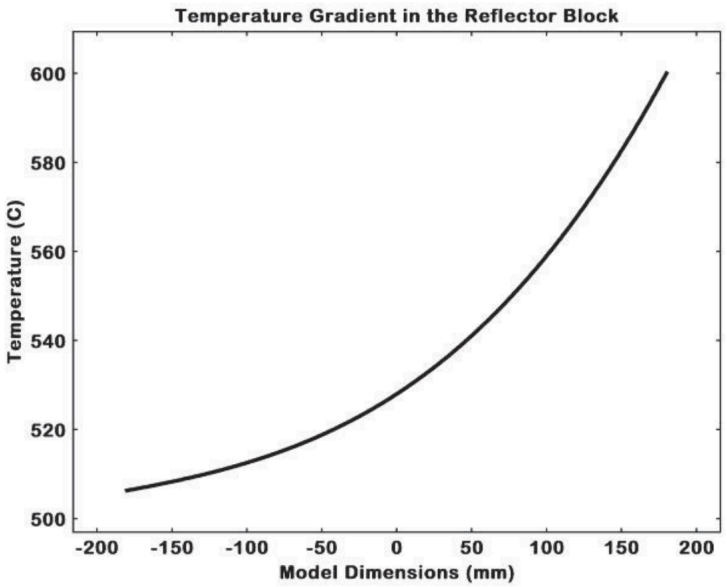


Dose Profile Rate



Input File: Implementing the Temperature Profile

Temperature profile from the literature



Plot Fit = 480.1*exp(-.0001681 x) + 26.25*exp(-.004799 x)

Fit from on left from: Bratton, R., "Modeling Mechanical Behavior of a Prismatic Replaceable Reflector Block", INL/EXT-09-15868, 2009.

Implementation in model

In Functions block

```
[./temp_fun]
  type = ParsedFunction
  value = 'a:=((x*1000+180)^2 +(y*1000)^2)^.5;
  480.1*exp(a*-0.0001681)+26.25*exp(a*.004799)'
[../]
```

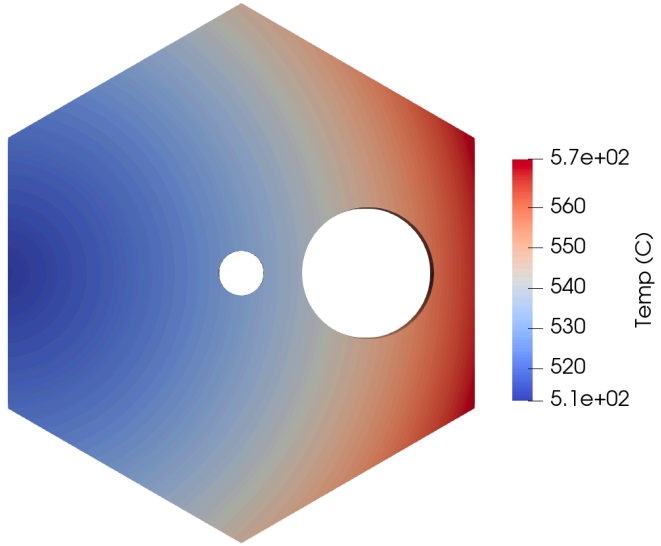
In AuxVariables block

```
[./temp_aux]
  order = FIRST
  family = LAGRANGE
[../]
```

In AuxKernels block

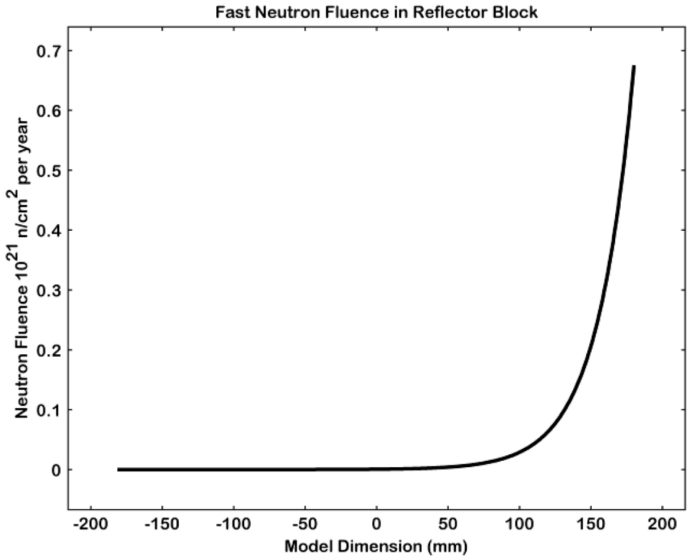
```
[./temp_aux]
  type = FunctionAux
  variable = temp_aux
  function = temp_fun
[../]
```

Resultant Profile



Input File: Implementing the Dose Profile

Dose Profile from the literature



Plot Fit = .001912 exp(.03224 x)

Implementation in model

In Function block

```
[./dose]
  type = ParsedFunction
  value = 'a1:=.001912*exp(.03224*x*1000)*t;
  a2:=.001912*exp(.03224*(x*.5+y*.866)*1000)*t;
  a3:=.001912*exp(.03224*(x*.5+y*-.866)*1000)*t;
  (a1+a2+a3)/1.37'
[../]
```

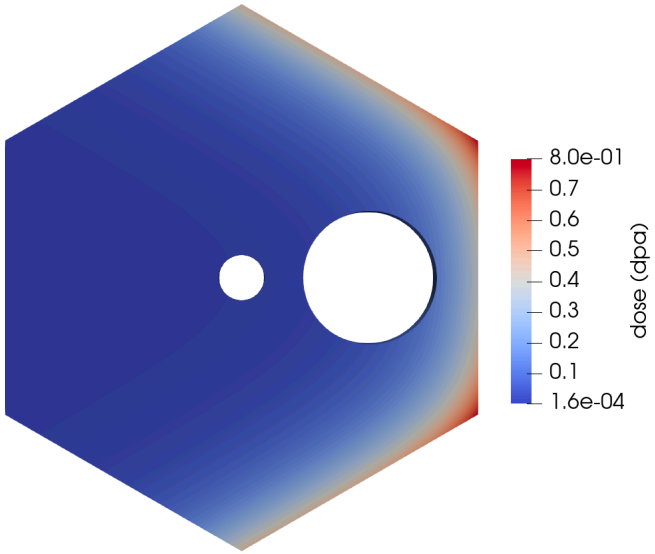
In AuxVariables block

```
[./rdose]
  order = FIRST
  family = LAGRANGE
[../]
```

In AuxKernels block

```
[./rdose]
  type = FunctionAux
  variable = rdose
  function = dose
[../]
```

Resultant Profile (dpa per year)



Note the dose time derivative needs to be implemented in the same way.

