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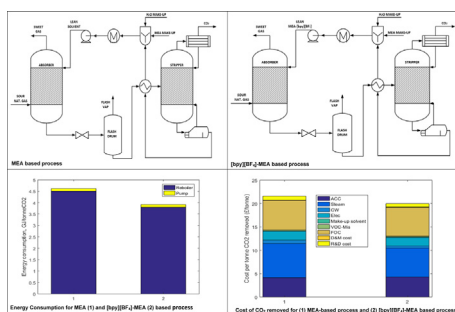
Study of CO₂ removal in natural gas process using mixture of ionic liquid and MEA through process simulation

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GRAPHICAL ABSTRACT



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ABSTRACT

There has been a shift to less carbon intensive fuels such as natural gas to meet energy demand due to increasing pressure to cut CO₂ emissions. This has prompted a need to assess unconventional and contaminated natural gas reserves (which contains CO₂ concentration of 20 mol% or more). The CO₂ capture process with MEA as the solvent is mostly adopted to treat contaminated natural gas. In this study, the option of using a blend of ionic liquids (IL) and MEA as a promising solvent in the process was investigated through modelling and simulation. A detailed rate-based model was developed for both MEA (30 wt%) solvent and IL (30 wt%)-MEA (30 wt%) blend using Aspen Plus® to assess both process and economic performances. The 1-Butylpyridinium ([bpy][BF₄]) ionic liquid was selected in this study. The physiochemical properties of [bpy][BF₄], predicted using Aspen Plus®, showed good accuracy compared with experimental data. The results from this study showed about 15% and 7.44% lower energy consumption in the reboiler duty and CO₂ removal cost respectively with aqueous [bpy][BF₄]-MEA solvent compared to 30 wt% MEA solvent. It is concluded that the aqueous [bpy][BF₄]-MEA solvent is therefore a promising solvent that could replace 30 wt% MEA solvent in this process.

Abbreviations: ACC, Annual Capital Cost; AOC, Annual Operating Cost; [bpy][BF₄], 1-butylpyridinium tetrafluoroborate; [bheaa], Bis(2-hydroxyethyl) ammonium acetate; [bmim][BF₄], 1-butyl-3-methylimidazolium tetrafluoroborate; [bmim][DCA], 1-butyl-3-methylimidazolium dicyanamide; CW, Cooling Water; DEA, Diethanolamine; DHVLB, Heat of Vaporization at T_b; D&M, Distribution and Marketing; Elec, Electricity; ENRTL, Electrolyte Non-Random Two Liquid; FC-CS, The Fragment contribution – corresponding states; FOC, Fixed Operating Cost; IL, Ionic Liquid; IEA, International Energy Agency; LNG, Liquefied Natural Gas; MDEA, Methyl-diethanolamine; MEA, Monoethanolamine; Mis, Miscellaneous; R&D, Research and Development; RK, Redlich Kwong; RKTZRA, Rackett/Campbell-Thodos Mixture Liquid Volume; RTILs, Room temperature ionic liquids; TSILs, Task specific ionic liquids; V_B, Liquid Molar Volume at T_b; VOC, Variable operating cost; VLSTD, Standard liquid Volume

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Nomenclature

$C_{1i}-C_{3i}$	Equation coefficients for (7)
$C'_{1i}-C'_{3i}$	Equation coefficients for (8)
Z_i^{RA} and d_i	Equation coefficients for (9)
A_i-C_i	Equation coefficients for (10)
$C_{1i}-C_{5i}$	Equation coefficients for (11)
D_i-D_{iii}	Equation coefficients for (12)
H_{ij}	Henry Constant
P_i^v	Vapour pressure of component i, Pa
P_c	Critical pressure, bar
Q_{reb}	Reboiler duty, kJ/kg _{co2}
Q_{cond}	Condenser duty, kJ/kg _{co2}
Q_{cooler}	Cooler duty, kJ/kg _{co2}
T	Temperature, K

