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Technical and Economic Assessments of Ionic Liquids for Pre-Combustion CO_2 Capture at IGCC Power Plants

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Abstract

This study evaluates the feasibility and cost of ionic liquids (ILs) for precombustion carbon dioxide (CO_2) capture at integrated gasification combined cycle power plants. The ionic liquid 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide is selected as a physical solvent for CO_2 capture. Using newly developed performance and cost models, our analysis shows that the energy penalty of the IL-based capture system mainly arises from powering various compressors and solvent pumps, and compressors and absorbers are the dominant capital cost components. Using the Integrated Environmental Control Model (IECM) for power plant assessments, the cost of CO_2 avoided by the IL-based capture system is estimated to be \$62/t CO_2 in constant 2011 USD. The preliminary comparisons of performance and cost between IL- and Selexol-based capture systems show that an IL-based capture system could be a viable alternative to current liquid solvent processes.

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Keywords: ionic liquid, carbon capture and storage, IGCC, performance, cost

1. Introduction and Research Objective

Ionic liquids (ILs) are being actively developed as an alternative to conventional solvents for carbon dioxide (CO_2) capture due to their favorable properties such as low volatility, high CO_2 solubility and selectivity, and endless tenability [1-2]. Chemical and physical properties of ILs can be tuned for CO_2 capture due to flexible combinations

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of cations and anions that yield ILs [1]. ILs can be used for CO_2 capture without water dilution, reducing parasitic energy requirements [1]. However, ILs have high viscosity, which poses a challenge for large-scale applications.

Current research on ILs is focused mainly on materials synthesis, laboratory experiments, molecular simulation, and phase equilibrium predictions [2-3]. Few efforts have explored the use of ILs for pre-combustion CO_2 capture at integrated gasification combined cycle (IGCC) power plants. Given that the shifted syngas stream mainly consists of CO_2 and hydrogen and has high CO_2 partial pressure, ILs that physically absorb CO_2 could be attractive for pre-combustion CO_2 capture [1,4]. Basha et al (2013, 2014) evaluated the technical feasibility of adiabatic absorption processes using ILs as a physical solvent for capturing CO_2 from the shifted gas stream at an E-Gas IGCC power plant [5-6]. However, techno-economic evaluations have been performed rarely for IL-based capture systems in the existing studies. The main objective of this study, therefore, is to investigate the feasibility and cost of IL-based CO_2 capture systems at IGCC plants. The ionic liquid 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([hmim][Tf_2N]) is selected as a physical solvent for CO_2 capture based on current literature [5-8].

Nomenclature

a	parameter in Redlich-Kwong equation of state
b	parameter in Redlich-Kwong equation of state
h:	enthalpy of liquid flow
H	enthalpy of gas flow
K	phase equilibrium ratio
L	solvent flow rate
Q	cooling duty
P	pressure
R	gas constant
T	temperature
V	gas flow rate
x	mole fraction in liquid phase
y	mole fraction in gas phase
Ø:	fugacity coefficient

Subscripts:

i:	component
j:	stage number
L:	liquid phase
V:	vapor phase

2. Performance Models of IL-based CO_2 Capture System

Figure 1 shows the process configuration for pre-combustion CO_2 capture and storage (CCS). The CO_2 is absorbed by [hmim][Tf_2N] in a packed vessel, while the CO_2-rich solvent stream out of the absorber enters multiple flash drums with low pressure for solvent regeneration. In addition to the absorption and stripping vessels, various compressors are used for liquid and gas streams, and pumps are used to transport solvent streams and offset any pressure drops. Using a pressure swing for solvent regeneration, some energy can be recovered by hydraulic power turbines from high-pressure solvent streams.

