Finite Element Based Surrogate Modeling and Irradiation Capsule Optimization for Large-Scale Neutron Irradiation Campaigns

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INTRODUCTION

Qualification of new materials for novel reactor designs requires experimental measurements of irradiation-dependent property changes such as thermal conductivity, swelling, stored energy, and tensile strength. Measurements of these properties are performed over a range of temperature and neutron fluence conditions in order to fully characterize thermophysical property changes for use in reactor analysis codes and in obtaining regulatory license approval. X-Energy and Oak Ridge National Laboratory (ORNL) have partnered under the US Department of Energy Advanced Reactor Concepts (ARC) program to perform a large-scale irradiation campaign to qualify a graphite for use in X-Energy's Xe-100 pebble-bed high-temperature gas-cooled reactor. This collaboration will irradiate graphite samples in the ORNL High Flux Isotope Reactor (HFIR) under specific temperature and neutron fluence conditions to encompass the operational envelope anticipated in the Xe-100 reactor. Post-irradiation mechanical testing will subsequently be performed on the graphite specimens to generate irradiation-induced property change data pursuant to the ASME Boiler and Pressure Vessel (B&PV) code recommendations.

Material irradiations in HFIR are typically achieved using small uninstrumented capsules colloquially referred to as *rabbits*, which are placed within the HFIR flux trap (FT), where fast neutron flux is maximized [1]. The material under investigation is machined into small specimens (disks in this case) and arranged in the center of the rabbit, inside of a hollow cylinder-shaped component called a *holder*. The temperature of the specimens within the holder is determined from several capsule design variables, including the choice of holder material, the radial distance between the holder and capsule wall (also referred to as the gas gap), gas thermal conductivity, and location in the FT. Finite element analysis (FEA) using ANSYS® is performed to predict specimen temperatures in the capsule using previously calculated material heat generation rates and boundary conditions imposed by the HFIR coolant. Design variables are then iteratively modified until the desired temperature is achieved in the specimen components.

The experimental scope for this campaign requires irradiating over a range of temperatures and neutron fluences that graphite will experience over the material's expected operational lifetime. Selection of these conditions, specimen geometry, and post-irradiation characterization has been developed according to the requirements provided in the ASME B&PV code, Section III Division 5 [2]. Multiple specimens are required for each experimental condition in order to achieve statistically significant measurements, but the limited internal volume (4.1 cm^3) of the irradiation capsules requires specimens to be distributed among many (> 100) rabbits. The large number of capsules can result in HFIR FT loading difficulties due to the reactor's limited space, particularly when there are additional campaigns competing for neutrons. To meet the campaign schedule, every position in the FT must be utilized. However, placing irradiation capsules at the FT's axial periphery can lead to large temperature distributions across specimens within the same rabbit, as well as variations between rabbits with similar design goals. Additionally, peripheral FT positions receive lower fast neutron flux, requiring longer irradiation times to reach required doses.

Traditionally, rabbits are designed by preselecting three variables (material, gas composition, location), modeling using FEA, and iteratively updating a fourth design variable (gas gap) until a desired temperature is achieved. This approach is not only time intensive but lacks the capability to explore all possible design options. Additionally, this technique decouples rabbit thermal modeling from neutron dose rate location dependence and location availability in the FT. To accommodate such large-scale irradiation campaigns, higher-level modeling is needed to not only accurately predict and optimize specimen conditions within each capsule, but to also account for the neutron dose rate axial profile and to forecast FT availability over many reactor cycles.

The first step in developing higher-level irradiation capsule models is to build parameterized thermal models, allowing for primary design variables to be explored and optimized according to the goals of the campaign. However, solving FEA models for an irradiation capsule can be time intensive, and solving for every possible combination of design variable is prohibitive. The work presented here

describes development of a surrogate model for predicting the thermal performance of irradiation capsules in HFIR. Use of this surrogate model allows for the complete exploration and optimization of rabbit design variables by fitting response surfaces to the outputs of FEA models.