T_b	Normal Boiling temperature, K
T_c	Critical temperature, K
T_r	Reduced temperature, K
V_c	Critical Volume, cc/mol
W_{pump}	Pump power kJ/kg _{co2}
Z_c	Critical Compressibility factor
σ_i	Surface tension, mN/m
η_i	Liquid Viscosity, cP
ρ_i	Liquid molar density, mol/cc
Ω	Omega
ΔH_f^0	Standard heat of formation, kJ/mol
ΔH_c^0	Standard heat of combustion, kJ/mol
λ_i	Thermal conductivity, kcal-m/hr-m ² -K

1. Introduction

1.1. Background

The need to reduce emissions has favoured a shift towards low carbon fuels such as natural gas for energy generation [1]. It is predicted that a switch to low carbon fuels will contribute about 15% in expected CO₂ emission cuts by 2050 [2]. Globally, mineable natural gas reserves are far smaller in comparison to that of carbon intensive fuels (*i.e.* coal) and as such, natural gas supply is less secured and expensive. This has prompted the need to re-assess the development of unconventional, stranded, contaminated and sour natural gas reserves [3]. However, raw natural gas is known to contain acid gas such as CO₂ with concentration of about 20 mol% and more, which makes these reserves economically unviable. These natural gas reserves are predominantly in SE Asia, NW Australia, Central USA, North Africa and the Middle East [4]. These locations are far from the established gas markets in Western Europe, Japan and South Korea. Thus, a large amount of natural gas must be conveyed either via long distance pipeline or as Liquefied Natural Gas (LNG) [3]. The presence of CO₂ in natural gas limits its quality (heating value) and the liquefaction process performance.

Natural gas sweetening technologies are adopted to remove CO₂, so natural gas can meet acceptable standards for pipeline transport to end-users and/or liquefaction process for LNG [5]. Natural gas sweetening process involves CO₂ separation from the gas mixture using techniques such as physical absorption, chemical absorption, adsorption, cryogenic separation and membrane separation among others [5]. Chemical absorption is the most commonly and widely used separation method in natural gas sweetening processes [6,7]. However, it is expensive especially due to the high energy penalty of the process [8]. Thus, there is a need to explore different options for reducing the high-energy penalty of the process.

1.2. Motivation

Amine-based CO₂ absorption/desorption process has been in use for decades in the industry for CO₂ removal from gas mixtures such as natural gas among others [3,6,9,10]. This is primarily due to its relatively rapid kinetics of the amine solvents [3,6]. However, amine solvents generally require high energy for regeneration. They also tend to stimulate equipment corrosion and degrade rapidly during operation. This makes the operating cost for amine-based process generally high