Dose profile plot from: Bratton, R., "Modeling Mechanical Behavior of a Prismatic Replaceable Reflector Block", INL/EXT-09-15868, 2009.

Tensor mechanics action

An “action” from the tensor mechanics module can be used to set up much of the groundwork for the problem and reduce the input file complexity. An example is shown below.

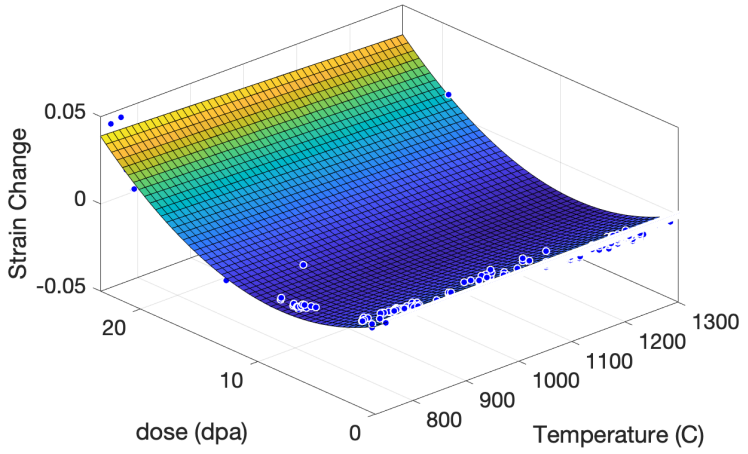
```
[Modules/TensorMechanics/Master]
  [./all]
    incremental =  true
    strain = SMALL                        # Small strains
    add_variables = true                  # Automatically add the displacement variables
    volumetric_locking_correction = true  # Bbar type method
    eigenstrain_names = 'eigen_swell_per eigen_swell_par eigen_therm_per'
    # Shortcut for making output
    generate_output = 'strain_xx strain_xy strain_xz strain_yx strain_yy strain_yz strain_zx strain_zy strain_zz
  [../]
[]
```

The action is useful for declaring eigenstrains and making stress related outputs.

Eigenstrains from Irradiation and Temperature

The eigenstrains will vary as a function of the states as shown in the plots below.

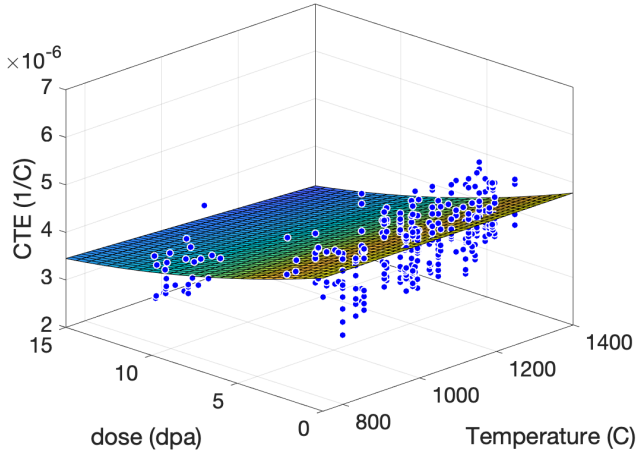
Irradiation induced dimensional change



Curve fit

$$\epsilon_{irr} = .0006351 - 6.23 * 10^{-7} T - .003476\,\gamma - 4.26 * 10^{-7}\,T\,\gamma - 0.0002324\gamma^2$$

Coefficient of Thermal Expansion



Curve fit

$$CTE = 4.827 * 10-6 - 3.9413 * 10-11\,T - 1.149 * 10-7\,\gamma - 2.648 * 10-11\,T\,\gamma + 3 * 10-9\,\gamma^2$$

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Implementing Eigenstrains from Irradiation and Temperature

The method for implementing both thermal and irradiation eigenstrains is the same:

1. Define the eigenstrains in the tensor mechanics action:
```
eigenstrain_names = 'eigen_swell_per eigen_swell_par eigen_therm_per'
```
2. Define AuxVariable and AuxKernels for the dimensional change.

In AuxVariables

```
[./cte_per]
  order = FIRST
  family = LAGRANGE
[../]
```

In AuxKernels

```
[./cte_per]
  type = ParsedAux
  args = 'temp_aux rdose'
  variable = cte_per
  function = '4.827e-6 - 3.9413e-11*temp_aux- 1.149e-7*rdose - 2.648e-11*temp_aux*rdose + 3e-9*rdose^2'
[../]
```

← User input fit

3. Define variable dependent eigenstrain object and compute the value (in the material block).

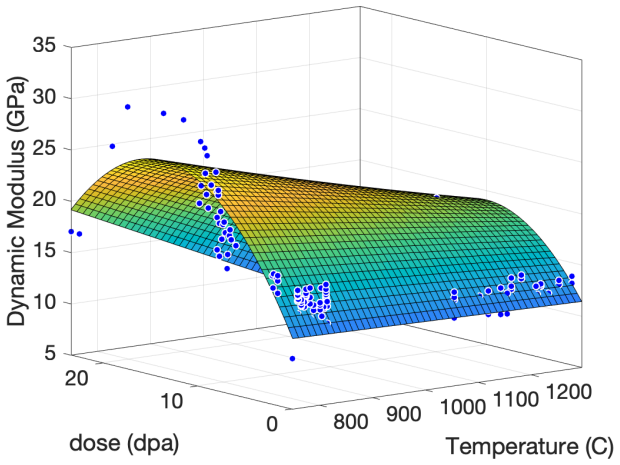
```
[./var_dependence_thermalPer]
  type = DerivativeParsedMaterial
  f_name = var_dep_thermalPer
  args = ' cte_per temp_aux'
  function = 'cte_per*temp_aux'
  outputs = exodus
  output_properties = 'var_dep_thermalPer'
  enable_jit = true
  derivative_order = 2
[../]
```

```
[./eigenstrainThermalPer]
  type = ComputeVariableEigenstrain
  eigen_base = '1 1 1 0 0 0'
  prefactor = var_dep_thermalPer
  args =  'cte_per temp_aux'
  eigenstrain_name = eigen_therm_per
[../]
```

Anisotropic behavior can be included by adjusting the “eigen_base”

Implementing an Isotropic Elastic Modulus

The elastic modulus will vary as a function of the states.



