Simulation-Based Analysis of Reactor Performance in Direct Air Capture Applications

Introduction

Carbon dioxide (CO_2) is the most dominant greenhouse gas, largely emitted through the burning of fossil fuels in sectors like electricity generation, cement manufacturing, and chemical processing. With increasing global concern over climate change, numerous technologies have emerged to capture CO_2 emissions. Among them, adsorption-based capture methods have gained attention due to their adaptability and promising performance. Direct Air Capture (DAC) represents a notable approach that targets atmospheric CO_2 directly. However, the success of these systems heavily relies on the design of the reactors and the techniques employed for sorbent regeneration. To improve CO_2 uptake while keeping energy use and costs low, researchers are focusing on advanced reactor engineering, precise control of operating conditions, and efficient regeneration methods. This pursuit has led to the exploration of various reactor types—including fixed-bed, fluidized-bed, and membrane reactors—each suited to particular process conditions. Additionally, regenerating the CO_2-absorbing materials for repeated use is a critical component under active investigation. Techniques such as thermal regeneration, pressure swing, and chemical regeneration present different benefits and trade-offs in terms of energy demand and long-term sustainability.

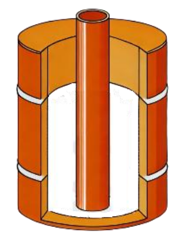

Fig. 1 Schematic of Reactor for Direct Air Capture (DAC) Systems

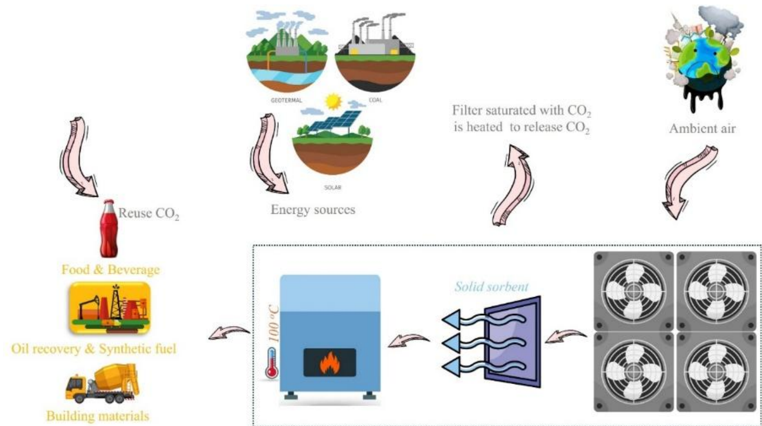

Fig. 2 Process flow of DAC using solid sorbent technology

Problem Statement

Despite ongoing advancements, there remains a significant gap in understanding how different reactor configurations, flow patterns, and thermal management strategies impact the overall performance and energy efficiency of DAC systems. Simulation tools such as CAMSOL and ANSYS provide a powerful means to model and optimize these systems, but comprehensive, validated models tailored for DAC applications are still limited. This project aims to address this gap by developing a detailed simulation model of a DAC reactor using CAMSOL or ANSYS. The objective is to evaluate and optimize parameters such as reactor geometry, airflow velocity, pressure drop, temperature distribution, and sorbent regeneration processes. The ultimate goal is to identify design and operational improvements that can enhance CO_2 capture efficiency while minimizing energy consumption and operational costs.

Research Objectives

1- To analyze the effects of reactor geometry and configuration (e.g., fixed-bed, packed-bed, or membrane-based) on CO_2 capture efficiency.

2- To investigate the impact of airflow dynamics, including velocity, Tmperature, pressure drop, and distribution, on system performance.

Your background

We are looking for excellent master students with a Mechanical Engineering or Sustainable Energy Technology background with a willingness to learn COMSOL Multiphysics/Ansys Fluent.

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