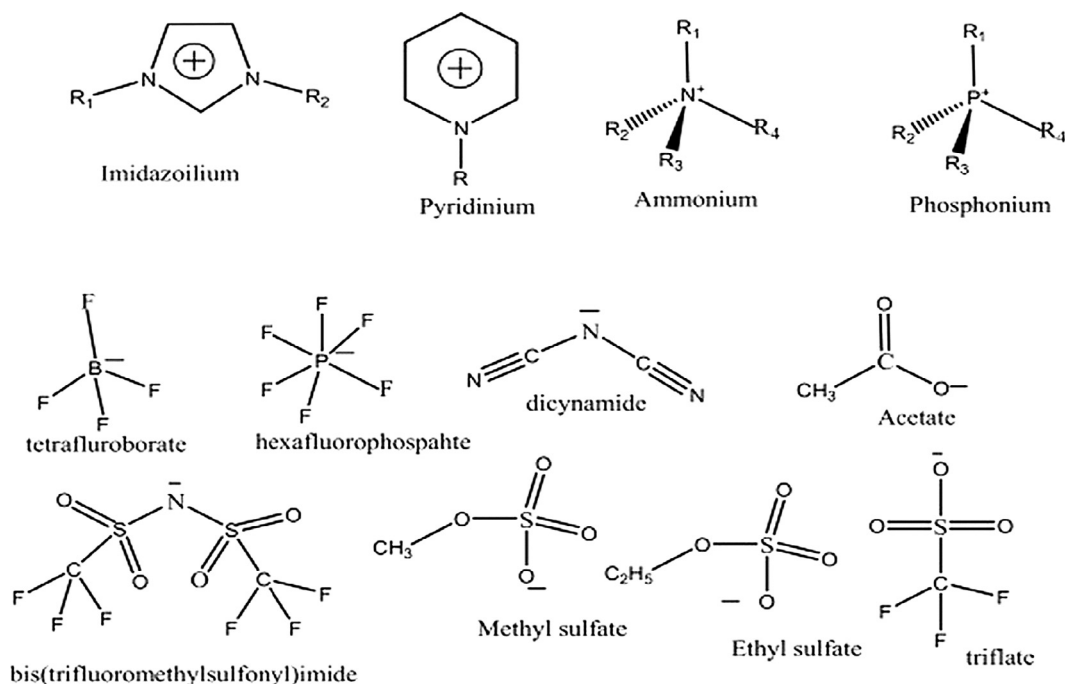


Fig. 1. General Structure of various cations and anions used for Ionic liquid formulation [5].

[6]. Thus, attention has shifted to development of new solvents that have less energy requirement for regeneration and are more stable, with less tendency to degrade and lower potential for stimulating corrosion. One of such solvents is ionic liquids (ILs).

Ionic liquids (ILs) are generally classified as compound composed entirely of ions (cations and anions). They tend to be liquids over a wide range of temperature and are non-volatile which makes them good solvents for a variety of materials. The tunability capability of the ionic liquid makes it possible to tune the ionic liquid structure to suit a specific process requirement by altering either the cation or anion. Some of the commonly encountered cations and anions are shown in Fig. 1. ILs requires less energy for regeneration and are environmentally friendly solvents [5]. In addition, they are thermally stable and have low vapour pressure among others. These qualities satisfy the requirements of a more energy-efficient solvent for CO₂ absorption/desorption process than amine solvents [5,11].

Several studies on the properties and application of various ILs for natural gas sweetening and carbon capture through experimental investigations have been carried out [11–18]. From these investigations, it was concluded that the use of ILs only as a solvent is less competitive when compared with MEA. This is due to its low CO₂ absorption capacity. In the quest to find a more competitive solvent, attention has been given to functionalized ILs, supported IL membranes and polymerized ILs [5]. These ILs formulation are considered more expensive than the traditional amine solvents [5]. Also, gas-liquid mass transfer rates are low with ILs due to their high viscosities, resulting in a low reaction rate with CO₂, making them less competitive than amine solvents [5]. These reasons have made IL solvents currently not industrially viable for CO₂ absorption/stripping processes in a large scale [5]. On the other hand, the option of blending ILs and amine solvents have shown a lot of promise [3,5,20]. This basically involves merging an eco-friendly IL with the high binding capacity amines [5]. It has been shown that this option requires less regeneration energy than conventional amine process, better process economics and substantially higher gas-liquid mass transfer rates than only ILs [11].

1.3. Previous studies

Use of IL-Amine blends for natural gas sweetening and carbon capture is driven by the need to develop new solvents with a CO₂ loading capacity comparable to the amine-based solvents and with great reduction in the energy required for regeneration [11]. The section gives a review on the application of IL-amine blends for natural gas sweetening and carbon capture.

Various researchers have carried out experimental investigations on the physical properties and absorption capacity of IL-amine blend. Investigation by Camper et al. [20] on the solubility of CO₂ in IL-amine blend revealed that the RTIL-amine (RTIL-MEA and RTIL-DEA) blends demonstrated rapid and reversible CO₂ capture performance, while the amine functionalised TSIL exhibited a slower CO₂ capture performance due to its high viscosity. Similar investigation carried out by Feng et al. [21] showed that temperature increase enhances the absorption rate. The influence of temperature on the absorption rate is said to diminish after a long period.

Study on CO₂ solubility using two ILs blended with MEA ([bheaa]-MEA and [bmim][BF₄]-MEA) by Taib and Murugesan [22] demonstrated that CO₂ solubility in MEA exhibit chemical solubility while the solubility of CO₂ in IL exhibits physical solubility, indicating that the CO₂ removal mechanism can both be physisorption and chemisorption [23]. Further details on the mechanism analysis for both solvents can be seen in Taib and Murugesan [22].

Experiment studies on CO₂ solubility and physical properties of IL-amine mixture highlighted the impact of H₂O and amine on the physical properties of the absorbents (particularly density and viscosity), which enhances CO₂ capture performance [24,25]. The CO₂ absorption capacity of the IL-amine blend was mainly a function of amine concentration and the presence of water reduces the IL-amine blend viscosity, which makes it an industrially viable solvent [24].