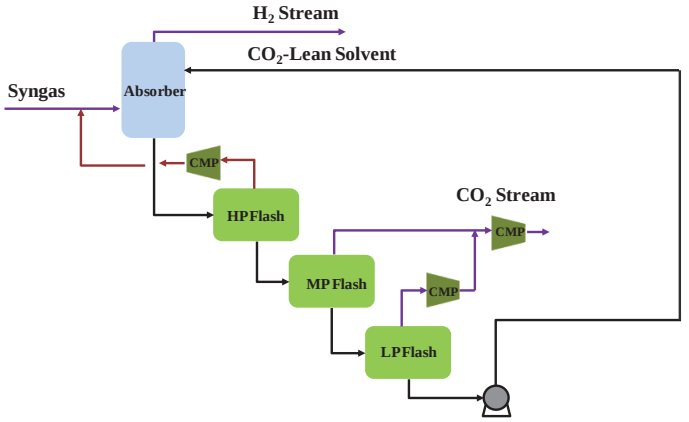

Fig. 1 Schematic of a pre-combustion CO_2 capture system using [hmim][Tf_2N]

2.1. Phase Equilibrium based on Equation of State

The generic Redlich-Kwong Equation of State (RK EOS) is employed to predict the phase behavior of gases in ILs under different pressures and temperatures. The RK EOS is modified and written as [7-8]:

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)} \tag{1}$$

For N-component mixtures, the parameters (a, b) in the RK EOS are calculated in terms of mixing rules, which are estimated as the function of mole fractions of the components in vapor-liquid equilibrium (VLE) [7-8]. Shiflett and Yokozeki (2007) estimated the binary interaction parameters in mixing rules for CO_2 and [hmim][Tf_2N] by using a nonlinear least-squares method to fit the solubility data [8]. Similarly, we also estimate the binary interaction parameters for hydrogen (H_2) and [hmim][Tf_2N] by fitting the solubility data measured by Raeissi et al [9].

The *K*-value of a component (*i*) in VLE is estimated as the ratio of liquid versus vapor fugacity coefficients ($\emptyset_i^L$, $\emptyset_i^V$) derived from the RK EOS and relates the vapor and liquid mole fractions of a given component as:

$$K_i = \frac{\emptyset_i^L}{\emptyset_i^V} = \frac{y_i}{x_i} \tag{2}$$

2.2. Multi-stage Equilibrium Process Model for Gas Absorption

Absorption of CO_2 is considered as a steady-state vapor-liquid process consisting of a number of equilibrium stages. Equilibrium is assumed to take place between vapor and liquid streams leaving each stage. The modified RK EOS is applied to predict the phase equilibrium of CO_2 and H_2 in [hmim][Tf_2N] under different pressure and temperature conditions and is then incorporated into the process model. A multi-stage equilibrium model is established to simulate the absorption process, which takes into account the mass balance (M), equilibrium (E), summation (S), and enthalpy balance (H) described in Equations (3) to (6). An inside-out (I/O) algorithm is applied to solve the coupled MESH equations and then estimate the vapor and liquid flow rates and compositions across the absorber.

***M**ass balance for each component for stage (j)*:

$$L_{j-1}x_{i,j-1} - L_j x_{i,j} + V_{j+1}y_{i,j+1} - V_j y_{i,j} = 0 \tag{3}$$

***E**quilibrium for each component for stage (j)*:

$$y_{i,j}=K_{i,j}\cdot x_{i,j} \quad (4)$$

***S**ummation based on mole fractions for stage (j)*:

$$\sum x_{i,j} = \sum y_{i,j} =1 \quad (5)$$

***E**nthalpy balance for stage (j)*:

$$L_{j-1}h_{j-1}-L_jh_j+V_{j+1}H_{j+1}-V_jH_j-Q=0 \quad (6)$$

To estimate the potential pressure drop, the Sherwood/Leva/Eckert correlation that describes the relation of column capacity with pressure drop rate is adopted in this study [10]. The absorber height is estimated based on the overall gas-phase mass transfer coefficient of physical absorption, in which the mass transfer coefficients of gas and liquid phases are estimated using empirical correlations developed by Onda et al (1968) for randomly packed columns [11].

2.3. Flashing for Solvent Regeneration

The CO_2-rich solvent stream exiting the absorber with a high pressure can enter multiple flash drums with lower pressures for solvent regeneration. The dissolved CO_2 is flashed off in a series of drums. The TP-flash calculation is conducted to model the stripping process in VLE.

