Analysis of Ionic Liquids for Post-combustion CO_2 Capture at a Coal-fired Power Plant

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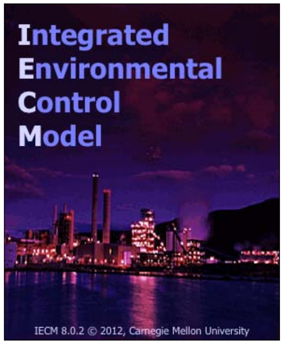
Background

IECM: A Tool for Analyzing Power Plant Design Options

- A desktop/laptop computer simulation model developed for DOE/NETL
- Provides systematic estimates of performance, emissions, costs and uncertainties for preliminary design of:
  - PC, IGCC and NGCC plants
  - All flue/fuel gas treatment systems
  - CO_2 capture and storage options (pre- and post-combustion, oxy-combustion; transport, storage)
- Free and publicly available at: **www.iecm-online.com**



Current IECM Technologies for CCS
(Version 8.0.2)

- CO_2 Capture Options
  - Pre-Combustion (IGCC):
    - » Water gas shift + Selexol
    - » Chemical looping
  - Oxy-Combustion (PC)
  - Post-Combustion (PC, NGCC):
    - » Amine systems (MEA, FG+)
    - » Chilled ammonia
    - » Membrane systems
    - » Auxiliary NG boiler or power plant (optional)
- CO_2 Transport Options
  - Pipelines (six U.S. regions)
- CO_2 Storage Options
  - Deep Saline or Other Formations
  - Enhanced Oil Recovery (EOR)

Advanced Capture Technology Models Under Development (Version 9.0)

Post-Combustion Capture
- Advanced membranes
- Calcium looping
- Solid sorbents
  - Amine-based
  - Activated carbon-based
  - Metal organic frameworks
- **Ionic liquids**

Oxy-Combustion Capture
- Low-sulfur coals
- High-sulfur coals

Pre-Combustion Capture
- Ionic liquids
- Chemical looping
- Sorbent-enhanced WGS

Why Ionic Liquids for CO_2 Capture?

- Ionic liquids (ILs) are among the new materials being developed for carbon dioxide (CO_2) capture because of their many favorable properties:
  - Non-volatile
  - High thermal stability
  - High CO_2 solubility and selectivity
  - Endless tunability
    - Both chemical and physical properties of ILs may be “tailored” by varying their structure and/or chemical composition *(Gurkan et al 2010, 2013)*

Source: Maginn and Brennecke, 2010.

Prior Research

- Current research on ILs is focused mainly on materials synthesis, laboratory experiments and molecular simulation of physical and chemical properties.
- Few efforts have been made to analyze IL-based CO_2 capture *processes*
  - Trimeric Corporation (2012) conducted a techno-economic analysis that indicated the economics of using ionic liquids for post-combustion CO_2 capture is comparable to that of the amine-based process
  - That analysis assumed the IL-based absorber tower had the same absorber packing height as the MEA base case; Liquid viscosity was not utilized for any critical calculations
  - Capture equipment cost estimates in the MEA base case were increased by a factor of 2.01 to agree with those of the NETL Baseline Report

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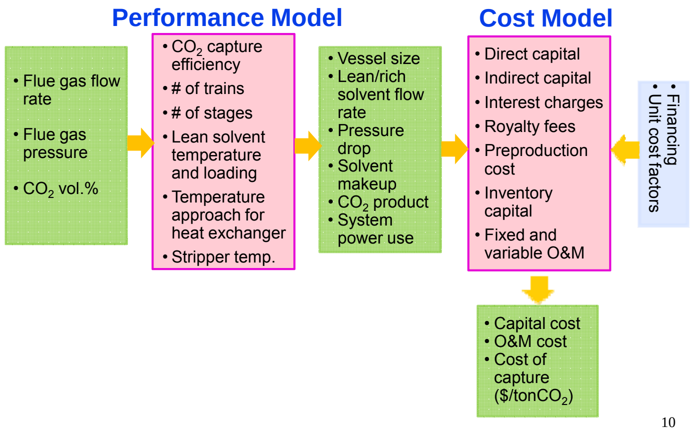
Objectives of This Study

- The main objectives of this study are to:
  - Develop preliminary performance and cost models of an IL-based process for post-combustion CO_2 capture suitable for integration into the IECM framework
  - Investigate system performance and cost for a current ionic liquid material
  - Explore approaches to enhance the technology’s viability

Techno-Economic Model

Techno-Economic Assessment Framework



Performance Model

- Flue gas flow rate
- Flue gas pressure
- CO_2 vol.%

- CO_2 capture efficiency
- # of trains
- # of stages
- Lean solvent temperature and loading
- Temperature approach for heat exchanger
- Stripper temp.

