NUCLEAR ENERGY UNIVERSITY PROGRAMS

Modeling Fission Product Sorption in Graphite Structures

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Abstract

The goal of this project is to determine changes in adsorption and desorption of fission products to/from nuclear-grade graphite in response to a changing chemical environment. First, the project team will employ principle calculations and thermodynamic analysis to predict stability of fission products on graphite in the presence of structural defects commonly observed in very high-temperature reactor (VHTR) graphites. Desorption rates will be determined as a function of partial pressure of oxygen and iodine, relative humidity, and temperature. They will then carry out experimental characterization to determine the statistical distribution of structural features. This structural information will yield distributions of binding sites to be used as an input for a sorption model. Sorption isotherms calculated under this project will contribute to understanding of the physical bases of the source terms that are used in higher-level codes that model fission product transport and retention in graphite. The project will include the following tasks:

- Perform structural characterization of the VHTR graphite to determine crystallographic phases, defect structures and their distribution, volume fraction of coke, and amount of sp^2 versus sp^3 bonding. This information will be used as guidance for *ab initio* modeling and as input for sorptivity models..
- Perform *ab initio* calculations of binding energies to determine stability of fission products on the different sorption sites present in nuclear graphite microstructures. The project will use density functional theory (DFT) methods to calculate binding energies in vacuum and in oxidizing environments. The team will also calculate stability of iodine complexes with fission products on graphite sorption sites.
- Model graphite sorption isotherms to quantify concentration of fission products in graphite. The binding energies will be combined with a Langmuir isotherm statistical model to predict the sorbed concentration of fission products on each type of graphite site. The model will include multiple simultaneous adsorbing species, which will allow for competitive adsorption effects between different fission product species and O and OH (for modeling accident conditions).