Further experimental investigation on IL-amine solvent revealed that the hybrid solvent achieved lower energy consumption compared to conventional solvent [26] and demonstrated better corrosion control with carbon steel material compared with aqueous amine [27]. More experimental studies on IL-amine solvents can be found in [28–31]. It

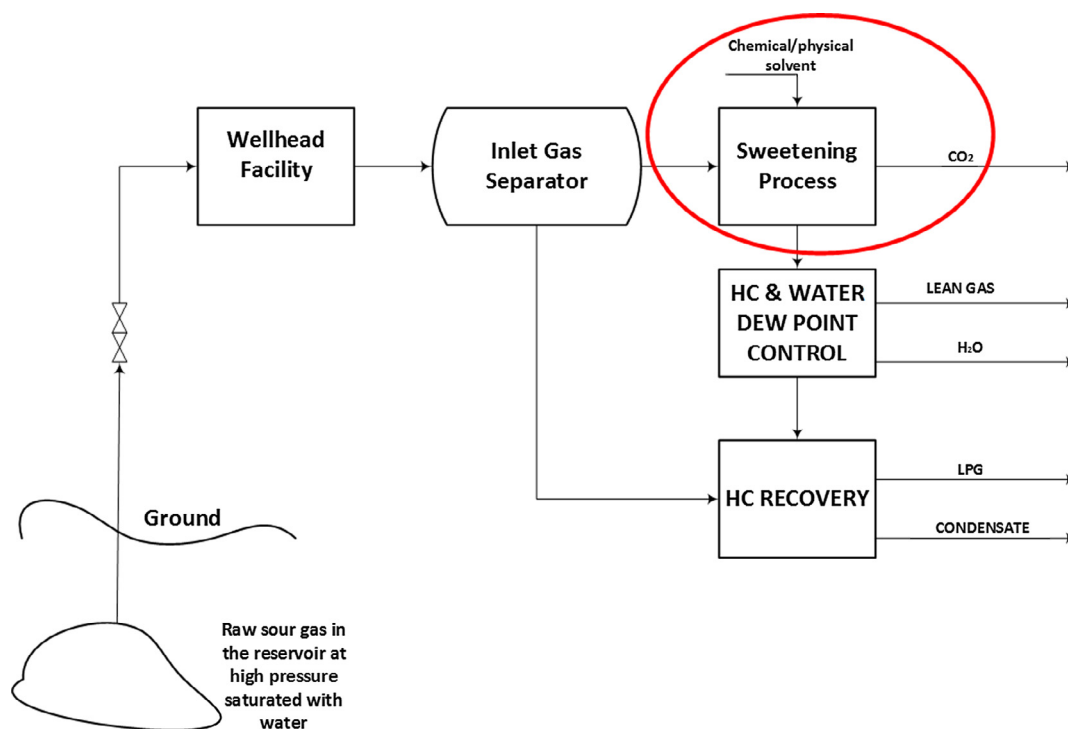


Fig. 2. Schematic diagram of sour natural gas production/processing [37].

can be seen that an industrially competitive hybrid solvent could be developed by blending ILs with amine solutions to enhance the CO₂ removal performance.

Studies involving whole process analysis of CO₂ removal from gas mixtures using IL-based solvents have also been reported [11,26]. Despite the successful experimental investigations on the application of IL-amine blends for CO₂ removal, there have been little research on modelling and simulation of the natural gas sweetening process/carbon capture process using the hybrid solvent to our knowledge. It is necessary that the thermodynamic model adopted accurately predict the hybrid solvent behaviour. This will ensure accurate configuration and operation selection [5]. Huang et al. [32] predicted the critical properties of various IL using the FC-CS method and then carried out thermodynamic modelling, process simulation and cost estimation of CO₂ removal (absorption) process from flue gas (6.37 mol% CO₂, 69.46 mol %N₂, 3.66 mol% O₂, 20.51 mol% H₂O) [11]. In the study, three (3) ILs ([bmim][BF₄], [bmim][DCA] and [bpy][BF₄]) blended with aqueous MEA solution were investigated. The physicochemical properties of the ILs were predicted by various temperature-dependent correlations. The phase equilibria were modelled based on the Henry's law and NRTL equation. The values calculated agree well with experimental solubility data from literature. From the process simulation assessment, the [bpy][BF₄]-MEA hybrid solvent (with 30 wt% IL and 30 wt% MEA) process gave savings of 15% and 11% regeneration duty and capture cost compared to the reference MEA based process. Other studies on process analysis of gas mixtures using IL-based solvents includes [33,34].