METHODS

Irradiation Capsule Design

Surrogate modeling of irradiation capsules begins with development of robust finite element models of the heat equation for a specific design based on the physical shape of specimens. Capsules placed in the HFIR flux trap generally consist of three primary components: specimens, a holder, and a housing. Specimens are small parts fabricated from an experimental material of interest and are arranged tightly within the holder. The holder is a hollow cylindrical component made from a material with well-characterized thermophysical properties that is machined to a precise outer diameter to control temperature in the capsule via an insulating gas gap. The housing is a hermetically sealed, fixed-size, aluminum cylindrical enclosure containing all capsule components and is in direct contact with the HFIR coolant.

Computer assisted design (CAD) models of these three primary components (Figure 1, left), along with secondary parts such as centering thimbles, small wires for aligning parts, and passive SiC thermometry for post-irradiation temperature measurement [3] were imported into ANSYS® finite element simulation software for steady-state thermal analysis. A 2-D axisymmetric geometry was created from the CAD model to reduce the problem's computational complexity (Figure 1, right). Material properties were assigned to each component, along with the heat generation rates determined from prior reactor neutronics calculations, and a convective heat transfer condition was applied to the aluminum housing surface based on separate thermal hydraulic calculations. Customized contact libraries [4] were used to model heat transfer between parts in close proximity by calculating thermally expanded gas gaps and accounting for thermal jump in lieu of meshing the capsule gas. Solving the finite element models yielded temperature populations for each component, giving important information on specimen average temperature, maximum temperature, and temperature ranges.

Temperatures in the specimens were controlled by selecting holder material, placing capsules closer or farther from the reactor midplane, altering the gas gap between the holder and housing, or changing the composition of the gas within the capsule (generally He, Ar, or a combination of these gases). The thermophysical properties of each holder material—such as melting temperature, thermal conductivity, and thermal expansion—influenced which material could be used in a capsule with a specific temperature goal, and the uniformity of specimen temperatures. Capsule location in the FT determined material heat generation rates in the capsule, with the FT midplane providing the highest heat generation rates. The gas gap distance and thermal conductivity of the fill gas mixture determined the temperature drop between the holder and housing wall, which typically remains within a few degrees of the HFIR coolant temperature (54°C).

