INTEGRATION OF HIGH-FIDELITY CO_2 SORBENT MODELS AT THE PROCESS SCALE USING DYNAMIC DISCREPANCY

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A high-fidelity model of a mesoporous silica supported, polyethylenimine (PEI)-impregnated solid sorbent for CO_2 capture has been incorporated into a model of a bubbling fluidized bed adsorber using Dynamic Discrepancy Reduced Modeling (DDRM). The sorbent model includes a detailed treatment of transport and amine-CO_2-H_2O interactions based on quantum chemistry calculations. Using a Bayesian approach, we calibrate the sorbent model to Thermogravimetric (TGA) data. Discrepancy functions are included within the diffusion coefficients for diffusive species within the PEI bulk, enabling a 20-fold reduction in model order. Additional discrepancy functions account for non-ideal behavior in the adsorption of CO_2 and H_2O. The discrepancy functions are based on a Gaussian process in the Bayesian Smoothing Splines ANOVA framework, which provides a convenient parametric form for calibration and upscaling. The dynamic discrepancy method for scale-bridging produces probabilistic predictions at larger scales, quantifying uncertainty due to model reduction and the extrapolation inherent in model upscaling. The dynamic discrepancy method is demonstrated using TGA data for a PEI-based sorbent and model of a bubbling fluidized bed adsorber.

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