1.4. Aim and novelty

The aim of this study is to analyse CO₂ removal from raw natural gas in the context of natural gas sweetening using [bpy][BF₄]-MEA mixture through modelling and simulation. [bpy][BF₄] is selected mainly due to its low cost [19] and low toxicity [35] compared to the imidazolium-based ionic liquids which has been experimentally investigated successfully for removal of CO₂.

In carrying out this study, we intend to carry out an energy and cost

performance analysis for the IL-MEA process in comparison to the MEA only process. Ionic liquid-amine blends have been reported for CO₂ removal from power plant flue gases by Huang et al. [11]. However, CO₂ removal from natural gas presents a unique scenario involving higher operating pressure (up to 69 bar) and a mixture of light hydrocarbons, namely methane, ethane, propane etc. This will affect the thermodynamics of the process and mass transfer performance and possibly lead to results that are dissimilar to Huang et al. [11]. Thus, it is necessary that a study dedicated to CO₂ removal from natural gas be carried out in the quest to discover a more energy efficient solvent to replace the amine based solvent. Physical properties of the IL in this study were obtained from experimental data available in [13,15,17,36].

2. Process benchmark

2.1. Description

The process schematic for sour natural gas production and processing is shown in Fig. 2. In this process, sour gas coming from the production well flows through a separator to knock out condensates in the gas before entering the sweetening process, which is of interest in this study (Fig. 3).

The Natural gas sweetening process mainly consists of absorption and regeneration columns (See Fig. 3). Sour gas (Table 1) flows in the absorber, from the bottom stage. The lean solvent absorbs CO₂ from the sour gas by forming weakly-bonded compounds while flowing in a counter-current manner. The treated gas exits from the top of the absorber while the CO₂ rich solvent exits from bottom [6,38]. The rich solvent leaving the absorber, flows to the flash drum to remove absorbed hydrocarbons. The rich solvent leaves the flash drum to the rich/lean exchanger, where heat is absorbed from the lean solution. The heated rich solvent flows to the stripper where CO₂ is recovered from the solvent through heat input to the reboiler. The lean solvent is recycled to the absorber as it flows from the regeneration column bottom through the rich/lean exchanger, cooler and pump. The process flow diagram shown in Fig. 3 is adopted for both MEA and hybrid solvent

