Xe-100 Graphite Engagement:
IGNIS Graphite Modeling Toolset used in Xe-100 Analyses and Qualification Approach

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Agenda & Objectives

Objectives:
- Understand how this work fits into the larger reactor and graphite qualification work.
- Understand the challenges of graphite modeling.
- Understand the capabilities and structure of IGNIS.
- Understand the pedigree of IGNIS.

Agenda

Open Portion:
- Framework Overview
- Phenomena Identification
- Review of Existing Data
- IGNIS Overview
- IGNIS Development Plan
- IGNIS Structure (open)
- IGNIS Closure Models (open)
- IGNIS Verification and Validation (open)

Closed Portion:
- IGNIS Structure (closed)
- IGNIS Closure Models (closed)
- IGNIS Verification and Validation (closed)
IGNIS Motivation

- The Xe-100 is a graphite-moderated reactor with multiple graphite core components
- These graphite core components must be analyzed to ensure safe operation of the reactor
- Irradiated graphite is a complex material that requires specialized tools to analyze
- X-energy is developing IGNIS to help analyze graphite structural behavior
- IGNIS = Irradiated Graphite Numerical Iterative Solver
Framework Overview

- IGNIS is developed in accordance with RG 1.203
- Element 1: Requirements for Capabilities: Discussed previously
- Element 2: Develop Assessment Base: Discussed previously
- Element 3: Model Development (Focus)
  - Establish evaluation model development plan
  - Establish evaluation model structure
  - Incorporate closure models
- Element 4: Model Adequacy
  - Bottom Up
  - Top Down
Phenomena Identification

- Key phenomena identified per NUREG/CR-6944 and X-energy’s Xe-100 PIRTs
- IGNIS designed to capture key *structural* phenomena
  - Elastic Strain
  - Irradiation creep strain
  - Dimensional change strain (Wigner strain)
  - Thermal strain
- Planned future work
  - Thermal conductivity
Review of Existing Data

• The existing data for the graphite grades are reviewed and relevant data is collected for the grades and the irradiation temperature and dose in which X-energy is designing the Xe-100 graphite reactor core components.

• More information regarding this effort can be found in the previous engagement with the NRC staff on the Xe-100 Graphite Material Model.
IGNIS Model Development Overview

- Development Plan
- IGNIS Structure
- Material Closure Models
- Verification and Validation
IGNIS Development Plan

- IGNIS is developed with guidance from NQA-1, NUREG/BR-0167, and industry best practices.

  - Prior to coding
    - Requirement specification
    - Architecture diagram
    - Roles and responsibilities
    - Style guide
  - During Coding
    - Source version control
    - Unit test development
    - Pair programming and peer checking
  - After coding
    - Verification
    - Validation
    - User documentation
    - Configuration management
    - Upgrades/Maintenance
IGNIS Structure

• A commercial finite element software (FEA tool) is used to evaluate the graphite reactor core components. These FEA tools are developed with NQA-1 & ISO-9001 certification and have long history of being used in various industries.

• The standard material models available in these FEA tools are insufficient to accurately reflect the changes that graphite undergoes due to irradiation.

• IGNIS is a user-defined material model that connects to an FEA tool in order to enhance the FEA tool with the modelling capabilities required to assess the structural performance of graphite reactor core components.
IGNIS Structure

- FEA Loads
- Force Balance
- FEA Tool
- Strain
- Stress
- Stiffness
- IGNIS
- Material Property Solvers
IGNIS Structure – Detailed Overview

- The FEA tool is fed a load case containing the loads and boundary conditions and checks the force balance.

- The tool calculates a displacement field and the resulting strain field.

- IGNIS then uses material property solvers, discussed in the Xe-100 Graphite Material Model presentation and will be revisited later, to find the stress and compliance matrices describing the 3D behavior at each integration point.

- These are fed back into the FEA tool, which will use them to evaluate the force balance and see if the equilibrium criteria are met.