Modulus fit

$$E = 12.41 - 0.0007386\,T + 2.839\,\gamma - 0.00102\,T\,\gamma - 0.0753\,\gamma^2\ (GPa)$$

Code Implementation

In Materials Block

```
[./ym]
type = DerivativeParsedMaterial
f_name = ym
function = '10^9*(12.41 - 0.0007386 * temp_aux + 2.839*rdose - 0.00102*rdose*temp_aux - 0.0753*rdose)'
args = 'rdose temp_aux'
[../]
[./elasticity_tensor]
  type = ComputeVariableIsotropicElasticityTensor
  args = 'rdose temp_aux'
  youngs_modulus = ym
  poissons_ratio = .2
[../]
```

If an anisotropic modulus is needed, the material "ComputeGraphiteElasticityTensor" can be used. In this case, two DeriviativeParsedMaterials are required. One to define the modulus parallel to the gain and one to define the modulus perpendicular to the grain.

The material property fits are computed from experimental data

Model Outputs

The full assessment required both element volumes and equivalent stresses which are computed from the principal stresses. These can be output in the following way

Principal Stresses

1. Include the principal stresses in the tensor mechanics action.

```
generate_output = 'min_principal_stress mid_principal_stress max_principal_stress'
```

2. In the VectorPostprocessor block, use the ElementValueSample

```
[max_principal]
  type = ElementValueSampler
  variable = max_principal_stress
  sort_by = id
  execute_on = TIMESTEP_END
[]
```

3. Output the values in a csv file by setting “csv= true” in the Outputs block.

Element Volumes

1. Create a volume AuxVariable and AuxKernel

```
[./volume]
  order = CONSTANT
  family = MONOMIAL
[../]
```

```
[./volume_aux]
  type = VolumeAux
  variable = volume
[../]
```

2. In the VectorPostprocessor block, use the ElementValueSample

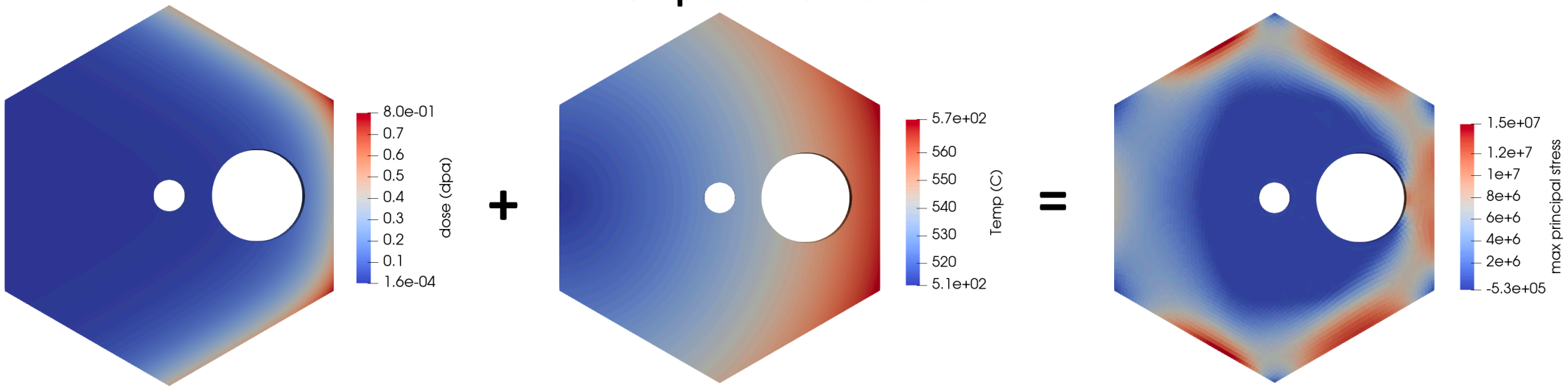
```
[volume]
  type = ElementValueSampler
  variable = volume
  sort_by = id
  execute_on = TIMESTEP_END
[]
```

3. Output the values in a csv file by setting “csv= true” in the Outputs block.

Simulation Results

The resultant stress distribution from the input temperature profiles, and irradiation effects are shown below. This results match well with previous studies which have simulated this problem.

Dose Profile **Temperature Profile** **Stress Distribution**



All variables and auxvariables can be output (including the outputs relevant the ASME code assessments)

Oxidation Model

Oxidation Model: 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.

$$\frac{\partial \varepsilon[CO_2]}{\partial t} = -\nabla \boldsymbol{N_{CO_2}} + (1 - x\,) k_{eff}^{''} \boldsymbol{S_A}[O_2] \qquad \frac{\partial \rho}{\partial t} = k_{eff}^{''} \boldsymbol{S_A}[O_2] \qquad \boldsymbol{N_i} \cong -[C_T] D_{eff} \nabla y_i + y_i\,(\boldsymbol{N_i} + \boldsymbol{N_m})$$

$$\frac{\partial \varepsilon[I]}{\partial t} = -\nabla \boldsymbol{N_I} \qquad \frac{\partial \varepsilon[CO]}{\partial t} = -\nabla \boldsymbol{N_{CO}} + x\, k_{eff}^{''} \boldsymbol{S_A}[O_2]$$

$$\frac{\partial \varepsilon[O_2]}{\partial t} = -\nabla \boldsymbol{N_{O_2}} - (1 - \frac{\boldsymbol{x}}{\boldsymbol{2}}) k_{eff}^{''} \boldsymbol{S_A}[O_2] \qquad \frac{\partial (\rho C_p T)}{\partial t} = \nabla \cdot (\boldsymbol{k_T} \nabla T) + k_{eff}^{''} \boldsymbol{S_A}[O_2\,]\, \Delta H_{rx}(\mathrm{x})$$

Microstructural evolution 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.

Oxidation Example Problem: Introduction

This example problem investigates the temperature-dependent density profiles generated in a graphite cylinder (2-inch length, L, and 1-inch diameter, D).

