the ENERGY lab

PROJECT FACTS

Existing Plants, Emissions & Capture

Carbon Dioxide Separation with Novel Microporous Metal Organic Frameworks

Background

UOP LLC, the University of Michigan, and Northwestern University are collaborating on a three-year program to develop novel microporous metal organic frameworks (MOFs) suitable for CO_2 capture and separation. MOFs are hybrid organic/inorganic structures in which the organic moiety is readily derivatized. This innovative program is using sophisticated molecular modeling to evaluate the structurally diverse, highly porous, thermally stable MOFs, which have shown exceptional storage capacity for methane. Selected MOFs will be optimized for CO_2 selectivity, adsorption capacity, and rates of adsorption and desorption.

Project Description

This partnership of industry and university researchers brings a novel approach and unique depth of experience to the problem of CO_2 separation and capture. The University of Michigan has extensive experience in the discovery and tailoring of novel MOFs for adsorption of gases, such as methane and hydrogen. In this project, the use of MOFs will be extended to CO_2 separation. UOP is a global leader in process chemistry and has developed a broad portfolio of technologies for separating CO_2 from gas streams. Northwestern University will provide expertise on molecular modeling.

MOFs are a structurally diverse family of materials with over 500 having been prepared. This project will use molecular modeling to identify MOFs with the best sorption properties for CO_2 and to predict the structures of new MOFs. Synthesis of the organic linker is an important part of the preparation of novel MOFs. In addition, detailed characterization of the novel materials will be performed to determine the active sorption sites. UOP will perform process modeling and economic analysis of processes designed for the separation and capture of CO_2 from gas mixtures produced by electric utilities.

CONTACTS

Jared P. Ciferno
Technology Manager
Existing Plants, Emissions & Capture
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-5862
jared.ciferno@netl.doe.gov

David Lang
Project Manager
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4881
david.lang @netl.doe.gov

Richard Willis
Principal Investigator
UOP LLC
50 East Algonquin Road
Des Plaines, IL 60016
847-391-3190
Richard.Willis@uop.com

PARTNERS

UOP LLC
University of Michigan
Northwestern University

PERFORMANCE PERIOD

Start Date	End Date
08/05/2004	02/04/2008

COMPLETED

COST

Total Project Value
$900,000

DOE/Non-DOE Share
$900,000 / $0

Goals/Objectives

The primary goal of this project is to develop a low-cost, novel sorbent to remove CO_2 from flue gas and gasifier streams in coal-fueled power plants. The sorbent will have high selectivity, high adsorption capacity, and good adsorption/desorption rates. In addition, the MOFs will be tailored to minimize the CO_2 binding energy in an effort to reduce the energy required for regeneration.

The objectives of the program are:

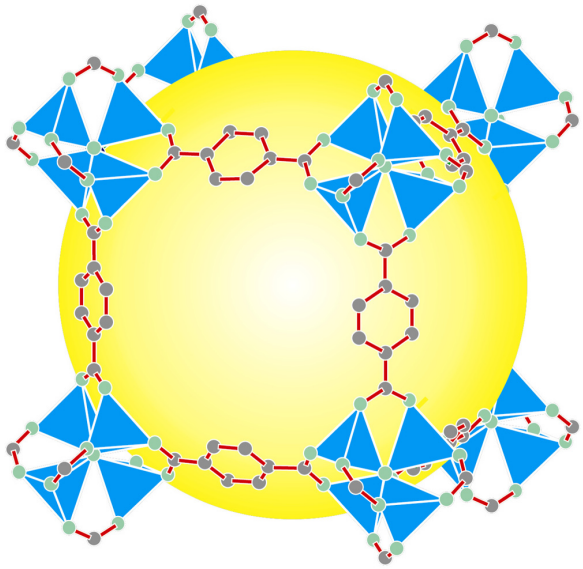
- To develop a theoretical model to predict the structure of MOFs with good CO_2 sorption properties. This model will allow for the efficient screening of existing MOFs and for the design of new MOFs and the prediction of their sorption properties.
- To develop an understanding of the sorption sites in MOFs.
- To develop MOFs tailored for CO_2 separation from flue gas.
- To develop MOFs tailored for CO_2 separation from gasifier streams.
- To assess the commercial potential of MOFs for separation and capture of CO_2.

Accomplishments

- A broad scoping study on CO_2, CH_4, and N_2 sorption properties for selected known MOFs was performed.
- A Theoretical Virtual High Throughput Screening (VHTS) isotherm model was developed and verified for known MOFs.
- Multiple MOFs with functionalized linkers to aid in CO_2 sorption were prepared and evaluated.
- MOFs based on literature reports were also prepared.
- A method of modeling hydrolysis on MOF materials that correlates with experimental data was developed and refined.
- Raman spectroscopy was developed as a useful tool to characterize MOF sorption behavior and sites.
- The hydrothermal stability and contaminant sensitivity of MOFs was determined. These results were critical in developing flow schemes for the incorporation of MOFs into flue gas and gasification streams.
- Two MOFs were identified for satisfactory pre-combustion CO_2 capture.
- Two MOFs identified for post-combustion CO_2 capture can be further optimized for low-temperature and low-pressure absorption.
- An assessment of the commercial potential for MOFs in gasifiers for pre-combustion CO_2 capture was performed.
- A preliminary techno-economic study to evaluate the capital and operating expenses for a MOF CO_2 capture process on synthesis gas in an IGCC power plant was completed.

Benefits

Although oil production in the U.S. has been gradually declining, there are huge reserves of coal available. Unfortunately, when coal is burned, it releases more CO_2 per unit of heat than any other fossil fuel, and anthropogenic CO_2 is believed to be contributing to global warming and climate change. Successful completion of this program could lead to a low-cost, novel sorbent to remove CO_2 from flue gas and gasifier streams in electric power plants. The captured CO_2 could then be sequestered to prevent its emission to the atmosphere. This would enable the use of our coal reserves as an energy source without contributing to global warming, while simultaneously creating jobs and reducing our dependence on imported oil.



Molecular structure of MOF-5

NT42121, August 2010–FINAL