- If imbalances exist, the strain is updated and the process iterates to convergence.
IGNIS Closure Models & Constitutive Equations

- Closure models relate stress/strain/fluence/temperature
- General form of closure models is based on literature
  - Graphite Material Model presentation
- Closure models are tuned based on experimental data
  - Detailed discussion will be provided in future engagement
- Details of the closure models are proprietary to X-energy and will be discussed further in the closed session
IGNIS Closure Models & Constitutive Equations

- Strain model based on combination of strains:
  \[ \varepsilon = \varepsilon_{\text{elastic}} + \varepsilon_{dc} + \varepsilon_{\text{th}} + \varepsilon_{\text{creep}} \]

  \[ \varepsilon_{\text{elastic}} = \frac{\sigma}{E} \]

  \[ E = E_0 \cdot \left(1 + (P_{em} - 1)(1 - e^{-k_{em}r})\right) \cdot (1 + C_{em} \cdot S_c) \cdot e^{-\beta_d \Delta \nu_d} \cdot e^{-\beta_{pg} \Delta \nu_{pg}} \]

  \[ \frac{d\varepsilon_{dc}}{d\gamma} = \frac{dG_{dc}}{d\gamma} + \frac{dF_{dc}}{d\gamma} \]

  \[ \frac{dG_{dc}}{d\gamma} = A_{dc} (1 - e^{-k_{dc}r}) \]

  \[ \frac{dF_{dc}}{d\gamma} = B_{dc} S_c \frac{dG_{dc}}{d\gamma} \]

  \[ S_c = \frac{1}{2} \left(1 + \text{erf} \left(\frac{\gamma - \mu_{Sc}}{\sigma_{Sc} \sqrt{2}}\right)\right) \]

  \[ \varepsilon_{\text{th}} = \text{CTE} \cdot (T - T_0) \]

  \[ \text{CTE} = (1 - D_{\text{CTE}} S_c) \cdot \left(1 + P_{\text{CTE}} \left(1 - e^{-k_{th}r}\right)\right) \cdot \text{CTE}_{\text{norad}} \cdot (1 + a_{\text{cte,p}} \varepsilon_{cr,p} + a_{\text{cte,r}} \varepsilon_{cr,r}) \]

All parameters are temperature and grade dependent. Some also depend on orientation.
IGNIS Verification and Validation

• Verification
  • The process of determining that a computer model, simulation, or federation of models and simulations implementations and their associated data accurately represent the developer's conceptual description and specifications. (Are we building the product right?)

• Validation
  • The process of determining the degree to which a model, simulation, or federation of models and simulations, and their associated data are accurate representations of the real world from the perspective of the intended use(s). (Are we building the right product?)

• Overall V&V approach aligned with NQA-1 and RG 1.203 practices.

• Details of these efforts are proprietary to X-energy and will be discussed in the closed session.
Conclusion | Next Steps

• IGNIS is a custom material model designed by X-energy to model irradiated graphite.
• IGNIS leverages experimental graphite testing data in combination with theoretical formulations to allow analysis of graphite core components.
• The software will be constructed, verified, and validated using industry standard guidance.
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Review of Existing Data

• [Proprietary – Withhold in accordance with 10 CFR 2.390]
IGNIS Structure
IGNIS Structure – Detailed Overview

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IGNIS Structure
IGNIS Structure – DETAIL

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IGNIS Structure – DETAIL

• $[[P^P]$
To calculate the strains from the stress tensor, temperature, and fluence the following procedure is followed.

In this series of slides, a \[ \text{[[ ]]}^P \text{ or “γ” in the box indicates that the quantity is calculated as a direct function of } \text{[[ ]]}^P \text{ or neutron fluence, respectively.} \]

First the structural connectivity is calculated. It is used as a basis for several of the strain equations.

\[
S_c = \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\gamma - \mu_{Sc}}{\sigma_{Sc} \sqrt{2}} \right) \right)
\]
IGNIS Structure

[[

]]
• The structural connectivity feeds into the equation for the densification and pore generation.

