



the **ENERGY** lab

## PROJECT FACTS

Existing Plants, Emissions & Capture

# CO<sub>2</sub> Capture from Flue Gas Using Solid Molecular Basket Sorbents

## Background

The mission of the U.S. Department of Energy/National Energy Technology Laboratory (DOE/NETL) Existing Plants, Emissions & Capture (EPEC) Research & Development (R&D) Program is to develop innovative environmental control technologies to enable full use of the nation's vast coal reserves, while at the same time allowing the current fleet of coal-fired power plants to comply with existing and emerging environmental regulations. The EPEC R&D Program portfolio of post- and oxy-combustion carbon dioxide (CO<sub>2</sub>) emissions control technologies and CO<sub>2</sub> compression is focused on advancing technological options for the existing fleet of coal-fired power plants in the event of carbon constraints.

Pulverized coal plants burn coal in air to produce steam and comprise 99 percent of all coal-fired power plants in the United States. CO<sub>2</sub> is exhausted in the flue gas at atmospheric pressure and a concentration of 10–15 percent by volume. Post-combustion separation and capture of CO<sub>2</sub> is a challenging application due to the low pressure and dilute concentration of CO<sub>2</sub> in the waste stream, trace impurities in the flue gas (nitrogen oxides, sulfur oxides, and particulate matter) that affect removal processes, and the parasitic energy cost associated with the capture and compression of CO<sub>2</sub>. An effective post-combustion CO<sub>2</sub> control technology being investigated for the capture of CO<sub>2</sub> from flue gas is the use of novel nanoporous polymer-based sorbents with high CO<sub>2</sub> adsorption capacities for application to existing and future power plants.

## Project Description

Pennsylvania State University (PSU) will develop a new generation of solid polymer-based sorbents for more efficient capture and separation of CO<sub>2</sub> from flue gas of coal-fired power plants. The project is based on the concept of a molecular basket sorbent (MBS), which was invented and developed at PSU. The idea of MBS development is to load CO<sub>2</sub>-philic polymers onto high surface area nanoporous materials. This process increases the number of approachable sorption sites on/in the sorbent and enhances the sorption/desorption rate by increasing the gas-sorbent contacting interface and by improving the mass transfer in the sorption/desorption process. The expected result of this project will be a concentrated CO<sub>2</sub> stream that can be directed to CO<sub>2</sub> sequestration or CO<sub>2</sub> utilization.

Development of the new generation of MBS involves the selection of the best performing, most cost-effective CO<sub>2</sub>-philic polymer and nanoporous materials. Different types of nanoporous materials will be purchased as support materials. A series of polymers will be immobilized in the nanoporous materials to prepare different sorbents. The prepared sorbents will be tested and evaluated for CO<sub>2</sub> capture in a fixed-bed flow system. The promising MBSs will be further characterized to determine their structure; surface properties; thermal, physical, and chemical properties; and CO<sub>2</sub>-sorption/desorption properties. Advanced molecular modeling will be used to facilitate the screening of the polymer sorbents and the design of novel polymers. Computational results will be utilized to guide project experimental approaches. A techno-economic analysis will also be performed on the new MBSs and CO<sub>2</sub> capture process. The analysis will focus on energy consumption and the cost of the sorbents in comparison to a conventional post-combustion CO<sub>2</sub> capture process.

