Development and Sensitivity Analysis of a Quantitative Phase-Field Model for Non-Equilibrium U-Zr

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U-Zr fuels are intended to be used in a several sodium fast reactor designs currently under development, but existing metallic fuel performance codes are too reliant on empirical correlations to be used confidently for new designs and safety analyses. Mesoscale methods are beginning to be used to study poorly understood U-Zr behaviors and address deficiencies in our understanding of the system. In the current work, we compile thermodynamic and kinetic properties for the β and γ phases of U-Zr into a quantitative phase-field model for non-equilibrium processes.

We simulate a full diffusion couple experiment and compare the results to published data to identify specific gaps in our current knowledge of the system and provide an objective assessment of our understanding of U-Zr behavior. Direct comparisons of predicted and experimental constituent, interdiffusion flux, and interdiffusion coefficient profiles show that model accuracy could be improved by refining the model's free energies and by accounting for composition dependence in its kinetic parameters.

Sensitivity analysis is then applied to justify recommendations for selection of phase-field modeling parameters and to identify the most impactful experimental data. These studies demonstrate that modeling parameters can be selected to limit their influence on the model's predictions. Results show that kinetic parameters are more influential than interfacial parameters for this type of problem and that model sensitivity is closely related to phase solubility and diffusion-limiting behaviors.

Procedures are established for comparison of quantitative phase-field predictions to diffusion couple experiments. The sensitivity analysis findings will guide future experiments and modeling efforts, promoting collaboration and enabling more efficient allocation of research time and funding. This will accelerate refinement of existing metallic fuel performance codes and expedite U-Zr fuel development.