Densification:
\[ \frac{dG_{dc}}{d\gamma} = A_{dc} \left(1 - e^{-k_{dc} \gamma}\right) \]

Pore generation:
\[ \frac{dF_{dc}}{d\gamma} = B_{dc} S_c \frac{dG_{dc}}{d\gamma} \]
IGNIS Structure
The Young’s modulus can then be calculated by virtue of the three aforementioned variables:

- Structural connectivity
- Densification
- Pore generation

As well as the fluence and the 

\[
E = E_0 \cdot \left(1 + (P_{em} - 1)(1 - e^{-k_{em}r})\right) \cdot (1 + C_{em} \cdot S_c) \cdot e^{-\beta_d \Delta v_d} \cdot e^{-\beta_{pg} \Delta v_{pg}}
\]
IGNIS Structure
• The 3D elastic strain is found by

\[ \varepsilon_{\text{elastic}} = \frac{\sigma}{E} \]
• By adding the densification and the pore generation, the dimensional change due to irradiation can be found.

\[
\frac{d\varepsilon_{dc}}{dy} = \frac{dG_{dc}}{dy} + \frac{dF_{dc}}{dy}
\]
IGNIS Structure
• The creep strain is then found by solving with the stress and the fluence:

\[
\varepsilon_c = \varepsilon_{c,p} + \varepsilon_{c,s} + \varepsilon_{c,r}
\]

\[
\varepsilon_{c,p} = k_{cr,p} \int_0^\gamma \frac{\alpha_{cr} \sigma}{E_0 S_{cr}} e^{k_{cr,p}(\gamma' - \gamma)} d\gamma'
\]

\[
\varepsilon_{c,s} = \int_0^\gamma \frac{\beta_{cr} \sigma}{E_0 S_{cr}} d\gamma'
\]

\[
\varepsilon_{c,r} = k_{cr,r} \int_0^\gamma \frac{\omega_{cr} \sigma}{E_0 S_{cr}} e^{k_{cr,r}(\gamma' - \gamma)} d\gamma'
\]
To calculate the Coefficient of Thermal Expansion (CTE) the creep strain is required:

\[
CTE = (1 - D_{CTE} S_c) \cdot \left( 1 + P_{CTE} \left( 1 - e^{-k_th \gamma} \right) \right) \cdot CTE_{norad} \cdot \left( 1 + a_{cte,p} \varepsilon_{cr,p} + a_{cte,r} \varepsilon_{cr,r} \right)
\]
• With the CTE found the thermal strain can be found:

\[ \epsilon_{th} = CTE \ (T - T_0) \]
Individual strain terms are then summed to determine the total strain:

\[ \varepsilon = \varepsilon_{el} + \varepsilon_{dc} + \varepsilon_{cr} + \varepsilon_{th} \]
IGNIS Closure Models/Constitutive Equations

- Closure models previously presented were for simplified, 1D strains.
- Each equation must be expanded to 3D and account for potential inter-direction dependencies (e.g., Poisson ratio effect)

\[
\varepsilon = \varepsilon_{\text{elastic}} + \varepsilon_{dc} + \varepsilon_{th} + \varepsilon_{\text{creep}}
\]

\[
\bar{\varepsilon} = \bar{\varepsilon}_{\text{elastic}} + \bar{\varepsilon}_{dc} + \bar{\varepsilon}_{th} + \bar{\varepsilon}_{\text{creep}}
\]

Overbars represent tensor quantities. Double overbar represents rank 2 tensor.
At the root of the changes in the material properties lies a scalar term named the structural connectivity. As graphite is irradiated, its overall structure changes as bonds between atoms are displaced and pores are filled. This underlying change in the microscopic structural connectivity ultimately affects many of the macroscopic properties of graphite.