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## PERIOD OF PERFORMANCE

Start Date	End Date
09/01/2009	08/31/2012

## COST

### Total Project Value

\$571,291

### DOE/Non-DOE Share

\$456,992 / \$114,299

## AWARD NUMBER

DE-FE0000458

## NATIONAL ENERGY TECHNOLOGY LABORATORY

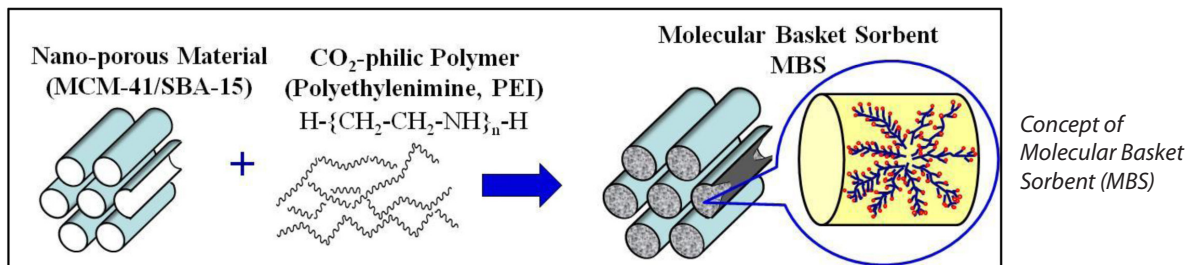
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## Project Goal

The project goal is to develop a new generation of solid polymer-based sorbents that can be used to capture and separate CO<sub>2</sub> from coal-fired power plant flue gas in an energy-efficient, economical, and environmentally-friendly manner.

## Objectives

The project objectives are to develop MBSs that have regenerable working sorption capacities higher than 70 milligrams of CO<sub>2</sub> per gram of sorbent, and to lower the sorbent preparation cost by 30 percent compared to the first and second generations of MBSs.

## Planned Activities

PSU will develop sorbent formulations, test developed MBSs, and analyze the effect of physical and chemical properties of the sorbents on the CO<sub>2</sub> sorption performance. Specific activities include:

- Optimizing the combination of CO<sub>2</sub>-philic polymers and nanoporous materials to further enhance CO<sub>2</sub> sorption capacity.
- Researching inexpensive and commercially available materials for preparation of the new generation of MBS to significantly reduce the sorbent cost.
- Evaluating the sorption performance of the developed MBSs in a laboratory-scale fixed-bed sorption system, including the capacity, selectivity, regenerability, and stability; and determining the best conditions for sorption and desorption.
- Improving the thermal stability of the developed MBSs through the cross-linking method.
- Conducting a computational chemistry approach to estimate the heats of sorption of CO<sub>2</sub> on different MBSs and the kinetic barriers for the diffusion of CO<sub>2</sub> sorbate in the bulk of the sorbent for fundamental understanding of the sorption mechanism, which can benefit the development, design, and modification of the sorbents and the process.
- On the basis of the experimental data, conducting a preliminary technical and economic analysis of the developed sorbent and process.

## Accomplishments

- Four types of nanoporous materials were selected for evaluation: silica gels, mesocellular silica foam (MCF), nanostructured fumed silica (FS), and hexagonal mesoporous silica (HMS).
- Several samples of each type of material were examined to determine the effect of various parameters, including pore size and particle size, and the molecular weight and loading of the polymer sorbent utilized (polyethylenimine [PEI]) on the sorption performance.
- For each material type the most favorable samples were selected and the best PEI molecular weight and PEI loading were determined for preparation of the MBSs for testing.
- Each prepared MBS was evaluated in a fixed-bed sorption system using simulated flue gas to obtain CO<sub>2</sub> sorption breakthrough curves, and measure CO<sub>2</sub> sorption breakthrough capacity and saturation capacity.
- Various crosslinking agents were investigated to improve the thermal stability of the PEI sorbent.
- The Temperature Programmed Desorption method was utilized to study the CO<sub>2</sub> sorption mechanism.

## Benefits

This project will provide valuable data on new material synthesis and preparation, novel process and operational experience on CO<sub>2</sub> capture, and processes of interest for application to large scale power plant flue gas control systems. The optimization of molecular basket sorbent performance to increase post-combustion CO<sub>2</sub> capture while significantly lowering costs can benefit both existing and new coal-fired power plants. Additionally, cost effective CO<sub>2</sub> capture will significantly contribute to the viability of power generation from the nation's abundant supplies of coal, thus enhancing U.S. energy security.