NUCLEAR ENERGY UNIVERSITY PROGRAMS

Simulations of the Thermodynamic and Diffusion Properties of Actinide Oxide Fuel Materials

PI: Becker, Udo - University of Michigan

Collaborators:
None

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Abstract

Spent nuclear fuel from commercial reactors is comprised of 95-99 percent UO_2 and 1-5 percent fission products and transuranic elements. Certain actinides and fission products are of particular interest in terms of fuel stability, which affects reprocessing and waste materials. The transuranics found in spent nuclear fuels are Np, Pu, Am, and Cm, some of which have long half-lives (e.g., 2.1 million years for ^{237}Np). These actinides can be separated and recycled into new fuel matrices, thereby reducing the nuclear waste inventory.

Oxides of these actinides are isostructural with UO_2, and are expected to form solid solutions. This project will use computational techniques to conduct a comprehensive study on thermodynamic properties of actinide-oxide solid solutions. The goals of this project are to:

- Determine the temperature-dependent mixing properties of actinide-oxide fuels.
- Validate computational methods by comparing results with experimental results.
- Expand research scope to complex (ternary and quaternary) mixed actinide oxide fuels.

After deriving phase diagrams and the stability of solid solutions as a function of temperature and pressure, the project team will determine whether potential phase separations or ordered phases can actually occur by studying diffusion of cations and the kinetics of potential phase separations or ordered phases. In addition, the team will investigate the diffusion of fission product gases that can also have a significant influence on fuel stability. Once the system has been established for binary solid solutions of Th, U, Np, and Pu oxides, the methodology can be quickly applied to new compositions that apply to ternaries and quaternaries, higher actinides (Am, Cm), burnable poisons (B, Gd, Hf), and fission products (Cs, Sr, Tc) to improve reactivity.