New Materials and Processes for Energy-Efficient Carbon Capture in the Presence of Water Vapor

Investigators
Randall Snurr and Fengqi You, Department of Chemical and Biological Engineering; Joseph Hupp and Omar Farha, Department of Chemistry, Northwestern University

Objective
The goal of this project is to develop new materials and processes for the economical capture of 90 percent of carbon dioxide (CO$_2$) emissions from power plants, with a particular focus on circumventing or overcoming competition from water vapor in the flue gas.

Background
Adsorption is a process that occurs when gas molecules adhere to the surface of a solid or within the channels of a porous solid. Adsorption processes are a promising technology for separating and removing CO$_2$ from combustion flue gas. Compared to traditional separation methods, such as solvent-based absorption, adsorption processes tend to use less energy and have lower operating and capital costs.

A major challenge to adsorption-based technology in power plants is the competitive adsorption of water vapor that is released simultaneously with CO$_2$. A key to solving this challenge is to develop or find a sorbent material that preferentially binds with CO$_2$. For effective carbon capture and separation, the sorbent must meet many stringent requirements, such as high selectivity for CO$_2$ over nitrogen, tolerance to water and impurities (including sulfates), rapid adsorption and desorption kinetics, and durability.

While some porous minerals, such as zeolites, show promise for CO$_2$ separation/removal at high pressure, most materials interact either too weakly or too strongly with CO$_2$ to be effective in combustion flue gas. Weak interactions result in low CO$_2$ capacity, whereas interactions that are too strong require too much energy for sorbent regeneration.

An attractive, emerging class of nanoporous materials is a group of compounds known as metal-organic frameworks (MOFs). MOFs consist of metal ion nodes interconnected by organic linker molecules to form crystalline frameworks, as shown in Figure 1. In contrast to other sorbent materials, MOFs can be prepared in an almost infinite variety of ways, providing enormous design flexibility.

Experiments have shown that MOFs with open metal sites can efficiently capture CO$_2$ from simulated dry flue gas. Unfortunately, the best CO$_2$-binding MOFs to date also interact strongly with water, which typically constitutes about 10 molar percent of industrial flue gas.

A key objective of the research is to identify the efficiency limits of MOF-based adsorption processes for carbon capture and separation with minimal environmental impact and cost.
Approach
The overall approach of this research is to combine materials synthesis and characterization; molecular-level modeling and materials design; and process-level modeling. The premise of the project is that the MOF material and the adsorption process must be developed together.

The research team will design, synthesize, characterize, and test new classes of MOFs to block water uptake yet preserve the otherwise outstanding carbon-capture properties of MOFs. One approach is to consider specially designed pockets that preferentially bind CO₂ over water.

Molecular-level modeling will play a key role in the design and screening of the new MOFs. Researchers will generate a database containing millions of hypothetical MOFs and use computer simulation to evaluate their ability to adsorb molecules of CO₂, nitrogen and water.

In addition, integrated process modeling and optimization will be performed. Adsorption-based separation schemes, such as pressure-, vacuum-, and temperature-swing adsorption (PSA, VSA, and TSA) have been widely used in large-scale separations processes, including air separation. The project will employ advanced process modeling tools and systems optimization techniques to explore the efficiency limits of MOF-based adsorption processes for carbon capture, while minimizing the associated life cycle environmental impact.