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ABSTRACT:

Further Advances in Machine Learning Aided Methodology for Constructal Design of Carbon Capture

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As the global energy transition from fossil hydrocarbons to renewable resources proceeds slower than predicted by Intergovernmental Panel on Climate Change (IPCC) projections, Carbon Capture and Sequestration (CCS) has emerged as a vital pathway to mitigate greenhouse gas emissions even in bioenergy systems (the so called BECSS), which are already advantageous in carbon footprint. While most common CO2 separation relies on liquid absorption, this technology is currently hindered by high energy penalties, low productivity, and generation of waste water. Dry adsorption routes offer a lower-cost alternative, yet identifying optimal materials remains a challenge due to the time-consuming nature of empirical trial-and-error and high cost of the new materials and the coupling with reactor design that takes the most potential of those materials. This paper details the so-called "Materials Informatics" approach that integrates Computational Fluid Dynamics (CFD) with Machine Learning (ML) and Design by Constructal Theory to accelerate the discovery and optimization of high-performance CC reactors either energywise, capture or costwise. The research departs from a one-dimensional, isothermal packed-bed reactor model to simulate chemical species mass balance. The transport phenomena are governed by transient convection-diffusion equations at the macro scale and diffusion at the pellet micro-scale, incorporating a Linear Driving Force (LDF) model and Langmuir isotherms. These equations were solved using an upwind explicit Euler scheme in a Python-based environment and in a commercial CFD calibrated with our own experimental results with low-cost biochar. The simulations and Machine Learning (ML) analysis were conducted using Python and then validated with those experimental data and the commercial CFD software. To generate a comprehensive dataset for the AI components, a Monte-Carlo approach was employed to select 101 numerical experiments from over 1,000 factorial combinations of key parameters, including bed porosity, gas velocity, and reactor length. Performance was evaluated based on two primary metrics: productivity (CCPr) and specific energy penalty (PE). The simulated data served as a training dataframe for several ML predictors, including Artificial Neural Networks (ANN), Random Forest (RFR), and Extreme Gradient Boosting (XGB).

Analytical results demonstrated that the XGB and ANN models provided the best predictive power for productivity, with Mean Absolute Percentage Errors (MAPE) of 25% and 30%, respectively. Conversely, the Random Forest Regressor proved most effective for predicting energy expenditure, achieving a MAPE of only 11%. The model was turned nondimensional, and the influence of the adapted Peclet, Biot, and Damkhöler number on the study of configurations (design) that matched the selected material to enhance the productivity and lower energy penalty This synergistic methodology proves that ML can significantly speed up the exploration of complex design spaces, identifying the requisite features of even "utopic" materials to guide future experimental development and industrial implementation.