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

Michael Saitta, Consultant (MPR Associates, Inc.)
X Energy, LLC

October 12, 2023

Department of Energy Acknowledgement and Disclaimer

This material is based upon work supported by the Department of Energy under Award Number DE-NE0009040.

This presentation was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Agenda & Objectives

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)

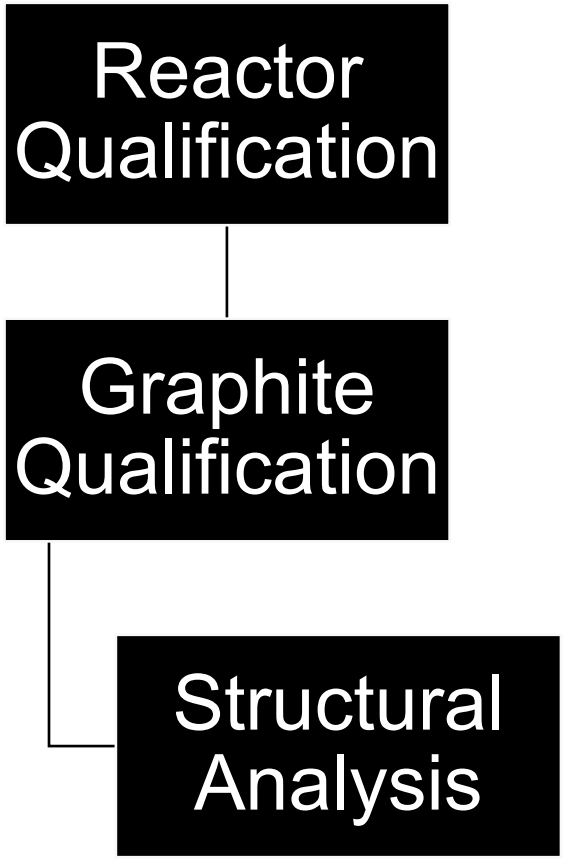
Objectives:

- 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.

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

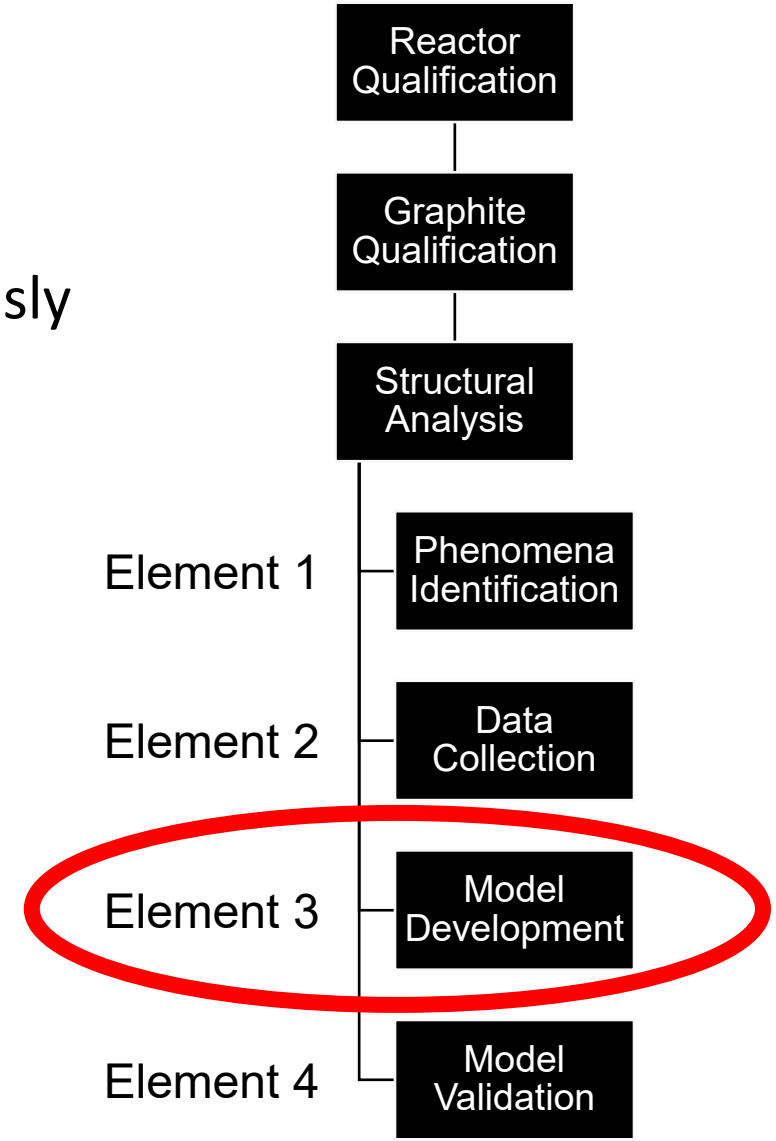
- X-energy is developing IGNIS to help analyze graphite structural behavior
- IGNIS = Irradiated Graphite Numerical Iterative Solver



