Project Title:

Reversible Ionic Liquids as Double-Action Solvents for Efficient CO_2 Capture

Technology Area:	**Technology Maturity:**
Post-Combustion Solvents	Laboratory-Scale, Simulated Flue Gas

Primary Project Goal:

To develop a novel class of solvents for the recovery of carbon dioxide (CO_2) from post-combustion flue gases that will achieve a substantial increase in CO_2 working capacity with a reduction in cost.

Technical Goals:

- Synthesis of silyl amine-based ionic liquids (ILs) with minimal viscosity.
- Measure heat of absorption and desorption.
- Measure rates of CO_2 absorption and desorption.
- Identify solvents that will consume the minimal amount of energy.
- Use simulation tools, such as ASPEN, to design an economic absorption/desorption process.

Technical Content:

Reversible ionic liquids (RevILs) are neutral molecules that react with CO_2 to form an IL, which then dissolves additional CO_2 by a physisorption mechanism. Subsequently, modest elevations in temperature reverse the reaction and yield pure CO_2 for disposal; because of this dual mode, capacity can be large.

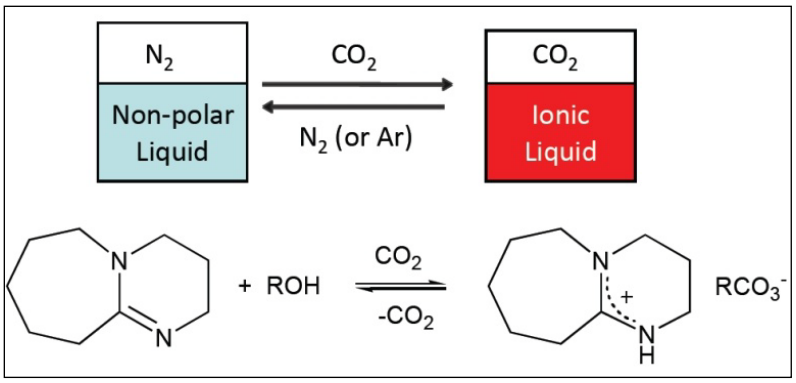

Figure 1: CO_2 Will Switch a Non-Polar Liquid to and Ionic Liquid

In a two-component RevIL, CO_2 at 1 atmosphere acts as a "switch," as shown in Figure 1.

Two-component RevILs have the disadvantage of being too complex and requiring alcohol. Light alcohol would evaporate with the CO_2, while a heavy alcohol would have too much heat capacity. A single component RevIL would eliminate the need for alcohol.

Figure 2 shows an example based on silylated amine. The chemistry must work well in the presence of water, considering that water is a component of flue gas. The RevILs will be tested for their chemical stability with 0% and 10% water present. Stability will also be tested at 4°C, 25°C, and 50°C. High viscosity could also be an issue; however, viscosity in RevILs is highly nonlinear (as shown in Figure 3) and can be reduced with impurities, such as water or dissolved gases.

