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ABSTRACT

Design of Carbon Dioxide Adsorption Systems with Machine Learning

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The demand for post-combustion carbon capture and sequestration (CCS) has dramatically increased in the last decade, and it will likely be an indispensable pathway in the overall global reduction of greenhouse gas emissions. Current established CCS technologies and materials are both energy and economically costly for most combustion applications. Therefore, there are opportunities for developing CCS systems design or uncovering materials to scale up the CCS deployment to contribute to the Intergovernmental Panel on Climate Change (IPCC) projections and socioeconomic shared pathways to mitigate atmospheric global warming. The search for new advanced materials for carbon capture (CC) considers the so-called productivity (CCPr), i.e., mols of CO2 per volume of CC-material per cycle for high levels of purity of CO2 recovery. It is possible to also investigate beforehand how those materials would perform energy-wise, otherwise known as the Energy Penalty (PE) (total energy expenditure by the total amount of CO2 mols captured) in the CC-reactor. This work presents a formulation based on the Constructal Theory and Machine Learning to explore how the features of the materials themselves (molecular diffusivity, density, and adsorptivity), the bed packing (effective diffusivity, specific capturing rate, pellets shape, and size), and the geometric configuration of a column packed-bed reactor affects the CC productivity (CCPr) and the energy penalty (PE). The approach is theoretical and numerical. The model takes into account the CO2 mass balance in a prescribed and constant mobile phase flow rate isothermal 1d tubular packed-bed reactor and the coupling with CO2 mass balance at the pellet level, both are saturated porous media. The simulations were performed in a Python code and a commercial software. The model was turned nondimensional, and the influence of the adapted Peclet, Biot, and Damkhöler number on the productivity and energy penalty was investigated employing Machine Learning algorithms such as the random forest (RFR), the polynomial regression, the extreme gradient boosting (XGB) and the artificial neural network (ANN). The results showed how the constructal principle of matching the small-scale flows and adsorption with the macro flow in the column reactor influences the performance and that the materials and design search based on the adopted dimensionless numbers can be more efficient by training the ML codes and using far less computational resources. The findings can be extended to separation systems in general.