Problem model setup:

Problem run to 10% mass loss in IG-110

BCs:

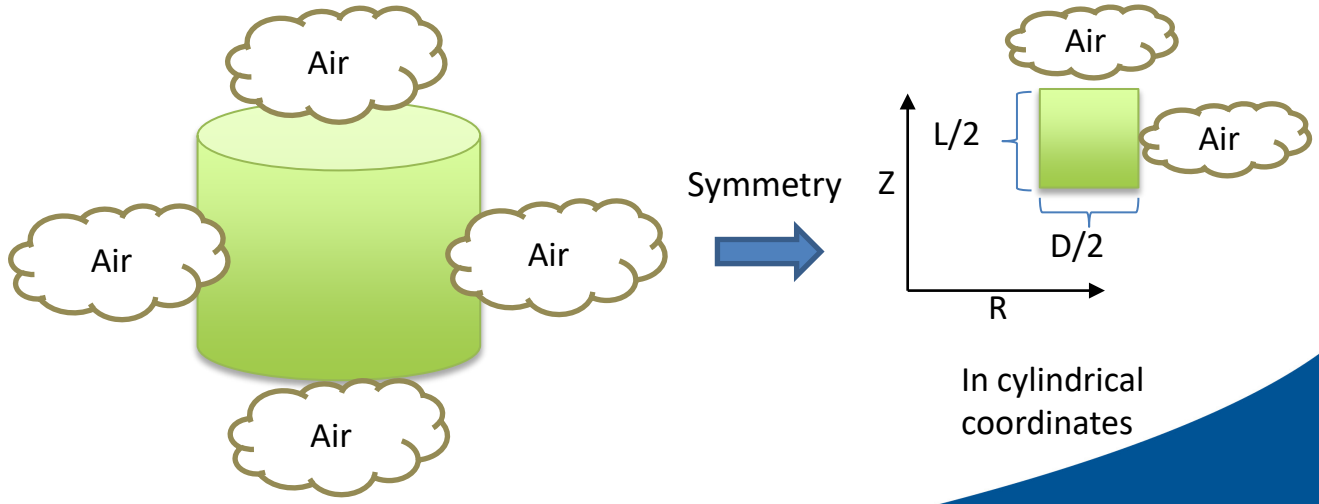
1) Air is on the outside of the cylinder

2) Temperature of 564, 645, and 744 °C

Wanted Result:

Density Profile

Problem Geometry:



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Example Problem: Input File Editing (1/6)

The coordinate system can be set to cylindrical by:

```
[Problem]
  coord_type = RZ
[]
```

This cylindrical geometry is very simple, so it can be implemented in the input file and does not require external mesh generation:

```
[Mesh]
  # mesh information:
  type = GeneratedMesh
  dim = 2
  nx = 100
  ny = 20
  xmax = 0.0127 # Test chamber radius
  ymax = 0.0254 # Length of test chamber
[]
```


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Example Problem: Input File Editing (2/5)

In the Variables block the initial conditions can be set for the species concentrations and temperature.

Problem Setup

Species Concentrations: The nitrogen is set at near the concentration of nitrogen in air.

Temperature: The temperature will have to be adjusted for each of the three simulated temperatures (564, 645, 744 °C).

```
[Variables]
  ### Molar concentration of oxygen gas [mol/m^3]
  [./O2]
    initial_condition = 0.0
  [../]

  ### Molar concentration of nitrogen gas [mol/m^3]
  [./N2]
    initial_condition = 35
  [../]

  ### Molar concentration of carbon-monoxide gas [mol/m^3]
  [./CO]
    initial_condition = 0.0
  [../]

  ### Molar concentration of carbon-dioxide gas [mol/m^3]
  [./CO2]
    initial_condition = 0.0
  [../]

  ### Molar concentration of helium gas [mol/m^3]
  [./He]
    initial_condition = .1
  [../]

  ### Temperature [K]
  [./T]
    initial_condition = 918.15
  [../]
[]
```

Set initial conditions for the species concentrations

Set initial Temperature in Kelvin

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Example Problem: Input File Editing (3/5)

Editing the AuxVariables, Kernels, AuxKernels and BCs blocks

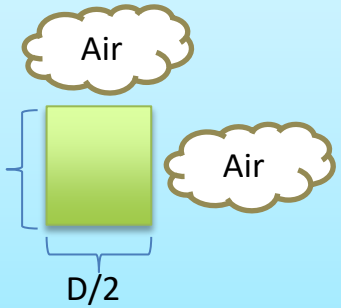
Block which normally don't need editing:

AuxVariables, Kernels, AuxKernels

The boundary condition block, BCs, editing:

The species concentration are set as constants approximately equal to air.

Problem Setup



BCs block

```
[BCs]
  [./O2]
    type = DirichletBC
    boundary = 'right top'
    variable = O2
    value = 9.375
  [../]
  [./CO2]
    type = DirichletBC
    boundary = 'right top'
    variable = CO2
    value = 0
  [../]
  [./CO]
    type = DirichletBC
    boundary = 'right top'
    variable = CO
    value = 0
  [../]
  [./N2]
    type = DirichletBC
    boundary = 'right top '
    variable = N2
    value = 35
  [../]
  [./He]
    type = DirichletBC
    boundary = 'right top '
    variable = He
    value = .1
  [../]
  [./T]
    type = DirichletBC
    boundary = 'right top'
    variable = T
    value = 918.15
  [../]
[]
```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Example Problem: Input File Editing (4/5)

The model is parameterized for IG-110 and NBG-18.

Material Block Edits:

1. Input “IG-110” or “NBG-18” for “graphite_type”.
2. Check that the initial pore fraction (initial_porosity) and bulk density (initial_bulk_denity) in g/cc match the selected graphite.
3. Input the system pressure in Pa.

