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## Predicting Adsorbent Performance for Carbon Capture using Machine Learning Models

Carbon capture is considered to be a promising way to slow down climate change from anthropogenic sources. One of the carbon capture technologies that is being actively researched is adsorption. Given the increasing amount of literature that present novel ideas, being able to predict adsorbents performance based on textural properties is desirable. Machine learning (ML) is used to construct a model to predict adsorbent performance.

Currently, many novel adsorbents are being researched simultaneously. While this is beneficial for adsorption technology, the organization of data varies between papers, as preparation and testing conditions affect the adsorbent performance. Determining the adsorbent data representative of the adsorbent is a difficult challenge, given that the presentation and availability are varied. Thus, there is a need to first determine which parameters are able to represent the adsorbents while being commonly reported in the literature. This presentation starts with a general review of what the textural properties represent, and the different types of adsorbents and their physical representation and key parameters.

A ML model will be created from the gathered adsorbent performance data. The model will use textural properties such as pore diameter and surface area along with the testing pressure and temperature to predict the adsorbent capacity and several isotherm parameters. The capacity will be predicted from several methods. The ML model will directly predict the adsorption capacity as well as predict the isotherm parameters. This will be compared against both the experimental adsorption capacity and the isotherm parameters fitted to the experimental data. This comparison distinguishes whether it is statistically better for the model to directly predict the adsorption capacity or use isotherm parameters. This results in different usages outside of the ML model. Simulation software typically uses either the adsorption capacity directly as an estimate or the isotherm parameters within prebuilt equation. Finally, identifying the effects of the key parameters based on the ML model structure can quicken design by establishing which design parameters should be focused on. Predicting adsorption performance with ML based on the textural properties can avoid extraneous experimental testing, as adsorbents with poorly predicted performance can avoid using additional experiments.

A section is dedicated to examining a sample adsorbent in more detail based on the ML model. Given typical flue gas conditions, the ML model will be evaluated against the experimental and simulated data in the original paper. These conclusions will be used to determine the effectiveness of the ML model.