2.4. Major Equipment Power Use

Electric power is required for equipment that involves process stream compression, CO_2 product compression, and solvent circulation. As shown in Figure 1, compressors are employed to achieve designated pressures for different streams, while pumps are used to elevate the CO_2-lean streams to absorbers, offset any possible pressure drop along the pipeline and increase the solvent stream pressure to the designed absorption pressure if needed. Given that pressure swing is used for solvent regeneration, some energy can be recovered from high-pressure streams by hydraulic power turbines [12].

3. Cost Models of IL-based CO_2 Capture System

The aforementioned performance models are linked to engineering-economic models that estimate the capital cost, annual operating and maintenance (O&M) costs, and total levelized cost of electricity (LCOE) for an IL-based CCS system applied to an IGCC power plant. This study employs the costing method and nomenclature of the Electric Power Research Institute's Technical Assessment Guide [13]. The total capital requirement (TCR) of a CO_2 capture system includes the direct process facilities cost plus various indirect cost categories such as the general facilities cost, engineering and home office fees, contingency costs, and owner's costs. The direct cost components mainly include the absorbers, flash drums, solvent circulation pumps, sump tanks, heat exchangers, process stream compressors, CO_2 product compressors, and hydraulic power recovery turbines. The cost estimation approach developed by Chen (2005) for Selxol-based CO_2 capture systems in the Integrated Environmental Control Model (IECM) was adopted to estimate the direct costs for the major components [12,14]. Variable O&M costs include IL makeup, power use, and CO_2 transport and storage where applicable, while fixed O&M costs include operating labor, maintenance costs, and administrative and support labor costs.

4. Case Study

The technical and economic models developed for IL-based CO_2 capture were employed in a case study. To evaluate the effects of CCS deployment on the overall plant performance and cost, the 2016 release of IECM

(Version 9.2) was applied to perform the plant-level analysis [14]. Table 1 summarizes the major technical and economic parameters and assumptions for the plant with an IL-based capture system in the IECM [14-15]. To incorporate CO_2 capture at an IGCC plant, as modeled, a two-stage water gas shift (WGS) reactor is added in addition to the CO_2 capture system [15]. At the plant with CCS, the WGS reactor was designed to achieve a CO to CO_2 conversion efficiency of 95%, while the CO_2 capture system was designed to achieve 90% CO_2 capture. The default IECM settings are adopted for all other IGCC power plant components.

4.1. Performance and Cost Results of IL-based CO_2 Capture System

The IL-based CO_2 capture system consists of two trains that are designed to be an isothermal process for 90% CO_2 capture. Both the absorption and stripping vessels are designed to operate at 29.4°C, which is similar to that of Selexol-based capture systems [12,15]. The CO_2 in the syngas is absorbed at 2960 kPa, whereas the CO_2-rich solvent is regenerated in the three flash drums with decreasing pressures from 1000 kPa to 80 kPa. As shown in Figure 1, two process compressors are used to boost the recycled gas stream exiting the HP flash drum from 1000 kPa to 2960 kPa in each train. The CO_2 product stream exiting the MP and LP flash drums are 500 kPa and 80kPa, respectively. The combined CO_2 product stream is then compressed to 15.3 MPa for transport and storage. A pump is used to deliver the CO_2-lean solvent stream back to the absorber and increase the stream pressure to 2960 kPa. Given a large decrease in the CO_2-rich solvent pressure from the absorber to the HP flash drum, a hydraulic turbine is used to recover energy from the solvent stream [12].

The process simulation results show that the H_2-rich stream delivered as the fuel to turbines has 94% H_2 and the combined CO_2 product stream has 99% CO_2. The gas stream out of the HP flash drum has 22% H_2 so it is recycled back to the absorber. The losses of hydrogen and [hmim][Tf_2N] along with the combined CO_2 product stream are ignorable. The pressure drop across the absorber operating under a high pressure is small (1.2 kPa).

The total power use and capital cost of the capture system are summarized in Table 2 for both the IL-based system and the Selexol-based system. The CO_2 product compression has the largest power requirement. The absorbers, process compressors, and product compressors dominate the capital investment, and account for about 20%, 22%, and 36% of the total direct capital cost, respectively, for the IL-based system.