- Vessel size
- Lean/rich solvent flow rate
- Pressure drop
- Solvent makeup
- CO_2 product
- System power use

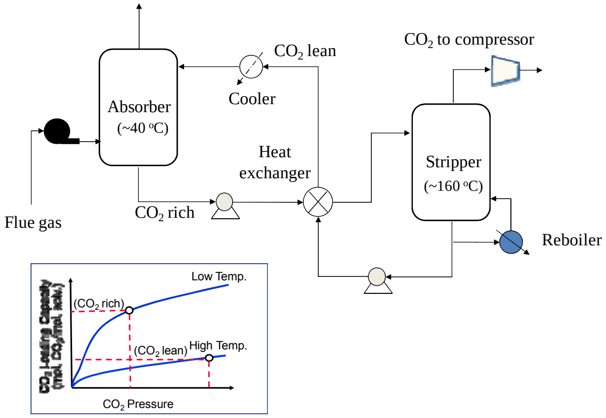
Cost Model

- Direct capital
- Indirect capital
- Interest charges
- Royalty fees
- Preproduction cost
- Inventory capital
- Fixed and variable O&M

- Financing
- Unit cost factors

- Capital cost
- O&M cost
- Cost of capture ($/tonCO$_2$)

Schematic of Ionic Liquid-based CO_2 Capture Process



Tunable Ionic Liquids for Post-Combustion CO_2 Capture

- The chemically tunable IL selected for this analysis is trihexyl-(tetradecyl)phosphonium 2-cyanopyrrolide ([P66614][2-CNpyr]) synthesized by researchers at the University of Notre Dame
- This IL achieves a 1:1 and reversible chemical reaction with CO_2, resulting in an efficient separation:

Absorption: CO_2 (g) + [2−CNpyr⁻] ↔ [2−CNpyr−CO$_2$⁻] (abs), $k_1(T)$

CO_2 (abs) ↔ CO_2 (g), $H(T)$

Regeneration: [2−CNpyr−CO$_2$⁻] (abs) ↔ CO_2 (g) + [2−CNpyr⁻]

Source: Gurkan et al 2010

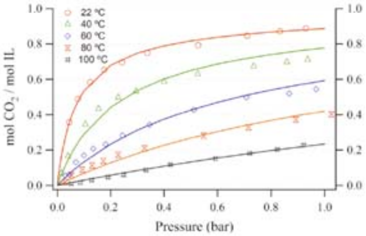
Solvent Properties: IL vs. MEA

Property	[P66614][2-CNpyr]*	30% MEA**
Molecular Weight (g/mole)	575	203
Heat Capacity @40°C (J/mole•°C)	1223	759
Viscosity @40°C (cp)	160	2.2
Surface Tension (mN/m)	30~40	48
Enthalpy of reaction (kJ/mole)	-43	-84

Source: * Gurkan et al. 2010; ** Wilcox, J. (2012)..

CO_2 Uptake Capacity

- Maximum CO_2 uptake (mole CO_2 per mole IL) is predicted using a Langmuir-type model as a function of CO_2 partial pressure, Henry constant, and reaction equilibrium constant (Gurkan et al 2010):



$$X_{co2} = \left[\frac{(P_{co2}/H)}{1-(P_{co2}/H)}\right] + \left[\frac{k_1 P_{co2} C_3}{1+k_1 P_{co2}}\right]$$

Isothermal Solubility of CO_2 in [P66614][2-CNpyr]

(*Source*: Gurkan et al 2010)

Multistage Equilibrium Process Model for Gas Absorption

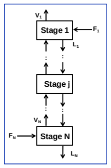
- Major assumptions:
  - Absorption of CO_2 is considered as a steady-state vapor-liquid process consisting of a number of equilibrium stages;
  - CO_2 is assumed to be the only component transferred from the gas phase to liquid phase (due to lack of multi-component data)
- A multistage equilibrium model simulates the adiabatic absorption process, including mass balance (M), equilibrium (E), summation (S), and enthalpy balance (H).

M: $L_{j-1}x_{i,j-1} - L_j x_{i,j} + V_{j+1} y_{i,j+1} - V_j y_{i,j} = 0$

E: $x_{co2,j} = \left[\frac{(P_{co2,j}/H_j)}{1-(P_{co2,j}/H_j)}\right] + \left[\frac{k_{1,j} P_{co2,j} C_3}{1+k_{1,j} P_{co2,j}}\right]$

S: $\sum y_{i,j} = 1 \quad \sum x_{i,j} = 1$

H: $L_{j-1}h_{j-1} - L_j h_j + V_{j+1} H_{j+1} - V_j H_j + \Delta H - Q = 0$



The Newton-Ralphson algorithm is applied to solve the MESH equations.