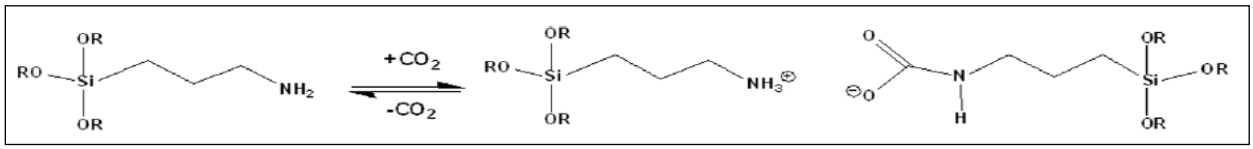

Figure 2: An Example of a Single Component RevIL

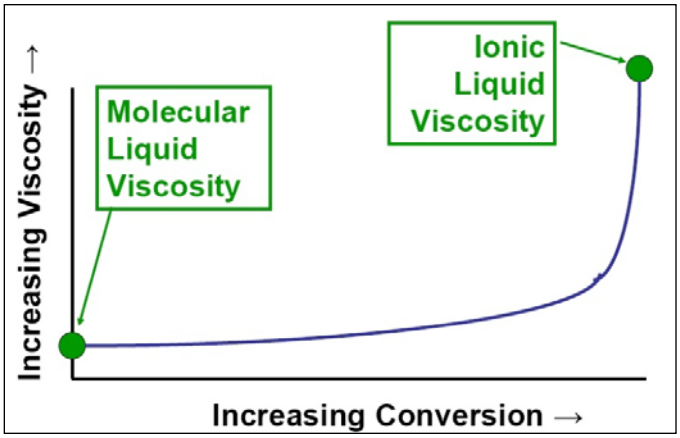

Figure 3: Ionic Liquids are more Viscous Than Their Respective Molecular Liquids

Table 1: Process Parameters for RevIL Solvents

	Parameter	Current R&D Value	Target R&D Value
Solvent Properties	Type of solvent	Reversible Ionic Liquid	
	Molecular weight	170-220	150
	Boiling point (^{0}C)	130	200
	Heat of reaction (kJ/mole CO_2)	Unknown	50
	CO_2 loading/working capacity*, wt.%	Unknown	100
	Solvent concentration to stripper (mol/liter)	4.5	7
	Heat capacity of solution (kJ/K/kg)	?	<4.2
	Viscosity, cP	>1,000	<80
Operating Conditions	Absorption temperature, °C	35	>50
	Absorption pressure, atm.	1.2	1.2
	CO_2 capture efficiency, %	?	90
	Regeneration method	Thermal	Thermal
	Regeneration temperature, °C	115	75
	Regeneration pressure, atm.	2	2
Heat Integration	Required regeneration steam temperature, °C	135	100
Miscellaneous	Solvent make-up rate, kg/kgCO_2	?	<0.003
Product Quality	CO_2 purity, %	?	>99
	N_2 concentration, %	?	<1
	Other contaminants, %	?	<<1
Process Performance	Electricity requirement, kJ/kgCO_2	?	500
	Heat requirement, kJ/kgCO_2	?	1,500
	Total energy (electricity equivalent), kJ/kgCO_2	?	950

*Working capacity is the loading difference CO_2-rich solution before and after it is regenerated.

Equations Describing Chemical Reaction

Chemical reaction for the CO_2 capture process is shown in Figure 2.

Solvent Contaminant Resistance

Since amine groups are involved in the reaction, sulfur oxides (SO_X) and nitrogen oxides (NO_X), as well as other acid gases, have to be removed. However, solvents have been shown to be stable in wet and oxygen-rich environments for a period of two months.

Flue Gas Pretreatment Requirements

Flue gas pretreatment should be similar to the amine-based absorption processes since the RevIL is resistant to moisture.

Technology Advantages:

- Use both physical absorption (dissolution in RevILs) and chemical absorption (reaction with RevILs); amines utilize only chemical absorption.
- Structure can be modified to optimize properties.
- Silylation will decrease viscosity.
- Function in the presence of water.
- Greater capacity than current solvents.
- Smaller energy penalty than current solvents.

R&D Challenges:

- New compounds must be designed, synthesized, and characterized.
- Optimum equilibria and heats must be achieved.
- Rapid reaction rates must be achieved.
- Favorable transport rates must be achieved.
- Results from new process must meet DOE goals.

Results To Date/Accomplishments:

- Have demonstrated greater capacity than current solvents.
- Successful synthesis and chemical characterization of three precursors for novel RevILs:
  - (3-aminopropyl) trimethoxysilane
  - (3-aminopropyl) triethoxysilane
  - (3-aminopropyl) triethylsilane

Next Steps:

- Successfully synthesize and characterize silylated one-component RevILs.
  - Demonstrate function in presence of water.
- Measure candidate RevILs' thermodynamic properties.
- Measure candidate RevILs' absorption and desorption rates.
- Identify and produce optimum capture solvent.
- Show that energy penalty is smaller than with current solvents.
- Design of capture process.
- Conduct an economic analysis.

Available Reports/Technical Papers/Presentations:	
Presentation from Kickoff Meeting held on December 2, 2009. Presentation: Annual NETL CO_2 Capture Technology for Existing Plants R&D Meeting, March 24-26, 2009, in Pittsburgh, Pennsylvania. Vittoria Blasucci, Cerag Dilek, Hillary Huttenhower, Ejae John, Veronica Llopis-Mestre, Pamela Pollet, Charles A. Eckert, and Charles L. Liotta, "One Component, Switchable, Neutral to Ionic Liquid Solvents Derived from Siloxylated Amines," Chem. Commun. 116-119, 2009. Vittoria Blasucci, Ryan Hart, Veronica Llopis Mestre, Dominique Julia Hahne, Melissa Burlager, Hillary Huttenhower, Beng Joo Reginald Thio, Charles L. Liotta, and Charles A. Eckert, "Single Component, Reversible Ionic Liquids for Energy Applications," *Fuel*, in press, 2010.	
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