Note that the above steps are only valid for IG-110 and NBG-18, modeling other grades will require additional editing.

```
[Materials]
  [./porous]
    type = PorousMediaBase

    gas_mixture  = 'O2 N2 CO CO2 He'
    molecular_weights = '31.9988 28.0134 28.0101 43.9987 4.0026'
    e_kb = '106.7 71.4 91.7 195.2 10.22'
    sigma = '3.467 3.798 3.69 3.941 2.551'
    dipole_moment = '0.0 0.0 0.122 0.0 0.0'
    polarizability = '1.562 1.71 1.9532 2.5070 0.2080'

    graphite_type = IG-110 # two types considered: IG-110 or NBG-18

    initial_porosity = 0.2114
    initial_bulk_density = 1779
    reactive_surface_area = 2.5e3
    rate_scaling_factor = 0.0056
    power_exponent = 1.0
    diffusivity_scaling_factor = 1

    system_pressure = 101325.0

    temperature_var = 'T'
  [../]
[]
```

Example Problem: Input File Editing (5/5)

Executioner block Edits:

1. The “end_time” (seconds) should be set to the total simulation time.
2. A user may want to adjust the initial time step (dt). Low temperature simulations can be set with a larger time step than high temperature simulations.

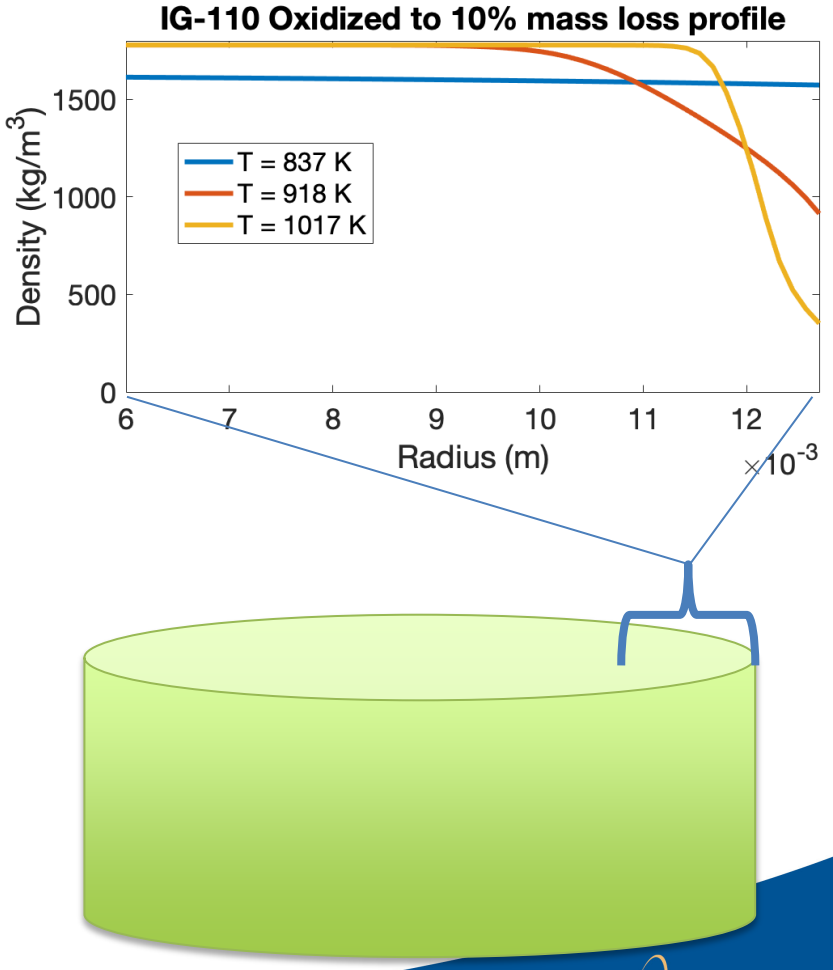
Generally, the other inputs need not be adjusted unless there are convergence issues.

```
[Executioner]
  type = Transient
  solve_type = 'NEWTON'

  petsc_options_iname = '-pc_type -pc_hypre_type -ksp_gmres_restart -snes_ls -pc_hypre_boomeramg_strong_threshold'
  petsc_options_value = 'hypre boomeramg 201 cubic 0.7'

  dtmax = 2000.0
  dtmin = 1.0e-10
  end_time = 300000 # = 70 hrs

  [./TimeStepper]
    type = SolutionTimeAdaptiveDT
    dt = 1
  [../]

  l_max_its = 30
  l_tol = 1e-5

  nl_max_its = 10
  nl_rel_tol = 1e-6
  nl_abs_tol = 1e-5
[]
```

Example Problem: Results

To create the input file for this problem we must:

1. Generate a mesh
2. Specify boundary conditions (species concentrations and temperature)
3. Select a graphite grade (IG-110 or NBG-18)
4. Set a simulation run time



The plot on the right shows the resultant density profiles at three temperatures each of which are at 10% mass loss. The main takeaways from this plot are:

1. The slope of the density profile increases with an increase in temperature
2. This is the experimentally observed temperature-dependent density profile behavior

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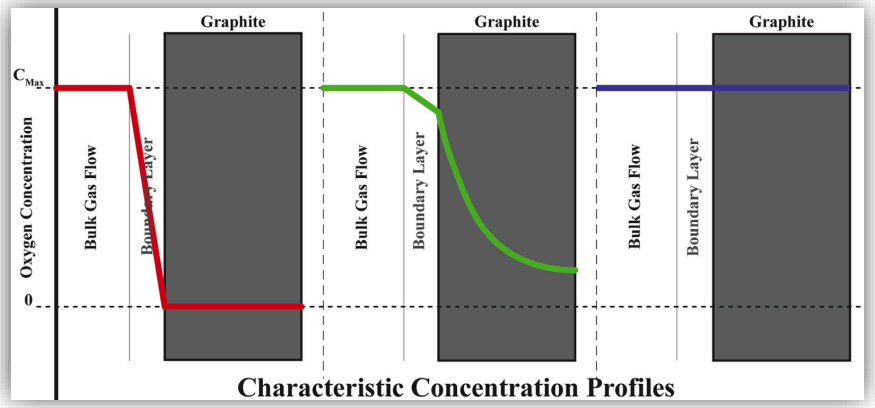
Modeling Reaction Kinetics

In order to model oxidation, we must know how the reaction kinetics vary as a function of mass loss.

