PROJECT facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Carbon Sequestration

04/2008

Design and Evaluation of Ionic Liquids as Novel Absorbents

CONTACTS

Sean Plasynski
Sequestration Technology Manager
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236
412-386-4867
sean.plasynski@netl.doe.gov

José Figueroa
Project Manager
National Energy Technology Laboratory
626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4966
jose.figueroa@netl.doe.gov

Edward Maginn
Principal Investigator
182 Fitzpatrick Hall
Dept. of Chem. & Biomolec. Eng.
University of Notre Dame
St. Joseph County, IN 46556
574-631-5687
ed@nd.edu

Background

There is growing concern among climate scientists that the buildup of greenhouse gases (GHG), particularly carbon dioxide (CO_2), in the atmosphere is affecting the global climate in ways that could have serious consequences. One approach to reducing GHG emissions is to scrub CO_2 from the flue gas of power plants and sequester it in geologic formations. Although it is technically feasible to remove CO_2 from flue gas, current processes are too expensive. New, less expensive processes are needed. This project is investigating the feasibility of using a novel class of compounds – ionic liquids – for the capture of CO_2 from the flue gas from coal and natural gas–fired power plants. The success of ionic liquids technology will be based on increasing the knowledge base on the chemical characteristics of ionic liquids and on the competitiveness of processes which utilize ionic liquid based absorbents for CO_2 capture from flue gas streams compared to commercial amine-based technologies. The successful ionic liquid absorbent will have high CO_2 selectivity and capacity (i.e., a Henry's law constant lower than 10 bar) with a low energy requirement for regeneration (i.e., an enthalpy of absorption less than 60 kJ/mol).

Description

The fundamental factors influencing the absorption of CO_2 and other gases present in flue gas streams will be determined, relevant thermo-physical and phase behavior properties measured, and a preliminary process design for the use of ionic liquids in an absorption separation system developed.

Primary Project Goal

The primary goal of this project is to provide a comprehensive evaluation of the feasibility of using a novel class of compounds – ionic liquids – for the capture of CO_2 from the flue gas of coal and natural gas – fired power plants.

Objectives

The objectives of the project are to:

- Produce a range of ionic liquid sorbents for further evaluation.
- Determine the fundamental factors influencing the absorption of CO_2 and other gases present in flue gas streams.

PARTNERS

University of Notre Dame

PERFORMANCE PERIOD

07/16/2004 to 07/15/2007

COST

Total Project Value
$434,076

DOE/Non-DOE Share
$434,076 / $0

ADDRESS

National Energy Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South
Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

One West Third Street,
Suite 1400
Tulsa, OK 74103-3519
918-699-2000

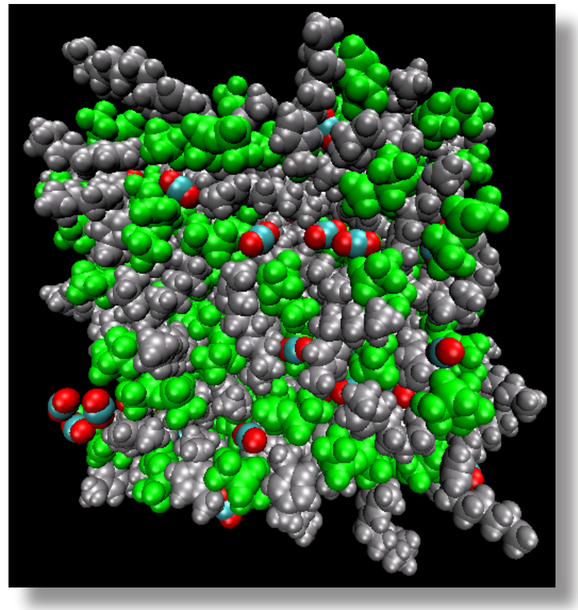
CUSTOMER SERVICE

1-800-553-7681

WEBSITE

www.netl.doe.gov

- Determine relevant thermo-physical and phase behavior properties.
- Develop a preliminary process design that uses ionic liquids in an absorption separation system.



Model of CO_2 absorption by an ionic liquid. The model shows that the anions are controlling absorption in ionic liquids. The green units represent anions and the grey units represent cations.

Benefits

If CO_2 capture from flue gas is 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 of these effects would lower process costs.

Accomplishments

Eleven ionic liquids have been synthesized or acquired. CO_2 solubility has been measured for five of these compounds, with 1-n-hexyl-3-methylimidazolium tris (pentafluoroethyl) trifluorophosphate showing the best performance to date, having a Henry's constant of 25 bar at 25 ^{o}C. By measuring the solubility of other gases in these liquids, including oxygen, ethylene and ethane, it was found that CO_2 is significantly more soluble in these ionic liquids than any of these other gases, Figure 1. Other physical properties, including viscosity and density, have been measured for these compounds. The viscosities vary widely at low temperature, but all fall to reasonable values above 40 ^{o}C.

First principles quantum mechanics calculations have been conducted to understand the nature of CO_2 absorption in these liquids. The calculations have shown that CO_2 associates primarily with the anion, but that the anion primarily associates with the cation. Thus, the CO_2 interacts most strongly with the secondary negatively charged regions of the anion, suggesting that greater negative charge delocalization could lead to enhanced CO_2 solubility. These concepts are being used to identify new targets for synthesis and testing.

Research has also demonstrated that SO_2 is highly soluble in ionic liquids, being 8 to 25 times more soluble than CO_2, depending upon pressure. NETL researchers have proven that ionic liquids can be used as the separating media in supported liquid membranes to separate CO_2.