Framework Overview

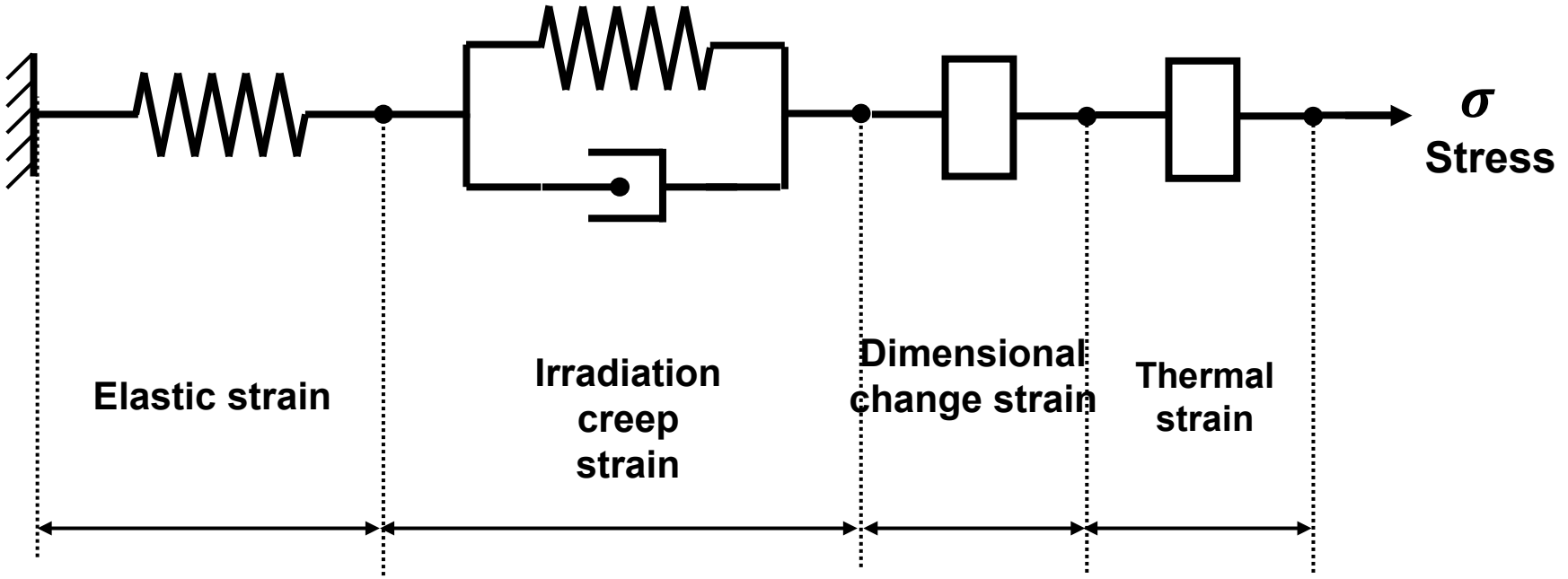
- IGNIS is developed in accordance with RG 1.203