4.2. Overall Plant-level Performance and Cost Results

To evaluate the effects of CCS deployment on the plant performance and cost, the IECM was employed to estimate the net plant efficiency, CO_2 emission rates, and LCOE for Shell-based IGCC plants with and without CCS. The implementation of IL-based CCS would decrease the net plant efficiency by more than 9 percentage points and increase the plant LCOE by $35/MWh (with all costs in constant 2011 dollars). To measure the overall cost for CCS, the cost of CO_2 avoided is a more appropriate metric than the separation cost, which employs an arbitrary electricity price assumption [16]. For the assumed total cost of $10/t for CO_2 transport and storage, the resulting cost of CO_2 avoided by the CCS system using [hmim][Tf_2N] is $62/t CO_2 relevant to the IGCC plant without CCS.

To further assess this technology, we compared it to a conventional Selexol-based two-stage system employing physical absorption for CO_2 capture [15]. The performance and cost of an IGCC plant with Selexol-based CCS were also estimated using the IECM, and the relevant results also are summarized in Table 2. To capture 90% CO_2 from the same inlet syngas as the IL-based system, the Selexol-based system requires 54 MW electric power for the equipment and has a resulting avoidance cost of $63 per ton of CO_2 avoided. In comparisons, both capture systems have similar effects on the overall plant and cost, resulting in a similar avoidance cost.

Table 1. Major technical and economic parameters and assumptions for IL-based CO_2 capture

Category	Parameter	Unit	Value
Performance	Syngas flow rate	kmol/hr	28300
	Syngas pressure	kPa	2960
	Syngas temperature	°C	29.4
	CO_2 concentration	%	37
	CO_2 removal efficiency	%	90
	Number of trains	#	2
	Capacity factor	%	75
	Absorber pressure	kPa	2960
	Lean-solvent temperature	°C	29.4
	Temperature in HP/MP/LP flash drums	°C	29.4
	Assumed solvent loss rate	kg IL/t CO_2	0.23
	Compressor efficiency	%	80
	Pump efficiency	%	75
	Power recovery turbine efficiency	%	75
	CO_2 product pressure	MPa	15.3
Cost	Fixed charge factor	fraction	0.113
	Discount rate	%	7.09
	Construction time	yr	3
	General facilities capital	% PFC	15
	Engineering & overhead fees	% PFC	10
	Process contingency cost	% PFC	10
	Project contingency cost	% (PFC+Overhead+Proc Contingency)	15
	Royalty fees	% PFC	0.5
	Misc. capital cost	%TPI	40
	Inventory capital	%TPC	30
	Total maintenance cost	%TPC	5.0
	Labor fee	$/hr	34.65
	Solvent makeup cost	$/t	10000
	Reclaimer waste disposal cost	$/t	260
	CO_2 transport and storage costs	$/t	10

Table 2. Comparisons of performance and costs of IGCC plants with and without CCS

Parameter	IGCC w/o CCS	IGCC w/ IL-CCS	IGCC w/ Selexol-CCS
Gross power output (MW)	681	656	656
Net power output (MW)	595	536	533
Net plant efficiency (HHV,%)	44.3	35.1	34.9
CO_2 emission rate (kg/kWh)	0.710	0.130	0.130
CO_2 capture system alone:			
Power use (MW)		51	54
TCR(2011$/kWnet)		318	349
Plant LCOE (2011$/MWh)	85.0	120.8	121.9
Cost of CO_2 avoided (2011$/t CO_2)		62	63

5. Conclusions

This study has developed and applied an integrated technical and economic assessment framework to examine the feasibility and cost of this ionic liquid [hmim][Tf_2N] as a physical solvent for pre-combustion CO_2 capture at IGCC power plants. The results indicate that the energy penalty of such an IL-based capture system arises mainly from powering the product and process compressors and solvent pumps. The product and process compressors and absorbers are shown to be the dominant cost components of the capture system. The preliminary comparisons between [hmim][Tf_2N]- and Selexol-based capture systems imply that an IL-based capture system could be a viable alternative to current liquid solvent processes. Further work is needed to assess other possible IL solvents and to

explore uncertainties and other capture process designs that might be less expensive and more cost-effective than the system analyzed here.

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