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Sorption Modeling and Verification for Off-Gas Treatment

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Program: Fuel Cycle R&D

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ABSTRACT

This project is focused on the development of modeling tools for off-gas capture from nuclearfuel recycling facilities. Target species include iodine, krypton, xenon, tritium, and carbon dioxide. This work will engage experts in adsorption and absorption to extend capabilities to develop open-source models that address goals of the Off-Gas Sigma Team and the Safeguarded Separations (SafeSeps) element of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. The proposed effort will extend available models and algorithms developed for gas sorption, and the results will be used to provide recommendations on a path forward for the development of sorbents and sorption processes for off-gas treatment.

Literature reports of iodine adsorption based on silver-exchanged inorganic sorbents will be initially used to guide model development efforts. Relevant data also exist for adsorption of noble gases, for tritium removal by adsorption, and for carbon removal by absorption due to the widespread applicability of industrial drying and caustic scrubbing processes. Additional experimental data for a wide range of temperature and gas partial pressures will be obtained in this project to complement existing data and aid in model development and verification. Experimental efforts in this project will be coordinated with those of the Off-Gas Sigma Team of the Fuel Cycle R&D Program's Separations and Waste Forms Campaign.

Extending available models and algorithms, this project intends to develop predictive models for simulating dynamic sorption processes of reactive, multi-component systems. Modeling and focused, fundamental experiments will be performed to develop algorithms and obtain parameters that are necessary to predict the performance of each sorbent in a mixture of gases.

The overall objectives of the project are:

1. Develop dynamic, reactive, multi-component adsorption models for iodine, krypton, xenon, and tritium capture. The predictive capabilities of the model will be validated via comparison with adsorption data from fixed-bed experiments.
2. Develop a dynamic absorption model for CO2 absorption in sodium hydroxide solutions. Model development and parameter estimation will be based on experimental information. The reactive, predictive model will be validated via comparison with absorption data obtained from absorption column experiments.