- 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

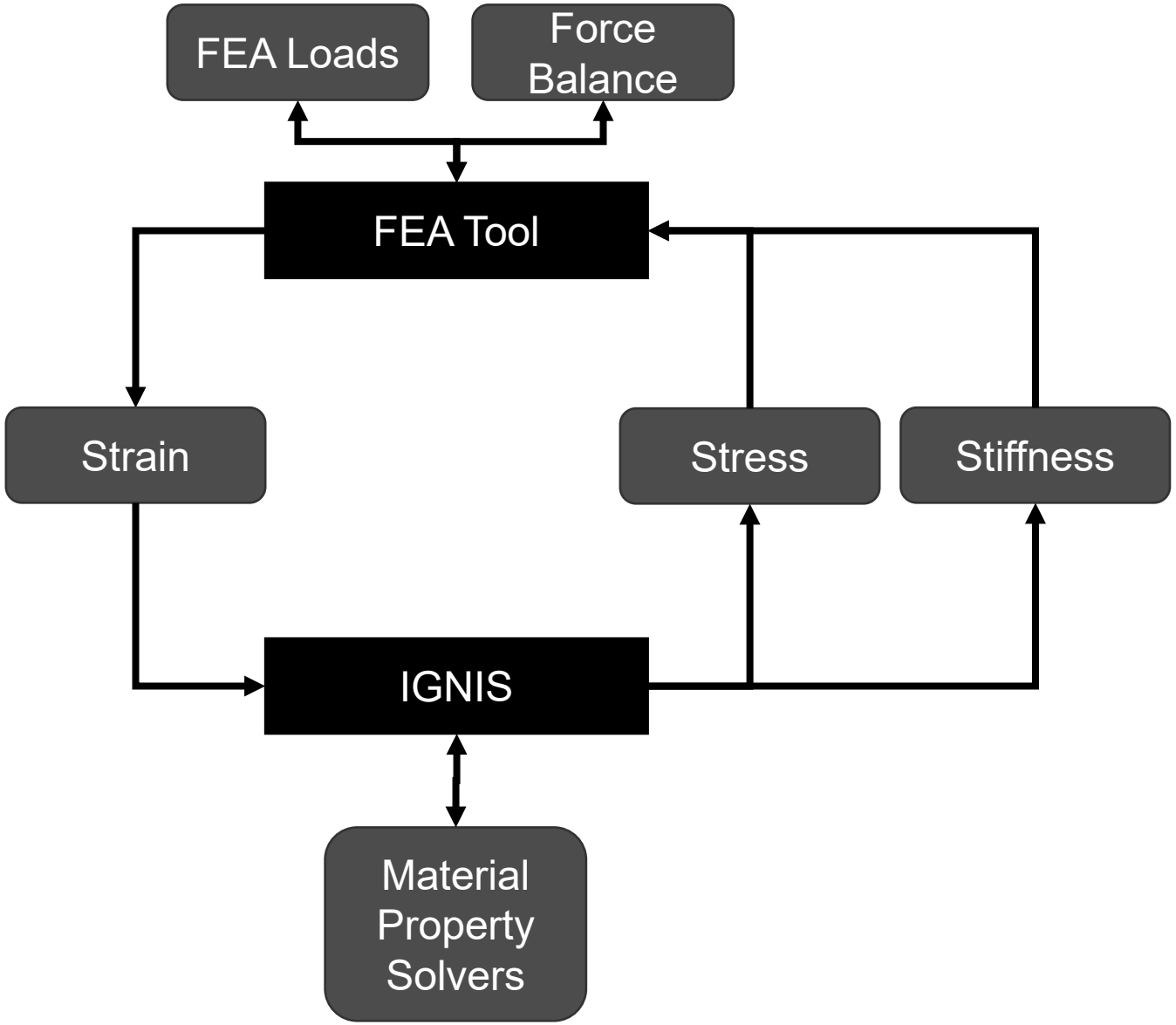
IGNIS Development Plan

- 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



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:

$$\varepsilon = \varepsilon_{elastic} + \varepsilon_{dc} + \varepsilon_{th} + \varepsilon_{creep}$$

$$\varepsilon_{elastic} = \frac{\sigma}{E}$$
$$E = E_0 \cdot \left(1 + (P_{em} - 1)\left(1 - e^{-k_{em}\gamma}\right)\right) \cdot (1 + C_{em} \cdot S_c) \cdot e^{-\beta_d \Delta v_d} \cdot e^{-\beta_{pg} \Delta v_{pg}}$$

