



PROJECT FACTS

Existing Plants,  
Emissions & Capture

# Ionic Liquids: Breakthrough Absorption Technology for Post-Combustion CO<sub>2</sub> Capture

## Background

Development of innovative environmental control technologies is key for maintaining coal as an affordable and environmentally sound energy source. Carbon dioxide (CO<sub>2</sub>) emissions control technologies, specifically post-combustion CO<sub>2</sub> capture, for coal-fired power plants is a major focus area in addressing climate change concerns. Post combustion CO<sub>2</sub> capture from flue gas is technically challenging as large volumes of gas at atmospheric pressure and with low CO<sub>2</sub> concentrations (10 to 15 volume percent) needs to be treated. In spite of this difficulty, post-combustion CO<sub>2</sub> capture offers the greatest near-term potential for reducing greenhouse gas emissions as the technology can be retrofitted to existing units and tuned for various capture levels.

One area of interest in post-combustion CO<sub>2</sub> capture is the use of solvent-based systems, which involves chemical or physical sorption of CO<sub>2</sub> from flue gas into a liquid carrier. Solvent-based systems are being used today for scrubbing CO<sub>2</sub> from industrial flue gases and process gases; however, scaling this type of CO<sub>2</sub> capture system to the size required for processing the large volumes of flue gas produced by a pulverized coal (PC) plant has not been achieved. DOE is funding research to develop low-cost and efficient, solvent-based CO<sub>2</sub> capture technologies that can significantly reduce CO<sub>2</sub> emissions from existing PC power plants.

## Description

The University of Notre Dame and its partners are working to continue development of novel ionic liquid absorbents and an associated process for the removal of CO<sub>2</sub> from coal-fired power plant flue gas. Ionic liquids (ILs) are salts that are liquid in their pure state near ambient conditions. In a previous NETL-funded project, Notre Dame demonstrated that ionic liquids can be engineered to have very high physical solubilities and can also be made to form chemical complexes with CO<sub>2</sub>. Due to their chemical diversity, ample opportunities should exist to tailor and optimize the properties of ionic liquids for CO<sub>2</sub> capture. Having shown their potential in the previous project, researchers will work in this project to take the next step in the development process.

In Phase I, the University of Notre Dame will carry out atomistic-level computer simulations of a series of ionic liquids and functional groups along with flue gas species. This will give researchers insight into what chemical and structural features will lead to favorable properties. Simultaneously, researchers will investigate known CO<sub>2</sub> - philic moieties, carry out synthesis of new ionic liquids,

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## PERFORMANCE PERIOD

Start Date	End Date
03/01/07	07/31/2011

## COST

**Total Project Value**  
\$3,641,420  
**DOE/Non-DOE Share**  
\$2,447,138 / \$1,194,282

## PARTNERS

University of Notre Dame  
Trimeric Corporation  
The Babcock and Wilcox Company  
DTE Energy  
Merck KGaA



and make preliminary measurements of physical properties and phase behavior. They will also begin work on setting up the process model for the system. In Phase II, researchers will refine development efforts for the “optimal” absorbent, exhaustively measure or estimate all relevant properties, and use this information to complete a detailed systems and economic analysis study. In Phase III, researchers will finalize the optimal ionic liquid(s), design a laboratory-scale test system, and continue to refine systems and economic analyses. During Phase IV, Notre Dame will construct and operate the lab-scale test system, finalize systems and economic analyses, and develop a path forward for pilot-scale testing and commercialization.

## Primary Project Goal

The overall goal of the project is to develop a new ionic liquid absorbent and accompanying process for post-combustion capture of CO<sub>2</sub> from coal-fired power plants with 90 percent capture efficiency and less than a 35 percent increase in the cost of energy services.

## Objectives

- Design and synthesize one or more ionic liquid absorbents having physical properties tailored for post-combustion CO<sub>2</sub> capture.
- Perform atomistic-level classical and quantum calculations to engineer ionic liquid structures that maximize CO<sub>2</sub> carrying capacity while minimizing regeneration costs.
- Measure or accurately estimate all physical properties of the ionic liquid that are essential for detailed engineering and design calculation.
- Complete a detailed systems and economic analysis.
- Demonstrate the CO<sub>2</sub> capture process with a continuous lab-scale unit.
- Develop a path forward for commercialization.

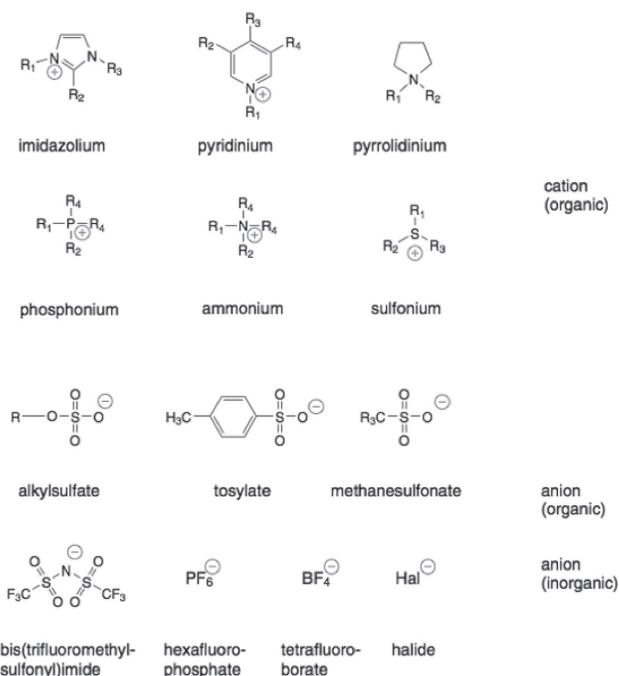
## Benefits

For CO<sub>2</sub> capture to become economically feasible, improved capture processes are needed. The use of ionic liquids as CO<sub>2</sub> absorbents holds promise for reducing costs by developing a process with higher CO<sub>2</sub> loading in the circulating liquid and lower heat requirements for regeneration. Both these effects would lower process costs.

## Accomplishments

- Synthesized and tested a total of 17 new “Generation 1” ionic liquids during the first year of the project; synthesized a total of 7 “Generation 2” ionic liquids during the second year of the project.

- Developed molecular modeling techniques that have enabled Notre Dame researchers to compute key properties of ionic liquids from first principles.
- Developed a way to tune the binding strength of CO<sub>2</sub> to optimize the ILs using process modeling as a guide.
- Developed unique experimental techniques, including the ability to monitor the infrared spectrum of the ionic liquid as it absorbs CO<sub>2</sub>, and then use this information to determine reaction rates and mechanisms.
- Evaluated alternative process configurations; selected a viscosity modified absorber stripper process for continued study.
- Completed assembly of a bench-scale absorber test system and initiated preliminary testing.
- Developed a detailed understanding of the mechanism responsible for the large viscosity increase observed upon complexing CO<sub>2</sub>, and designed new molecules that do not show viscosity increases.
- Synthesized several “Generation 3” ILs that exhibit low viscosity and do not demonstrate a significant increase in viscosity upon reaction with CO<sub>2</sub>, unlike the case with “Generation 2” ILs.



Examples of commercially available ionic liquids.

