Sorption Modeling and Verification for Off-Gas Treatment

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ABSTRACT:

Objective: This project is focused on the development of modeling tools for off-gas capture from nuclear-fuel recycling facilities. Target species include tritium, iodine, carbon dioxide, krypton, and xenon. The proposed effort will extend models and algorithms developed for gas sorption during the past three years, and the resulting tools will be useful for engineers to develop a path forward for off-gas treatment processes.

Approach: The development of off-gas models supports the goals of the Off-Gas Sigma Team of the Material Recovery & Waste Form Development Campaign of the Fuel Cycle Technologies Program. The Off-Gas Sigma team has four primary volatile radionuclides of interest: iodine-129 (^{129}I), carbon-14 (^{14}C), krypton-85 (^{85}Kr), and tritium (^{3}H). Adsorption modeling for the separation and recovery of these gases can be divided into three main categories at different physical scales: (1) macroscopic mass transport, (2) microscopic kinetics, and (3) microscopic equilibrium. A number of kernels have been developed in the past three years, comprising a FLOCK, i.e., FundamentaL Off-gas Collection of Kernels, which can be used to predict adsorption efficiency of an adsorption bed column for single or multiple adsorbing gas species. The FLOCK will be further developed and expanded in the proposed work to include reaction kinetics for some gaseous species, such as ^{129}I, and experimental information will be obtained to validate the models. Modeling and experimental work on carbon dioxide absorption, which is relevant to ^{14}C separation, will also be performed to yield validated models for flowsheet analysis.

Benefits: Future fuel recycling systems will need to capture volatile fission products from dilute streams with exceedingly high separation factors. Process modeling is expected to accelerate the development of environmentally compliant recycle systems. Models of key unit operations can generate dynamic source terms of gaseous streams and enable prediction of the performance of off-gas treatment components. Models will enable prediction of gaseous emissions of fuel recycling plants under a variety of alternative configurations and operating conditions, resulting in the capability to evaluate options for environmentally acceptable recycle systems. The work proposed will build on the progress made in the past three years to extend the capability to include chemisorption and demonstrate the capability of these multicomponent models for use in flowsheet analysis.