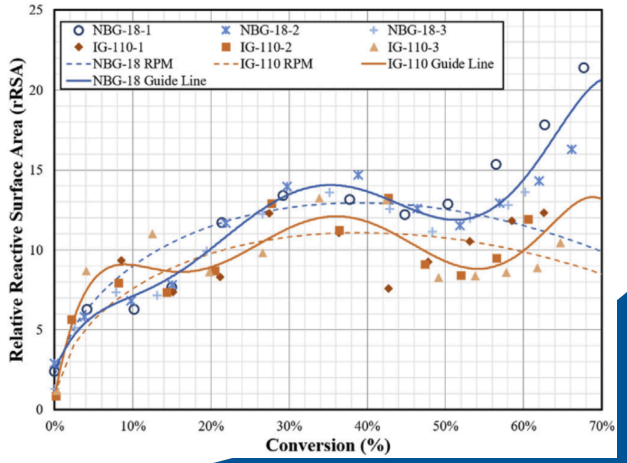
A macroscale understanding of the local reaction kinetics within a component can approximated using the following logic:

1. The local reaction rate within a component is a function of the reactive surface area density.
2. The reactive surface area density varies as function mass loss
3. At low temperatures, diffusion does not have an appreciable effect on the experimentally observed reaction rate

Therefore, **low temperature oxidation experiments can provide a relative reactive surface area density as a function of mass loss**.



RSA evolution with mass loss



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Modeling Oxidant Diffusion

The oxidant diffusion in the model is controlled by a mass loss dependent effective diffusion, D_{eff}.

An effective diffusion of unoxidized graphite can be experimentally measured. Measurements used in this work were done by Josh Kane[1].

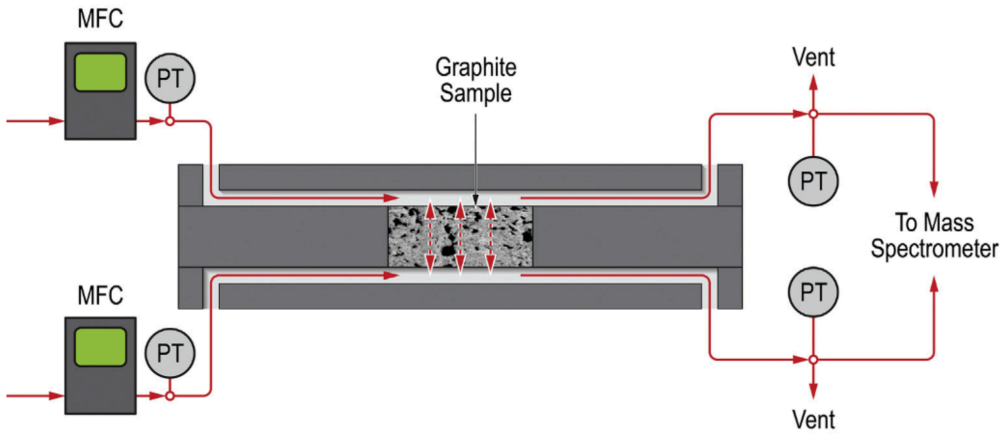
The effective diffusivity is implemented as

$$D_{eff} = D_{unox} + f(\rho)(D_{bulk} - D_{unox})$$

$$f(\rho) = (1-\rho)^2$$

Here D_{unox} is the unoxidized diffusivity, D_{bulk} is the bulk gas diffusion, and ρ is the normalized density.

Experiments are currently being conducted to confirm the effect of mass loss on diffusivity.



[1] J. Kane et al. (2018) Effective gaseous diffusion coefficients of select ultra-fine, super-fine and medium grain nuclear graphite. *Carbon,* Volume (136), pp. 369-379.

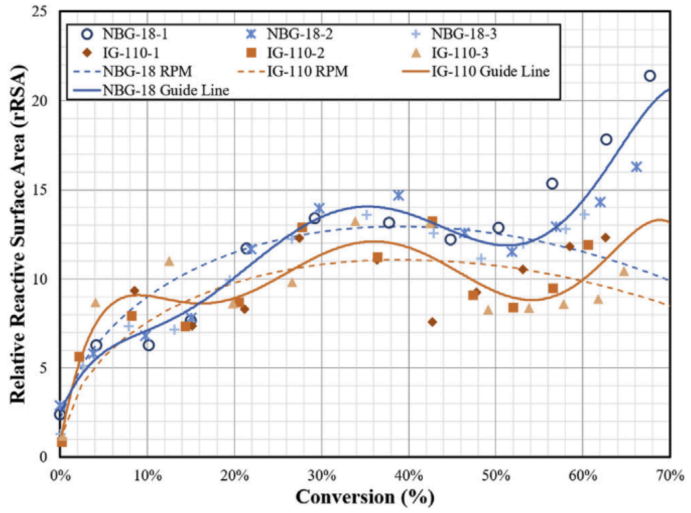
Model parameterization: Reaction kinetics

The model assumes that the active surface area varies as a function of mass loss.

Needed Experiment

Low temperature oxidation mass loss versus time data. This data can be used to:

1. Set the parameter related to active surface area in the model
2. Determine the evolution of the RSA

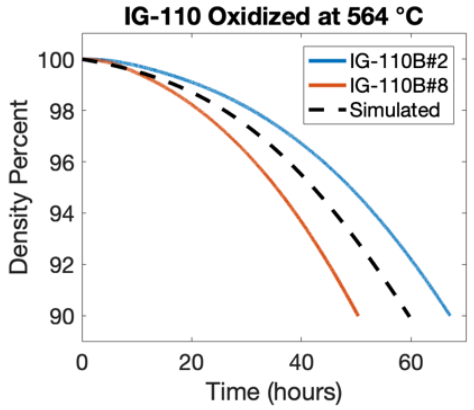


Implementation

The RSA evolution equation is input in the GraphiteThermalGaseous.C source file using the form:

$$\_SA[qp] = init\_area * f(kalfa)$$

where $\_SA$ is the reactive surface area variable. *init_area* is an internal parameter which need not be adjusted, and *f(kalfa)* is the RSA evolution equation where kalfa is the mass loss fraction.



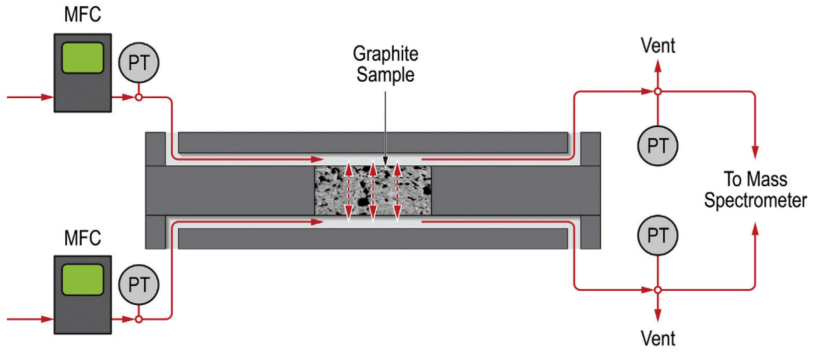
The rate_scaling_factor in the GraphiteThermalGaseous material need to be adjusted so that the simulation matches the low temperature mass loss.