$$\varepsilon_c = \varepsilon_{c,p} + \varepsilon_{c,s} + \varepsilon_{c,r}$$
$$\varepsilon_{c,p} = k_{cr,p} \int_0^{\gamma} \frac{\alpha_{cr}\sigma}{E_0 S_{cr}} e^{k_{cr,p}(\gamma' - \gamma)} d\gamma'$$
$$\varepsilon_{c,s} = \int_0^{\gamma} \frac{\beta_{cr}\sigma}{E_0 S_{cr}} d\gamma'$$
$$\varepsilon_{c,r} = k_{cr,r} \int_0^{\gamma} \frac{\omega_{cr}\sigma}{E_0 S_{cr}} e^{k_{cr,r}(\gamma' - \gamma)} d\gamma'$$

$$\frac{d\varepsilon_{dc}}{d\gamma} = \frac{dG_{dc}}{d\gamma} + \frac{dF_{dc}}{d\gamma}$$
$$\frac{dG_{dc}}{d\gamma} = A_{dc}(1 - e^{-k_{dc}\gamma})$$
$$\frac{dF_{dc}}{d\gamma} = B_{dc}\, S_c \frac{dG_{dc}}{d\gamma}$$

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

$$\varepsilon_{th} = CTE\ (T - T_0)$$
$$CTE = (1 - D_{CTE}\, S_c) \cdot \left(1 + P_{CTE}\left(1 - e^{-k_{th}\gamma}\right)\right) \cdot CTE_{norad} \cdot \left(1 + a_{cte,p}\varepsilon_{cr,p} + a_{cte,r}\varepsilon_{cr,r}\right)$$

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.

Closed Portion

energy

X-energy Proprietary Information

This document contains business confidential and proprietary information of X Energy, LLC ("X-energy"), and is not to be disclosed outside of X-energy except in accordance with a fully executed non-disclosure agreement. This document should be protected according to X-energy policies for protecting company proprietary information. Unauthorized disclosure or use of X-energy proprietary information is strictly prohibited and may be subject to civil and criminal penalties. Nonproprietary versions of this presentation indicate the redaction of such information through the use of [[ ]]P.

Export-Controlled Information

This document was reviewed by X-energy and determined to contain information designated as export-controlled per Title 10 of the Code of Federal Regulations (CFR) Part 810 and 10 CFR 110. This information must be withheld from disclosure. Non-export-controlled versions of this document indicate the redaction of such information through the use of [[ ]]E.

Review of Existing Data

- [[

]]P,E

IGNIS Closure Models – Overview

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – Detailed Overview

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – Detailed Overview

- [[

]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[ ]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- [[

]]P

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- To calculate the strains from the stress tensor, temperature, and fluence the following procedure is followed.
- In this series of slides, a [[ ]]^{P} or "γ" in the box indicates that the quantity is calculated as a direct function of [[ ]]^{P} or neutron fluence, respectively.
- First the structural connectivity is calculated. It is used as a basis for several of the strain equations.

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

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

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

Densification:

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

Pore generation:

$$\frac{dF_{dc}}{d\gamma} = B_{dc}\, S_c \frac{dG_{dc}}{d\gamma}$$

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- 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 [[ ]]P

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

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- The 3D elastic strain is found by

$$\varepsilon_{elastic} = \frac{\sigma}{E}$$

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- By adding the densification and the pore generation, the dimensional change due to irradiation can be found.

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

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- The creep strain is then found by solving with the stress and the fluence:

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

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

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

$$\varepsilon_{c,r} = k_{cr,r} \int_0^{\gamma} \frac{\omega_{cr}\sigma}{E_0 S_{cr}} e^{k_{cr,r}(\gamma' - \gamma)} d\gamma'$$

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- To calculate the Coefficient of Thermal Expansion (CTE) the creep strain is required:

