PROJECT facts

U.S. DEPARTMENT OF ENERGY
OFFICE OF FOSSIL ENERGY
NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Sequestration

08/2007

IONIC LIQUIDS: BREAKTHROUGH ABSORPTION TECHNOLOGY FOR POST-COMBUSTION CO_2 CAPTURE

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Background

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_2 from coal-fired power plant flue gas. Ionic liquids 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 chemically complex CO_2. Due to their chemical diversity, ample opportunities should exist to tailor and optimize the properties of ionic liquids for CO_2 capture. Having shown their potential in the previous project, researchers will work in this project to take the next step in the development process.

Description

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_2 - phillic moieties, carry out synthesis of new ionic liquids, and make preliminary measurements of physical properties and phase behavior. We will also begin work on setting up the process model for the system. In Phase II, we will refine our 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. We will also design a lab-scale continuous absorption and regeneration system. During Phase III, we will construct and operate the lab-scale absorption and regeneration system, finalize process designs 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 that enables 90% of the post-combustion CO_2 to be removed from a coal-fired power plant while attaining the 2012 capture cost target of less than a 20% increase in the cost of energy services according to the NETL Carbon Capture and Sequestration Systems Analysis Guidelines.

PARTNERS

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

PROJECT DURATION

03/01/07 to 06/30/10

COST

Total Project Value
$3,005,165

DOE/Non-DOE Share
$2,221,304 / $793,861

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Objectives

- Design and synthesize one or more ionic liquid absorbents having physical properties tailored for post-combustion CO_2 capture.
- Perform atomistic-level classical and quantum calculations to engineer ionic liquid structures that maximize CO_2 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_2 capture process with a continuous lab-scale unit.
- Develop a path forward for commercialization.

Benefits

If CO_2 capture is ever to become economically feasible, improved capture processes are needed. The use of ionic liquids as CO_2 absorbents holds promise for reducing costs by developing a process with higher CO_2 loading in the circulating liquid and lower heat requirements for regeneration. Both these effects would lower process costs.

Accomplishments

This is a new project. To date, researchers have initiated molecular modeling efforts and have already obtained quantitative agreement between simulated and experimental liquid densities for one ionic liquid. Researchers have also synthesized three new ionic liquids.