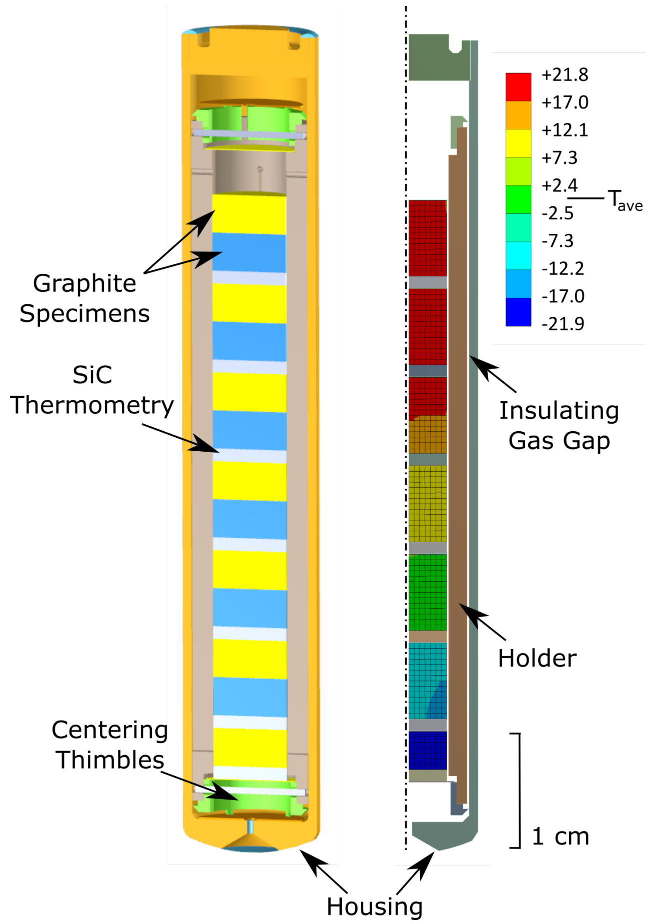

Figure 1. CAD model of rabbit capsule containing graphite disk specimens with primary components labeled (left) and associated 2D-axisymetric model of capsule with a representative graphite specimen temperature overlay from FEA solution (right) with a V-4Cr4Ti holder.

Design of Experiments

After constructing an FEA model of capsule components, a design of experiments was established to understand temperature response as a function of design variables. A design of experiments is a systematic approach to surrogate model development where individual or combinations of independent variables are perturbed or modified, and the output is observed. Discrete variables in the design of experiments included holder material (Al-6061, V-4Cr4Ti, Mo, or Nb-1Zr) and FT position (between 1 and 7). FT position corresponds to an integer number of

rabbit capsules stacked in the FT, beginning 27.9 cm below the core midplane and increasing 6.55 cm per capsule position, with 1 and 7 corresponding to the lowest and highest vertical positions, respectively, and 4 corresponding to the midplane. The rabbit holder outer diameter (8.9–9.48 mm) and gas composition (0–100 mole % He, balance Ar) were selected as continuous variables.

A central-composite design [5] was applied to each combination of discrete variables (28 combinations in all), giving experiment points at the bounds and midpoints of each continuous variable, for a total of 9 data points per discrete variable combination. FEA models were solved with ANSYS for each experiment point, and temperature results for each capsule component were aggregated for surrogate modeling.

Model Fitting

Thermal results for each ANSYS solution were compiled using custom python scripts and analyzed using a surface response methodology [5]. For each combination of discrete data points, the average temperature of graphite specimens in the capsule was fit to a 2^{nd} order, nondimensionalized polynomial in two dimensions, given by:

$$T = c_0 + c_1 x + c_2 y + c_3 xy + c_4 x^2 + c_5 y^2, \qquad (1)$$

where x corresponds to the holder diameter, and y corresponds to the mole percent of helium in the capsule fill gas (balance Ar). A linear least-squares regression was used to determine the coefficients of this function. A similar least-squares regression was performed on specimen temperature range, defined as the difference between the maximum and minimum temperatures of all specimens in a single capsule. Coefficients of the T_{ave} response surface were then used to solve for design diameters and fill gas compositions which yield a specific average temperature in the capsule specimens. Finding these corresponding values on the temperature range response surface then gave the anticipated specimen temperature range in the capsule.

RESULTS

Using the temperature conditions (T_1, T_2, T_3, and T_4, in order of increasing temperature) specified for this graphite irradiation, isothermal curves for each reactor position and holder material were calculated by solving the polynomials described above. A sample of results using this process for V-4Cr4Ti holders in FT positions 1–4 can be seen in Figure 2. The lower figure 2(b) depicts holder diameter/fill gas combinations which achieved a given average specimen temperature goal, indicated by different colors for each of the four target temperatures. The width of the lines corresponds to the reactor positions where the irradiation capsules were located in the model. For example, the thickest cyan-colored line in the upper right corner of Figure 2(b) corresponds to fill gas compositions and holder diameters which yield an average specimen temperature of T_1 in position 4 of the FT. Moving to the lower left of the figure, it becomes obvious that larger radial gas gaps (smaller holder diameters) and more thermally insulating fill gas blends (less helium) are required to achieve a higher temperature, particularly if the capsule is located at the FT periphery (position 1).