Parameterization: Diffusion and Heat Generation

Diffusion

Experiment

An effective diffusion value needs to be determined. This can be done using experiments like the one shown on right.



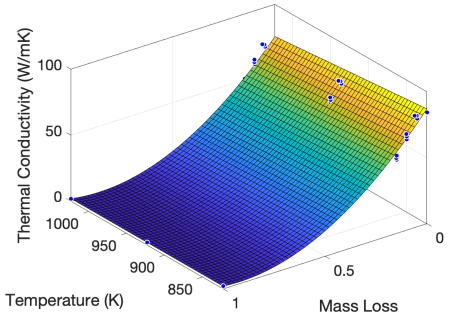
Implementation

In the GraphiteThermalGaseous.C source file the variable “Z” should be set to equal to the ratio of the unoxidized diffusivity to the bulk diffusivity

Heat Generation

Experiment

Thermal conductivity experiments as a function of mass loss should be run.



Implementation

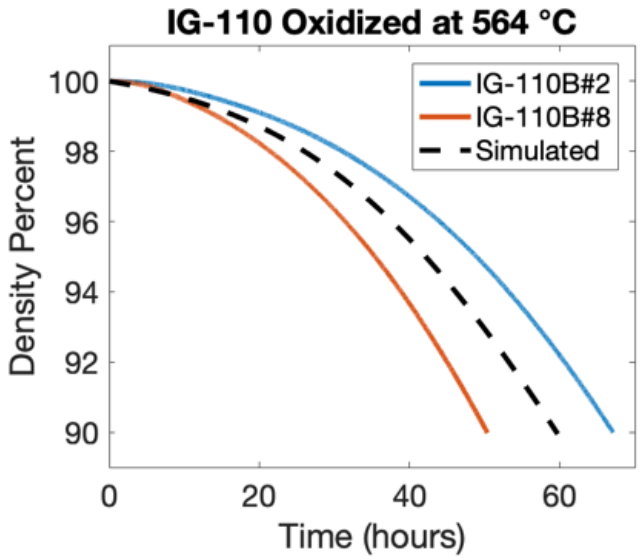
In the thermal conductivity, kT, should be input as a function of the states in the PorousMediaBase.C file. For example:

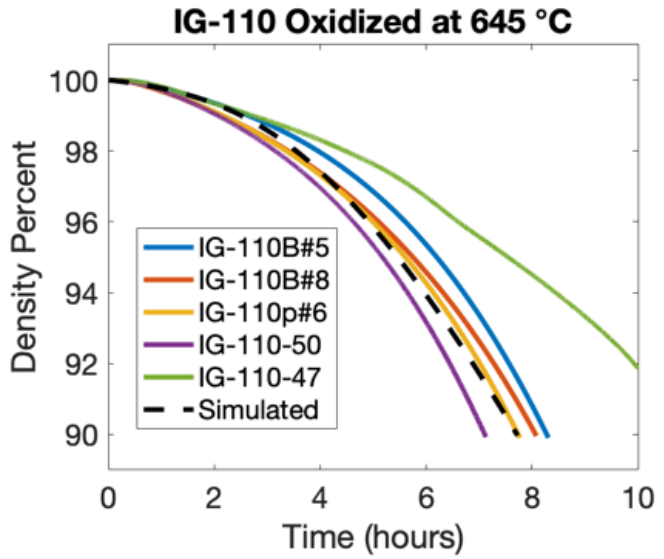
```
_kT[qp] = 134 + -0.05719 * T - 233.4 * kalfa + 0.05731 * T * kalfa + 101.3 * kalfa*kalfa;
```

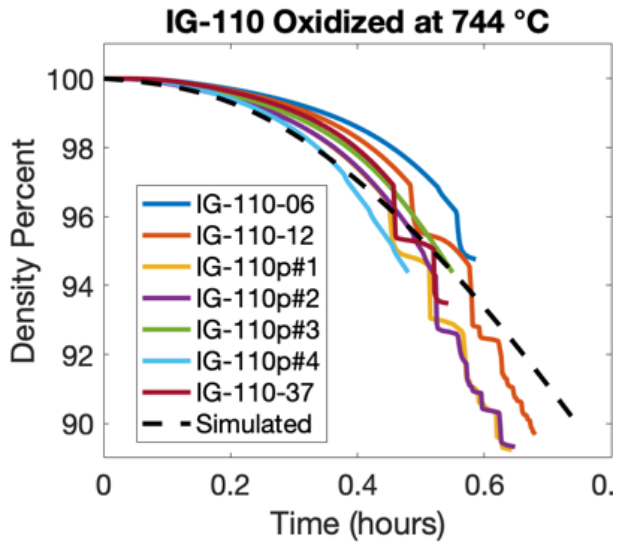
Validation of the Oxidation Model

Simple Validation:

The model can be compared to mass loss at multiple temperatures to validate the oxidation model.







Better Validation:

The best validation would be to compare the computed density profile to an experimentally determined density profile.

Molten Salt

MSR Modeling

Currently the ASME Code does not provide significant guidance related to MSR graphite assessment. Most of the discussion on MSR graphite is shown to the right.

What do we need to know in order to model graphite in an MSR?

1. **Material properties**
    - These must be determined as a function of the states (temperature, dose, salt concentration, etc.)
2. **Salt Penetration**
    - Penetration depth will be grade dependent
    - This is essential as it will dictate where property changes occur.
3. **Degradation mechanisms**
    - Chemical interaction (fluorination and chemical attack)
    - Abrasion/erosion rates

Currently, we don't know which aspects of the interaction between graphite and molten salt are most important to model.

