Seminar

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Institute for Plasma Research

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Title: Studies on Cryosorption of Hydrogen Isotopes on Zeolites for Application in Nuclear Fusion Systems

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Abstract

The selective recovery of trace levels of hydrogen isotopologues from helium is crucial to ensure tritium self sufficiency in the fusion reactor. One of the raw materials of the fusion reactor is tritium, a scarce radioactive isotope of hydrogen. This tritium is produced inside the fusion reactor with the aid of breeder blanket systems. The outlet stream from the breeder blanket system consists of trace levels of hydrogen isotopologues in helium gas. The separation and removal of these gases from helium presents a unique challenge due to their identical chemical nature of the hydrogen isotopologues. Adsorption on microporous materials is a promising approach for the selective removal of hydrogen isotopologues from helium enabling reversible hydrogen adsorption by physisorption at low temperatures. Room temperature adsorption is ineffective in the present application because of the absence of hydrogen isotopologues quantum sieving effects and negligible physisorption interactions at higher temperatures. Hence, cryosorption performed at liquid nitrogen temperature (77.4 K) is necessary to achieve reversible and effective hydrogen isotopologues adsorption. In addition, cryosorption enables effective hydrogen isotopologues recovery through rapid desorption kinetics, minimizes permeation of hydrogen isotopologues, reduces energy consumption, and ensures operational simplicity. Hence, cryosorption is considered as the potential technology for the removal of trace levels of hydrogen isotopologues from helium in the tritium extraction system (TES) of the Indian breeder blanket system.

This thesis investigates the adsorption and separation of 100-1000 ppm level hydrogen isotopes such as hydrogen and deuterium in helium using commercial zeolite beads (MS 3A, 5A and 13X) in a cryogenic molecular sieve bed (CMSB) operating at 77.4 K. A numerical model using the extended Langmuir dual-site and linear driving force approach was developed to predict the binary and ternary breakthrough curves for radioactive hydrogen isotopologues removal from helium gas. The heavier isotopologues consistently exhibited higher adsorbent affinities than the lighter ones, which can be attributed to differences in the zero-point energies of the isotopologues. From the insights obtained from the lab experiments and simulations, engineering scale-up design of a large-scale CMSB at International Thermonuclear Experimental Reactor (ITER) relevant conditions has been carried out.

Rapid and precise monitoring of the effluent concentrations in CMSB is challenging due to trace levels of hydrogen isotopes, their similar electronic properties, and identical masses of He and D_2. Hence, Al_2O_3 (activated thermally or with plasma) as well as transition metal (Mn and Ni) impregnated Al_2O_3 based novel gas chromatograph stationary phases were developed for the effective resolution of trace levels of hydrogen isotopes in helium with retention times less than 6 minutes.

In addition to macroscopic adsorption modeling, ab initio quantum mechanical and molecular modeling studies were also performed. Grand canonical Monte Carlo (GCMC) simulations were carried out on zeolites 4A - hydrogen isotopologue systems for evaluating the theoretical adsorption isotherms. The simulation results indicate that isotopic mass and cation number significantly affect equilibrium loading at a given temperature. An ab-initio periodic DFT study on transition metal ions functionalized ZSM-5 was conducted to identify the potential sites for metal ion inclusion and evaluate the hydrogen interaction characteristics with the active sites. Periodic DFT studies on metal ion-modified ZSM-5 revealed a significant improvement in binding energies, increasing from -10 kJ/mol to a range of ~ -45 to -80 kJ/mol, due to enhanced dihydrogen binding on the metal-ion active sites.

The primary findings from this research work highlights that the experiment-simulation dual approach provides rich insights into the nature of interactions, characterization of the active sites, dynamic bed capacities and selectivities. This, in turn, enables the design of an actual CMSB and the optimization of adsorbents for future CMSB applications in both inner and outer fuel cycle systems of a fusion reactor.

References:

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