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

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- With the CTE found the thermal strain can be found:

$$\varepsilon_{th} = CTE\ (T - T_0)$$

IGNIS Structure

[[

]]P

IGNIS Structure – DETAIL

- 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)

$$\varepsilon = \varepsilon_{elastic} + \varepsilon_{dc} + \varepsilon_{th} + \varepsilon_{creep} \rightarrow \bar{\bar{\varepsilon}} = \bar{\bar{\varepsilon}}_{elastic} + \bar{\bar{\varepsilon}}_{dc} + \bar{\bar{\varepsilon}}_{th} + \bar{\bar{\varepsilon}}_{creep}$$

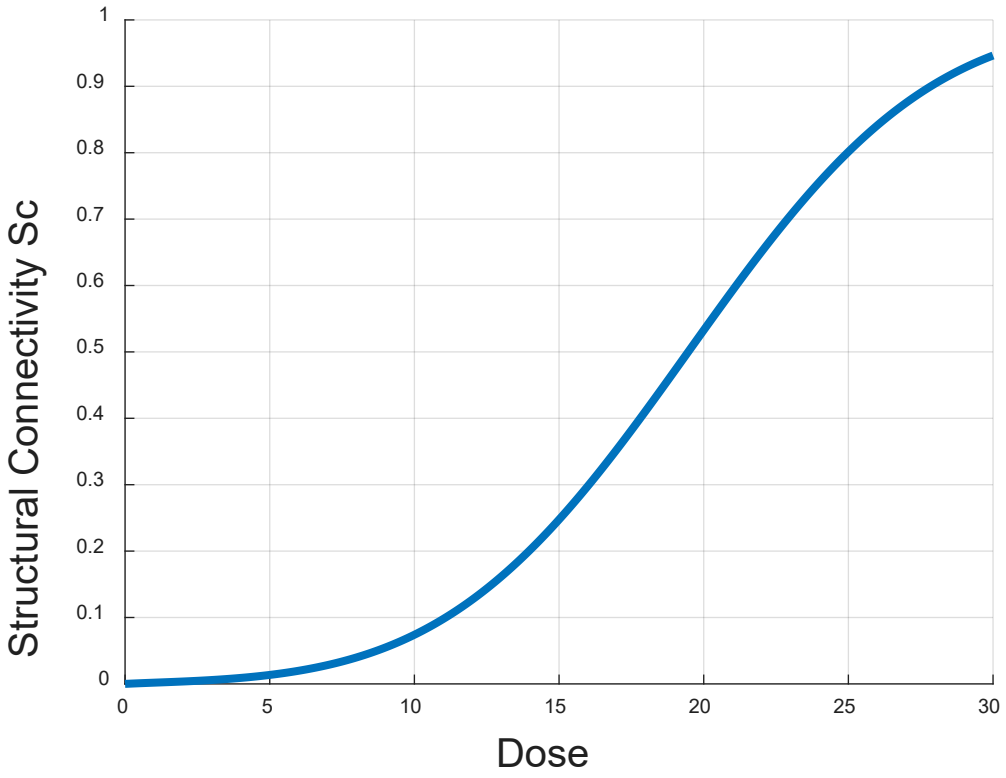
$$\bar{\bar{\varepsilon}} = \begin{pmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \end{pmatrix}$$

Overbars represent tensor quantities. Double overbar represents rank 2 tensor.

IGNIS Closure Models – Structural Connectivity

- 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

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



IGNIS Closure Models – Pore Generation and Densification

- The densification and the pore generation are found as:

$$\frac{d\bar{G}_{dc}}{d\gamma} = \bar{A}_{dc}\left(1 - e^{-k_{dc}\gamma}\right) \qquad \frac{d\bar{F}_{dc}}{d\gamma} = B_{dc}\, S_c \frac{d\bar{G}_{dc}}{d\gamma}$$

- 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 $\bar{A}_{dc}$.
- Integration with respect to fluence is used.

