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MODELING OF A RECTANGULAR CHANNEL MONOLITH REACTOR FOR SORPTION-ENHANCED WATER-GAS SHIFT

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Abstract

As CO_2 concentration levels in the atmosphere are steadily reaching a point of no return, it is paramount that actions are taken towards mitigating emissions by improving the efficiency of existing processes. Sorption-enhanced water-gas shift (SEWGS) combines the water-gas shift reaction with in-situ adsorption of CO_2 on potassium-promoted hydrotalcite (K-HTC). This enables a direct conversion of syngas into separate hot streams of H_2 at feed pressure and CO_2 at regeneration pressure, making the process attractive for pre-combustion carbon capture and storage (CCS) and reduction of greenhouse gas emissions. The current work is evaluating the high-temperature, high-pressure adsorption step of the SEWGS process enhanced by a novel technology which replaces common packed bed reactors with 3D-printed monolithic structures. This approach would enable an overall increase in process productivity. To this extent, innovative dynamic models based on validated competitive adsorption isotherms were developed in this work. COMSOL Multiphysics was used to develop a 1D computational fluid dynamics (CFD) model of adsorption for a fixed bed reactor in order to verify the model accuracy against existing studies. Subsequently, 2D CFD simulations were developed to describe adsorption inside monolith structures, both free and porous regions. The multi-component adsorption isotherm used in the simulations was validated with published breakthrough capacities for CO_2 and H_2O at different pressures. Model predictions are in agreement with expected behavior, as monolith reactors provide a more efficient mass transfer, and will be used to enhance the performance of experimental monolith structures used in SEWGS.

Key words: adsorption isotherm, carbon capture and storage, computational fluid dynamics, sorption-enhanced water-gas shift

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