# Machine Learning and Bayesian Optimization for Integrated Energy Material and Process Design

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With fossil fuels expected to be a significant portion of the world's energy mix for the near future, it is important to minimize $CO_2$ emissions from current power plants through carbon capture and sequestration (CCS). In post-combustion CCS, $CO_2$ is separated from the power plant flue gas emissions, containing mainly $N_2$ and $CO_2$. Of the technologies currently available for CCS, pressure swing adsorption (PSA) is one of the more promising due to low energy requirements and short cycle times compared to other adsorption based technologies. However, one challenge that exists in using PSA for CCS is designing the cycle to match newly developed materials for this application. Although the steps in all PSA cycles can be classified into six different possibilities (pressurization, feed, depressurization, light reflux, heavy reflux and pressure equilibration), the arrangement of the steps and interactions between steps lead to hundreds of potential different combinations. The objective of this work is to develop a new approach that is capable of synthesizing PSA cycles to capture the CO2 from flue gas at the required purities and recoveries while minimizing energy requirements and maximizing adsorbent productivities.

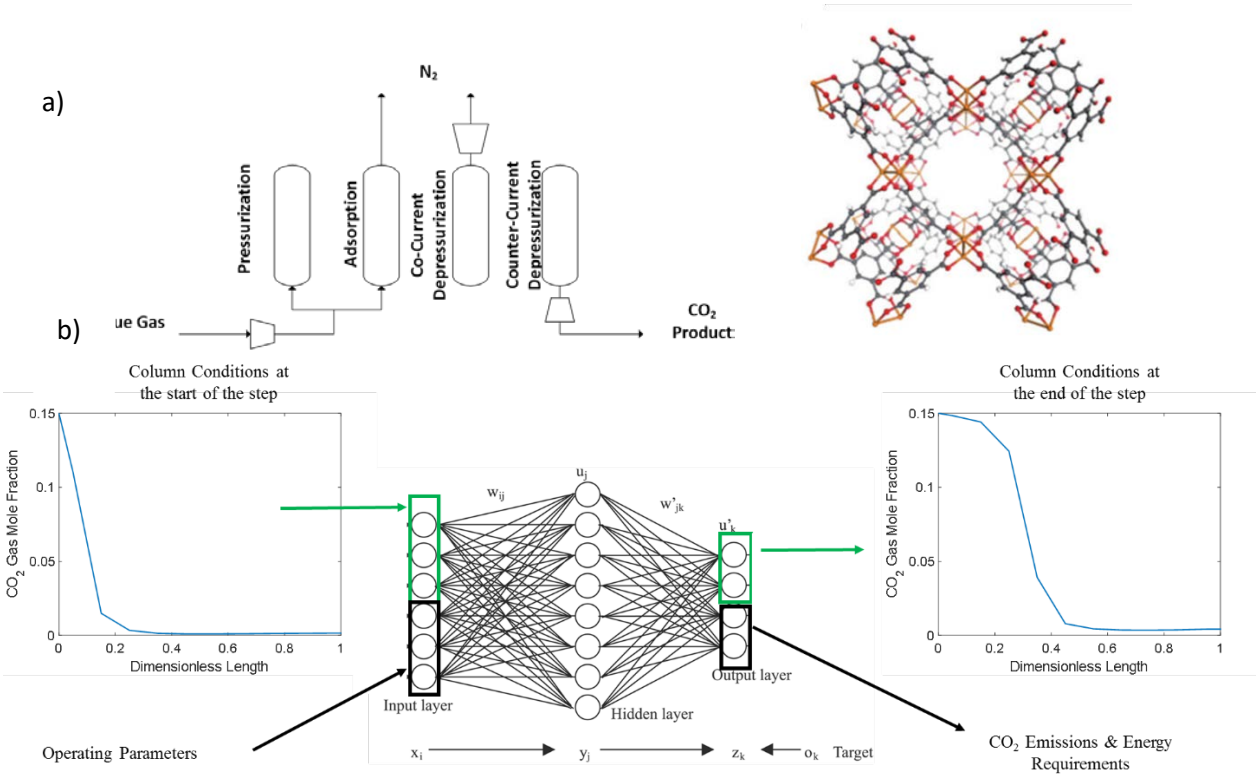

**Figure 1.** (a) Diagram of one potential PSA cycle and the metal organic framework (MOF) material; (b) schematic of the ANN surrogate model. For each step, the ANN surrogate model will take the initial conditions of the column along with operating parameters for that step (e.g. length of column, operating pressure, time length) and will estimate the conditions of the column after the step along with the gas emitted/consumed during the step and the energy requirements.

In this project, our goal is to develop a new framework for synthesizing the PSA cycle with the lowest predicted CO2 capture costs. In this framework, we train artificial neural networks (ANNs) using Bayesian regularization methods as surrogate models for the various PSA steps. The ANNs are trained on simulation data collected from our PSA model consisting of a system of partial differential algebraic equations incorporating mass and energy balances, pressure drop across the column, competitive multi-site Langmuir isotherms and the linear driving force model. With the ANN surrogate models, we propose a mixed integer nonlinear programming model to determine the ideal ordering and duration of steps in order to minimize the energy requirements and maximize the adsorbent productivity. We will evaluate this model with several adsorbents, including Ni-MOF-74, UTSA-16 and zeolite 13X in order to compare the adsorbents under optimized cycle conditions.