

Chemical Engineering Thesis Defense

Open-Source Python Code for Modeling of Adsorption Breakthrough
Performance of Direct Air Capture of CO₂

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Abstract

The objective of this thesis is to create a program in python that can describe the adsorption breakthrough performance of direct air capture of CO₂ by zeolite adsorbents. The purpose of creating this open-source code is because many commercial simulation software for adsorption process simulation can be extremely expensive and typically are yearly subscriptions which can be a costly expenditure for academic research labs and chemical engineers working on adsorption processes development and design. The simulation models are generated by solving the governing mass and energy transfer equations and providing experimental data. The typical inputs for the adsorption process simulation include adsorption equilibrium of both CO₂ and N₂ on selected adsorbents, mass transfer coefficients information, PBR length and void fraction, and other physical and chemical properties of the adsorbent being tested. The outputs of the simulation package are the dimensionless CO₂ concentration profile as a function of dimensionless time, which is usually used for evaluating the adsorbent performance for CO₂ capture. This M.S. research is part of the major research efforts for developing an open-source adsorption process simulation package for carbon capture and conversion in Prof. Deng's group at ASU. The goal of this research is to reduce carbon emissions and develop a sustainable solution for a future carbon-free economy.



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Zoom Link: <https://asu.zoom.us/j/3887586011>