ARTICLE HHA-B-4000
SALT COOLANT-GRAPHITE INTERACTIONS

The interest in salt-cooled power reactors commenced in the 1960s with the advent of the Molten Salt Reactor Experiment (MSRE) at Oak Ridge National Laboratory. More recently, there has been interest in the Fluoride Salt Reactors (FSR). Salt-cooled reactors are planned to be constructed in the next few years. Salt-graphite interactions include potential salt intrusion into the graphite porosity, buildup of tritium gas, and changes in properties. In instances where the coolant salt also contains the dissolved fuel, salt impregnation of the graphite can also lead to hot spots in the graphite. Salt coolant-graphite interactions and molten salt reactor literature is given in the references ([29]–[37]).

How could we implement MSR effect in the current tool?

We should model the interaction which has the largest effect on the graphite behavior.

The most important effect may be graphite grade and reactor design dependent.

If salt penetration is going to occur, we can model its effects by

1. Introducing an AuxVariable and function which describe the salt concentration.

AuxVariable block

```
[./salt_concentration]
  order = FIRST
  family = LAGRANGE
[../]
```

Function block

```
[./salt_fun]
  type = ParsedFunction
  value = 'salt concentration function'
[../]
```

AuxKernels block

```
[./salt_concentration]
  type = FunctionAux
  variable = salt_concentration
  function = salt_fun
[../]
```

2. Edit material properties as a function of salt_concentration auxvariable. For example, the CTE AuxKernel may look like:

Note: abrasion and erosion may be modeled in a similar manner to regime 3 oxidation.

```
[./cte_per]
  type = ParsedAux
  args = 'temp_aux rdose salt_concentration'
  variable = cte_per
  function = 'function of states including salt concentration'
[../]
```

ASME

ASME Code Considerations

- Weibull statistics for failure probability
- Distribution of loading in the graphite component includes stresses from irradiation dimensional changes and temperature gradients
- Oxidation loss of strength and irradiation property changes are to be considered

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.

Graphite Data for Assessment

- Graphite properties depend on the grade

e.g., Form MDS-1 Material Data Sheet

FORM MDS-1 MATERIAL DATA SHEET (SI UNITS)

Grade Designation

Material Grade ① Material spec. ID ② ASTM spec. ③

Max. grain size (mm) ④ Designation ⑤

Temperature-Dependent Parameters

Property	Units	Orientation	20°C	200°C	400°C	600°C	800°C	1000°C [Note (1)]
Bulk density ⑥	$kg \cdot m^{-3}$	...						
Strength – tensile ⑦	MPa	WG, AG						
Strength – flexural ⑧ (4-point)	MPa	WG, AG						
Strength – compressive ⑨	MPa	WG, AG						
Elastic modulus ⑩ (dynamic)	GPa	WG, AG						
Elastic modulus (static) ⑪	GPa	WG, AG						
Coefficient of thermal ⑫ expansion	$°C^{-1}$	WG, AG						
Thermal conductivity ⑬	W/m•k	WG, AG						

Temperature-Independent Parameters

Poisson's ratio ⑭ Anisotropy factor ⑮ Critical stress intensity factor K_{IC} MPa•$m^{½}$ ⑯

Design Strength and Material Reliability Curve Values

Ratio of compressive to tensile strength (R_{tc}) ⑰ Ratio of flexural to tensile strength (R_{tf}) ⑱ $S_{c95\%}$ MPa ⑲ $m_{95\%}$ ⑳

S_0 MPa ㉑ $S_{c095\%}$ MPa ㉒ $m_{095\%}$ ㉓

$S_g(10^{-4})$ MPa ㉔ $S_g(10^{-3})$ MPa ㉕ $S_g(10^{-2})$ MPa ㉖ $S_g(5 \times 10^{-2})$ MPa ㉗

Temperature-Independent Parameters

Poisson's ratio ⑭ Anisotropy factor ⑮ Critical stress intensity factor K_{IC} MPa•$m^{½}$ ⑯

Design Strength and Material Reliability Curve Values

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S_0 MPa ㉑ $S_{c095\%}$ MPa ㉒ $m_{095\%}$ ㉓

$S_g(10^{-4})$ MPa ㉔ $S_g(10^{-3})$ MPa ㉕ $S_g(10^{-2})$ MPa ㉖ $S_g(5 \times 10^{-2})$ MPa ㉗

Graphite Oxidation – Effect

Property	Units	2%	4%	6%	8%	10%
Strength [.] ㉘						
Elastic modulus (dynamic) [.] ㉙						
Thermal conductivity [.] ㉚						

Irradiated Graphite

Property	Units	WG	AG
Dimensional change [.] ㉛			
Creep coefficient [.] ㉜			
Coefficient of thermal expansion [.] ㉝			
Strength [.] ㉞			
Elastic modulus [.] ㉟			
Thermal conductivity [.] ㊱			

GENERAL NOTES:
(a) WG, AG refers to the with- and against-grain direction of the material.
(b) [.] indicates a dimensionless quantity.

NOTE:
(1) If the maximum intended use temperature exceeds 1 000°C, then the temperature dependent data shall be extended to cover the property values at the maximum intended use temperature.

Oxidation Modeling in the ASME Code

The ASME Code does:

1. Identify what can cause oxidation
2. Identify how oxidation affects strength
3. Provide guidance on how an FEA analysis should be conducted on oxidized graphite
4. Identify limitations to the oxidation rules (oxidation rules are not applicable to graphite irradiated past .25 dpa)

The ASME Code does not:

Provide a method for assessing an oxidized component. Therefore, it is the designer's responsibility to show that oxidation is appropriately accounted for.

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. Assessment of oxidized Graphite Core Components shall comply with (a) through (d) below.

(a) Material is considered oxidized if the weight loss is greater than 1%.

(b) Strength Reduction. The strength (both tensile and compressive) decreases as a function of weight loss as shown in Figures HHA-3141-1 and HHA-3141-2 (or alternatively from the Material Data Sheet HHA-2200). The stress evaluation shall be made according to this relation. The region where strength decreases to less than 50% shall not be credited in the stress evaluation.

(c) Geometry Reduction. The region where the amount of weight loss exceeds 30% shall be regarded as completely removed from the structure for both oxidation and strength calculations.

(d) Combinations of weight loss and irradiation where the resulting strength is lower than the nonirradiated strength are excluded from the scope of these code requirements. Oxidation to high weight loss (>1%) occurring simultaneously with significant irradiation (>0.25 dpa) is excluded from the scope of these code requirements. Note that large-scale oxidation resulting from accidental air or water ingress occurs over a short time scale without significant irradiation of the material and thus still falls within the scope of these rules.