IGNIS Closure Models – Dimensional Change Strain

- The dimensional change is found as the summation of densification and pore generation:

$$\frac{d\bar{\varepsilon}_{dc}}{d\gamma} = \frac{d\bar{G}_{dc}}{d\gamma} + \frac{d\bar{F}_{dc}}{d\gamma}$$

IGNIS Closure Models – Elastic Strain

- The Young's modulus is defined as, based on the work of Bradford and Steer:

$$\bar{\bar{E}} = \bar{\bar{E}}_0 \cdot \left(1 + (P_{em} - 1)\left(1 - e^{-k_1 \gamma}\right)\right) \cdot (1 + C_{em} \cdot S_c) \cdot e^{-\beta_d \Delta v_d} \cdot e^{-\beta_{pg} \Delta v_{pg}}$$

$$\Delta v_d = (1 + G_{dc,x})(1 + G_{dc,y})(1 + G_{dc,z}) - 1$$

$$\Delta v_{pg} = (1 + F_{dc,x})(1 + F_{dc,y})(1 + F_{dc,z}) - 1$$

- The densification (G_{dc}), pore generation (F_{dc}), and structural connectivity (S_c) are used with the orthotropic $\bar{\bar{E}}_0$ resulting in an orthotropic irradiated Young's modulus $\bar{\bar{E}}$:

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

IGNIS Closure Models – Elastic Strain

- The irradiated Young's modulus is used to find the mechanical strain:

$$\bar{\varepsilon}_{elastic} = \bar{\bar{J}}_{elastic}\bar{\sigma}$$

$$\bar{\bar{J}}_{elastic} = \begin{pmatrix} 1/E_{xx} & -\nu_{yx}/E_{yy} & -\nu_{zx}/E_{zz} & 0 & 0 & 0 \\ -\nu_{xy}/E_{xx} & 1/E_{yy} & -\nu_{zy}/E_{zz} & 0 & 0 & 0 \\ -\nu_{xz}/E_{xx} & -\nu_{yz}/E_{yy} & 1/E_{zz} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/2G_{yz} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2G_{zx} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2G_{xy} \end{pmatrix}$$

IGNIS Closure Models – Creep Strain

- The creep is a function of the primary, secondary and recoverable creep based on the work of Davies and Bradford

$$\bar{\varepsilon}_{creep} = \bar{\varepsilon}_{creep,p} + \bar{\varepsilon}_{creep,s} + \bar{\varepsilon}_{creep,r}$$

$$\bar{\varepsilon}_{c,p} = k_{cr,p} e^{-k_{cr,p}\gamma} \bar{\bar{J}}_c \int_0^{\gamma} \frac{\alpha_{cr}\bar{\sigma}}{S_{cr}} e^{k_{cr,p}\gamma'} d\gamma'$$

$$\bar{\varepsilon}_{c,s} = \bar{\bar{J}}_c \int_0^{\gamma} \frac{\beta_{cr}\bar{\sigma}}{S_{cr}} d\gamma'$$

$$\bar{\varepsilon}_{c,r} = k_{cr,r} e^{-k_{cr,r}\gamma} \bar{\bar{J}}_c \int_0^{\gamma} \frac{\omega_{cr}\bar{\sigma}}{S_{cr}} e^{k_{cr,r}\gamma'} d\gamma'$$

$$\bar{\bar{J}}_c = \begin{pmatrix} \frac{1}{E_{x,0}} & -\frac{\nu_{yx,c}}{E_{y,0}} & -\frac{\nu_{zx,c}}{E_{z,0}} & 0 & 0 & 0 \\ -\frac{\nu_{xy,c}}{E_{x,0}} & \frac{1}{E_{y,0}} & -\frac{\nu_{zy,c}}{E_{z,0}} & 0 & 0 & 0 \\ -\frac{\nu_{xz,c}}{E_{x,0}} & -\frac{\nu_{yz,c}}{E_{y,0}} & \frac{1}{E_{z,0}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2G_{xy,0}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2G_{yz,0}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2G_{xz,0}} \end{pmatrix}$$

IGNIS Closure Models – Creep Strain

- 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

$$\bar{\bar{J}}_{creep} = \bar{\bar{J}}_{creep,p} + \bar{\bar{J}}_{creep,s} + \bar{\bar{J}}_{creep,r}$$

[[

]]P

IGNIS Closure Models – Thermal Strain

- Based on the work of Bradford and Steer the irradiated thermal strain can be found by:

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

- Due to the anisotropic nature of graphite:

[[

]]P

IGNIS Closure Models – Thermal Strain

- The thermal compliance matrix can be found with the previously calculated compliance matrices.

[[ ]]^{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.
  - [[

]]P

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?

[[

]]P