Structural connectivity is a scalar and remains unchanged from previous discussion

\[ S_c = \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\gamma - \mu_{Sc}}{\sigma_{Sc} \sqrt{2}} \right) \right) \]
The densification and the pore generation are found as:

\[
\frac{d\tilde{G}_{dc}}{dy} = \tilde{A}_{dc}(1 - e^{-k_{dc}y})
\]

\[
\frac{d\tilde{F}_{dc}}{dy} = B_{dc} S_c \frac{d\tilde{G}_{dc}}{dy}
\]

These terms occur in the three normal directions and may be orthotropic due to the anisotropic behavior of the graphite, this is reflected in the coefficient \(\tilde{A}_{dc}\).

Integration with respect to fluence is used.
The dimensional change is found as the summation of densification and pore generation:

\[
\frac{d\epsilon_{dc}}{d\gamma} = \frac{d\tilde{G}_{dc}}{d\gamma} + \frac{d\tilde{F}_{dc}}{d\gamma}
\]
The Young’s modulus is defined as, based on the work of Bradford and Steer:

\[
\bar{E} = E_0 \cdot \left(1 + (P_{em} - 1)(1 - e^{-k_1 \gamma})\right) \cdot (1 + C_{em} \cdot S_c) \cdot e^{-\beta_d \Delta v_d} \cdot e^{-\beta_{pg} \Delta v_{pg}}
\]

\[
\Delta v_d = \left(1 + G_{dc,x}\right)\left(1 + G_{dc,y}\right)\left(1 + G_{dc,z}\right) - 1
\]

\[
\Delta v_{pg} = \left(1 + F_{dc,x}\right)\left(1 + F_{dc,y}\right)\left(1 + F_{dc,z}\right) - 1
\]

The densification \(G_{dc}\), pore generation \(F_{dc}\), and structural connectivity \(S_c\) are used with the orthotropic \(E_0\) resulting in an orthotropic irradiated Young’s modulus \(\bar{E}\):

\[
\bar{E}_0 = \begin{bmatrix}
E_{0,xx} \\
E_{0,yy} \\
E_{0,zz} \\
G_{0,yz} \\
G_{0,zx} \\
G_{0,xy}
\end{bmatrix}
\]

\[
\bar{E} = \begin{bmatrix}
E_{xx} \\
E_{yy} \\
E_{zz} \\
G_{yz} \\
G_{zx} \\
G_{xy}
\end{bmatrix}
\]
IGNIS Closure Models – Elastic Strain

• The irradiated Young’s modulus is used to find the mechanical strain:

\[ \bar{\varepsilon}_{\text{elastic}} = \bar{J}_{\text{elastic}} \bar{\sigma} \]

\[
\bar{J}_{\text{elastic}} = \begin{pmatrix}
1/E_{xx} & -\nu_{yx}/E_{yy} & -\nu_{zx}/E_{zz} & 0 & 0 & 0 \\
-\nu_{xy}/E_{xx} & 1/E_{yy} & -\nu_{zy}/E_{zz} & 0 & 0 & 0 \\
-\nu_{xz}/E_{xx} & -\nu_{yz}/E_{yy} & 1/E_{zz} & 0 & 0 & 0 \\
0 & 0 & 0 & 1/2G_{yz} & 0 & 0 \\
0 & 0 & 0 & 0 & 1/2G_{zx} & 0 \\
0 & 0 & 0 & 0 & 0 & 1/2G_{xy}
\end{pmatrix}
\]
The creep is a function of the primary, secondary and recoverable creep based on the work of Davies and Bradford

\[ \varepsilon_{\text{creep}} = \varepsilon_{\text{creep,p}} + \varepsilon_{\text{creep,s}} + \varepsilon_{\text{creep,r}} \]