Mass Transfer in Gas Absorption

- Absorber height is estimated in terms of the overall gas-phase mass transfer coefficient, in which the liquid-phase physical mass transfer coefficient is adjusted by an enhancement factor reflecting the reaction kinetics: $\frac{1}{K_G} = \frac{1}{k_G} + \frac{H_{co2}}{k_L E}$
- The physical mass transfer coefficients of gas and liquid phases are estimated using empirical mass transfer correlations developed by Onda *et al.* for randomly packed columns:

Interfacial area : $\frac{a}{a_p} = 1 - \exp\left\{-1.45\left(\frac{\sigma_c}{\sigma_L}\right)^{0.75}\left(\frac{v_L}{a_p \mu_L}\right)^{0.1}\left(\frac{v_L^2 a_p}{\rho_L^2 g}\right)^{-0.05}\left(\frac{v_L^2}{\rho_L \sigma_L a_p}\right)^{0.2}\right\}$

Gas-phase mass transfer: $\frac{k_G RT}{a_p D_G} = \epsilon\left(\frac{v_G}{a_p \mu_G}\right)^{0.7}\left(\frac{\mu_G}{\rho_G D_G}\right)^{1/3}(a_p d_p)^{-2}$

Liquid-phase mass transfer: $k_L\left(\frac{\rho_L}{\mu_L g}\right)^{1/3} = 0.0051\left(\frac{v_L}{a \mu_L}\right)^{2/3}\left(\frac{\mu_L}{\rho_L D_L}\right)^{-0.5}(a_p d_p)^{0.4}$

Solvent Regeneration

- Since no water is used to dilute the solvent, and there are no solvent vapor losses, a single-stage vessel in equilibrium is employed for the stripping process
- The thermal energy requirements for solvent regeneration mainly include the solvent heating and enthalpy of reaction
- The size of the stripper is determined using empirical vapor velocity and liquid surge time designs

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Case Study Results

Case Study Assumptions for 90% CO_2 Capture at a 650 MW_g Coal-Fired Plant

Performance Parameter	Units	Value
Flue gas flow rate	kmole/hr	94,980
Number of trains	#	4
CO_2 in flue gas	mol. fraction	0.12
Flue gas temperature	°C	40
Lean solvent temperature	°C	40
Absorber pressure*	bar	1.0
Number of equilibrium stages	#	5
CO_2 in lean solvent	mol. fraction	0.050
Temp. approach, rich/lean heat exchg.	°C	5
Stripping temperature	°C	160
CO_2 product pressure	bar	153

* Based on Sherwood/Leva/Eckert correlation

Preliminary Performance Results for an IL-based System for 90% CO_2 Capture

Parameter	Unit	Value
CO_2 concentration in rich solvent stream	mol. fraction	0.19
Lean solvent flow rate per train	kmole/hr	15,232
Liquid-to-gas ratio	mole ratio	0.64
Pressure drop across absorber	kPa	12
Absorber height	m	45.5
Absorber diameter	m	11.1
Stripping pressure	bar	1.03
Stripper height	m	27.1
Stripper diameter	m	8.7
Steam use for solvent regeneration	kJ/kg CO_2	3627
Steam use, electrical equivalent	MW	113.9
Total equipment power use	MW	68.7
Net power plant efficiency	**HHV, %**	**27**

Case Study Assumptions for 90% CO_2 Capture at a 650 MW_g Coal-Fired Plant

Cost Parameter	Units	Value
Cost year	Constant US $	2011
Capacity factor	%	75
Fixed charge factor	fraction	0.113
Construction time	yr	3
General facilities	% PFC	10
Engr. & overhead fees	% PFC	7
Project contingency	**% PFC**	**30***
Process contingency	**% PFC**	**30***
Misc. capital cost	%TPI	2
Inventory capital	%TPC	0.5
Total maintenance cost	%TPC	2.5
Labor fee	$/hr	34.65
Solvent makeup cost	$/t	10,000

[*] Reflects first-of-a-kind (FOAK) costs

Preliminary Cost Results for First-of-a-Kind (FOAK) Plant with 90% CO_2 Capture

Parameter	Unit	Value
Total capital requirement	**2011$/kW**	**2,637**
Fixed O&M cost	2011$/MWh	10.5
Variable O&M cost	2011$/MWh	10.6
Total O&M cost[*]	2011$/MWh	21.1
Cost of CO_2 captured [**]	**2011$/t**	**62.4**

[*] This item does not include CO_2 transport and storage costs.