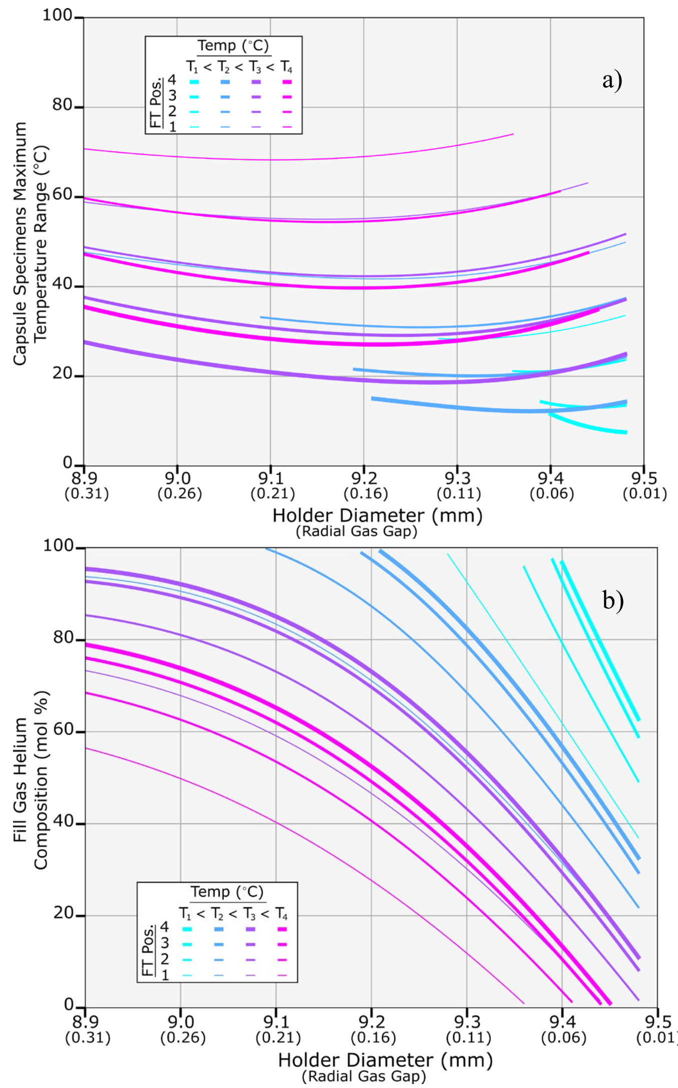

Figure 2. Isothermal curves for various design temperatures and FT positions using a V-4Cr4Ti holder: (a) specimen maximum temperature range within the capsule for the same conditions (b) fill gas composition and gas gap distances which will achieve a target temperature.

Using the isothermal solutions from the average temperature response surface, the maximum specimen temperature range was calculated for the same material and FT position. As Figure 2(a) shows, smaller temperature

ranges were observed in lower temperature capsules and in capsules near the reactor midplane. Moving further from the midplane and to higher capsule temperatures yields larger specimen temperature ranges. However, minima exist for each curve, allowing each discrete design point to be optimized for specimen temperature range. This ability allows direct comparison between holder materials at every reactor position and at every target temperature so that the most effective combination can be chosen. Similar isothermal solutions have been generated for other holder materials and for FT positions 5, 6, and 7.

CONCLUSIONS AND FUTURE WORK

Large-scale material irradiations like the graphite qualification project between ORNL and X-Energy require efficient utilization of all available reactor positions to achieve temperature and fluence experiment goals in a timely manner. Designing and optimizing uninstrumented irradiation capsules for multiple positions using multiple materials and dimensions can be time intensive and unsystematic. This work describes a surrogate model developed to characterize and predict irradiation capsule thermal performance which covers the primary design variables. This model uses a central composite design of experiments to solve FEA models and fit those results to a 2^{nd} order polynomial response surface using linear least square regression. Optimizing the response surfaces for two capsule parameters (average temperature and temperature range) provides confidence that the best capsule designs are being utilized. Future optimization work will expand these techniques to 3-D capsule models and incorporate core dose rate location dependence and discrete reactor position availability.

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