\[ \varepsilon_{c,p} = k_{cr,p}e^{-k_{cr,p}c} \int_0^\gamma \frac{a_{cr}\bar{\sigma}}{S_{cr}} e^{k_{cr,p}c'} dc' \]

\[ \varepsilon_{c,s} = \int_0^\gamma \frac{\beta_{cr}\bar{\sigma}}{S_{cr}} dc' \]

\[ \varepsilon_{c,r} = k_{cr,r}e^{-k_{cr,r}c} \int_0^\gamma \frac{\omega_{cr}\bar{\sigma}}{S_{cr}} e^{k_{cr,r}c'} dc' \]

\[ f_c = \begin{pmatrix}
\frac{1}{E_{x,0}} & -\frac{v_{yx,c}}{E_{y,0}} & -\frac{v_{zx,c}}{E_{z,0}} & 0 & 0 & 0 \\
-\frac{v_{xy,c}}{E_{x,0}} & \frac{1}{E_{y,0}} & -\frac{v_{zy,c}}{E_{z,0}} & 0 & 0 & 0 \\
-\frac{v_{xz,c}}{E_{x,0}} & -\frac{v_{yz,c}}{E_{y,0}} & \frac{1}{E_{z,0}} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2G_{xy,0}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2G_{yz,0}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{xz,0}}
\end{pmatrix} \]
The creep compliance matrix is a function of the primary, secondary and recoverable creep.

Found by taking partial derivative of strain with respect to stress:

\[
\bar{J}_{\text{creep}} = \bar{J}_{\text{creep,p}} + \bar{J}_{\text{creep,s}} + \bar{J}_{\text{creep,r}}
\]
Based on the work of Bradford and Steer the irradiated thermal strain can be found by:

\[ \varepsilon_{th} = \Delta T \cdot (1 - D_{CTE} S_c) \cdot \left(1 + P_{CTE}(1 - e^{-k_{th}Y})\right) \cdot CTE_{norad} \cdot \left(1 + a_{cte,p}\varepsilon_{cr,p} + a_{cte,r}\varepsilon_{cr,r}\right) \]

Due to the anisotropic nature of graphite:

\[ ]^{P} \]
• The thermal compliance matrix can be found with the previously calculated compliance matrices.

\[
\begin{bmatrix}
\end{bmatrix}^P
\]
IGNIS Numerical Integration

• IGNIS is heavily reliant on complex definite integrals.
  • Dimensional change components (densification and pore generation)
  • Creep strains

• Gaussian-Legendre quadrature is employed. The integral over an arbitrary interval \([a,b]\) can be found through:

\[
\int_{a}^{b} f(x) \, dx \approx \frac{b - a}{2} \sum_{i}^{n} w_{i} f(x_{i})
\]

• Where the knots \(x_{i}\) are derived from the normalized knots (on interval \([-1,1]\)):

\[
x_{i} = \frac{b - a}{2} x_{i,norm} + \frac{a + b}{2}
\]
IGNIS Verification and Validation

• Verification
  • Ensures that IGNIS solves equations correctly.
  • Compares simple scenario IGNIS model against hand-calculated reference value.
  • Several tests very different code execution paths.

• Validation
  • Ensures that IGNIS correctly captures physical phenomena.
  • Comparison to experimental data.
  • Experimental specimen is recreated within FEA software and resulting modeled strains are compared to experimental strains
  • Hundreds of individual experimental specimens are modeled.
  • ...
IGNIS Conclusion

- IGNIS interacts with the ANSYS FEA tool to provide mechanical properties of irradiated graphite.
- IGNIS is capable of modeling key physical phenomena:
  - Change in Young’s modulus under irradiation
  - Irradiation induced dimensional change
  - Irradiation induced creep
  - Change in thermal expansion under irradiation and strain
- IGNIS is developed in accordance with industry best practices.
- The primary governing equations of IGNIS have been presented.
- IGNIS has a robust verification and validation plan.
Questions?