[**] Estimated as the total annualized cost divided by the total mass of CO_2 captured.

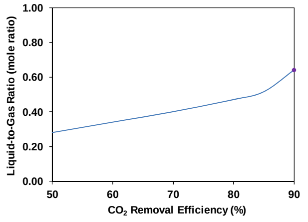
Alternative Cases

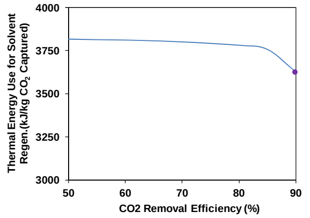
Sensitivity Analyses for IL-based CO_2 Capture: Performance Variables

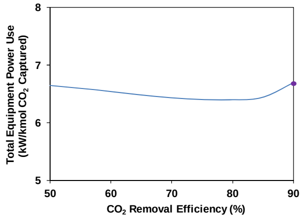
- Process Operating Design
  - Lean solvent temperature
  - Lean solvent loading
  - Stripping temperature
- Solvent Properties
  - Viscosity
  - Heat capacity
- CO_2 Removal Efficiency
- Cost and Financial Factors
  - Contingency costs
  - Fixed charge factor

Full details are available in the preprint. The following slides show a few of those results.

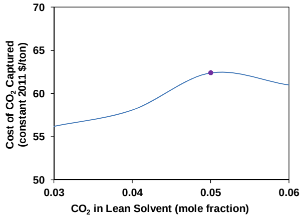
Effects of CO_2 Removal Efficiency on Process Design Parameters

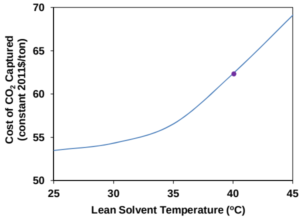


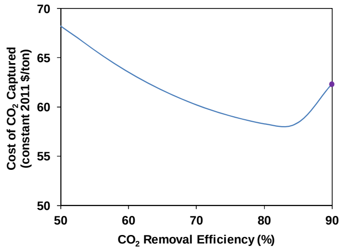




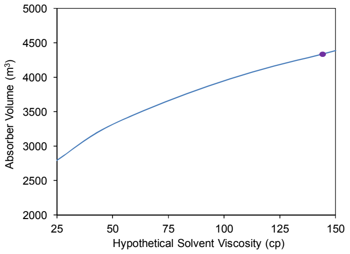
Effects of IL Process Variables on Cost of CO_2 Captured

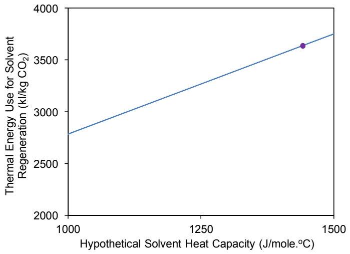




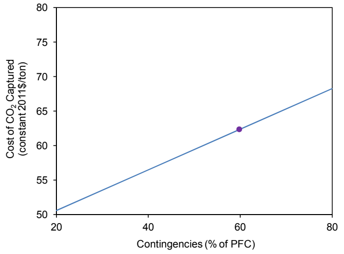


Effects of Solvent Properties

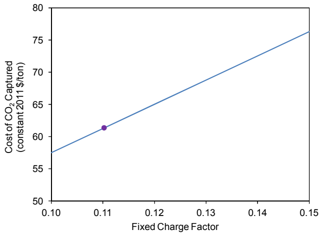




Effect of Contingency Costs and Fixed Charge Factor on Cost of CO_2 Captured



These factors will be lower for an *Nth*-of-a-kind (NOAK) plant than a FOAK plant. *But …*



First you have to build N plants!

Conclusions

Conclusions

- The preliminary results for the case study IL showed that the most cost-effective “cost of CO_2 captured” occurred at a removal efficiency of about 85%
- The overall cost of capture is higher than the U.S. DOE’s cost target of $40/t for new technologies, mainly due to high capital cost of vessels. However, current process designs for IL systems are not yet optimized.
- Improvement in solvent properties would improve the technology’s viability.
- The impacts of other flue gas constituents such as sulfur and water vapor remain to be studied and could alter conclusions shown here.
- Other important cost metrics for such as added LCOE and CO_2 avoidance cost will be reported in future cost assessments.

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Thank You

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