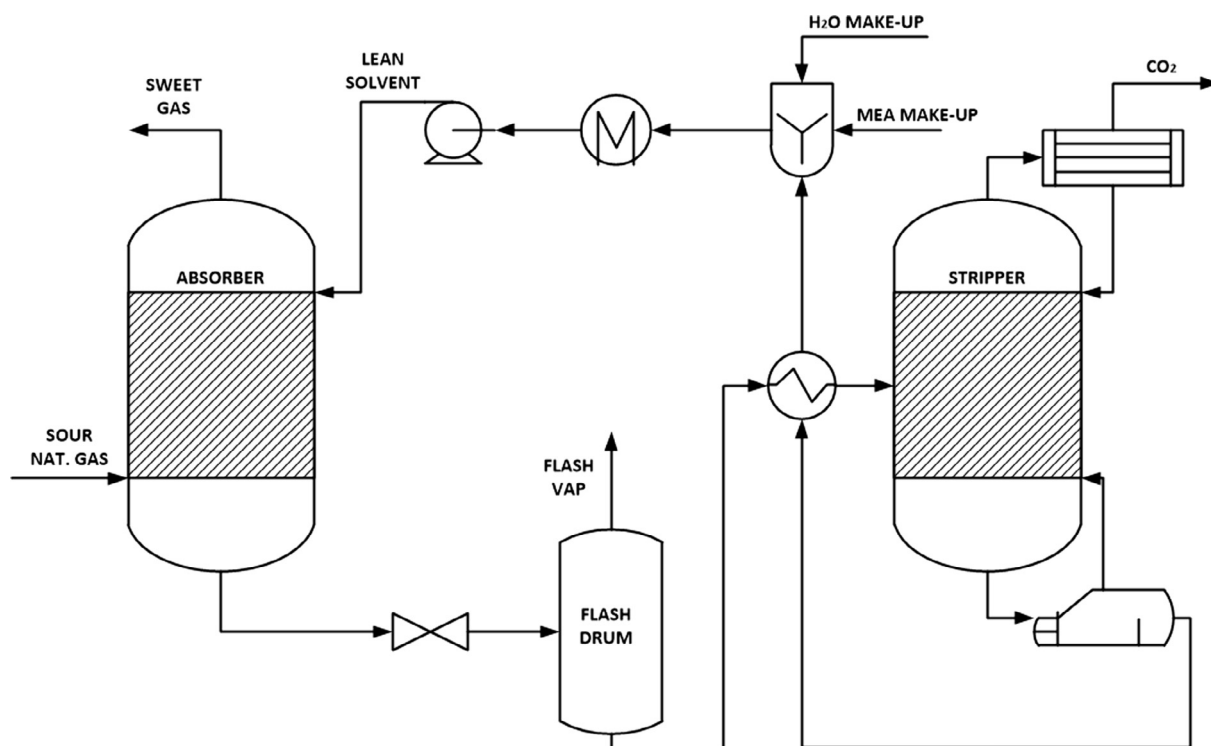


Fig. 3. CO₂ removal process Flow diagram [9].

Table 1
Sour Gas Conditions (Obtained from HYSYS [40] with modifications).

Parameters	Unit	Value
Temperature	°C	35
Pressure	bar	69
Flowrate	MMSCFD (Million Standard cubic feet per day)	25
<i>Component</i>		
Nitrogen	mol%	0.16
Water	mol%	1.22
Methane	mol%	73.76
Ethane	mol%	3.93
Propane	mol%	0.93
Carbon dioxide	mol%	20.00

based process.

3. Methodology

3.1. Model development

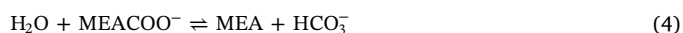
The absorber and stripper model were developed using RADFRAC model in Aspen Plus®. RADFRAC supports both equilibrium-based and rate-based approaches for mass transfer modelling. Models based on both approaches were developed in this study. In the equilibrium-based model, the liquid and gas phases are assumed to be in equilibrium [39]. On this basis, heat and mass transfer calculations are then based on estimated efficiency parameters. The rate-based model on the other hand includes detailed mass transfer calculations based on the two-film theory (Fig. 4). The following assumptions were made during the model development [39]:

- Mixed flow regime.
- Negligible heat loss to the surroundings.
- N₂ and hydrocarbon not readily soluble in IL and MEA.
- Chemical reactions are completed in the liquid film only.

3.2. Thermodynamic model

3.2.1. CO₂ removal process with MEA

Thermodynamic modelling of the conventional CO₂ removal process that involves physicochemical properties, phase equilibrium and chemical reactions of the component system was carried out using the Electrolyte Non-Random Two Liquid model (ELECRTL). The ELECRTL model is commonly used for thermodynamic modelling of MEA scrubbing process [11,39,42] and has been verified through industrial applications. The following are the set of chemical reactions considered for the system [6,9].



Temperature dependent correlations are used for estimating equilibrium constants as follows:

$$\ln k_j = A + \frac{B}{T} + \text{Cln}T + \text{DT} \quad 6$$

The reaction equilibrium constants as well as physicochemical properties (both scalar and temperature dependent) of each component, binary parameters and electrolyte pairs were retrieved from the Aspen properties databank.

3.2.2. CO₂ removal process using [bpy][BF₄]-MEA

3.2.2.1. Physicochemical properties. The properties of MEA are available in ASPEN properties databank as previously described. However, there is little information on pyridinium based ionic liquid properties in the databank. Thus, the properties of [bpy][BF₄] were obtained from literature. The scalar properties of [bpy][BF₄] such as the properties were obtained from literature (Table 2). Aspen Plus simulation software was used to estimate other relevant scalar properties of [bpy][BF₄].

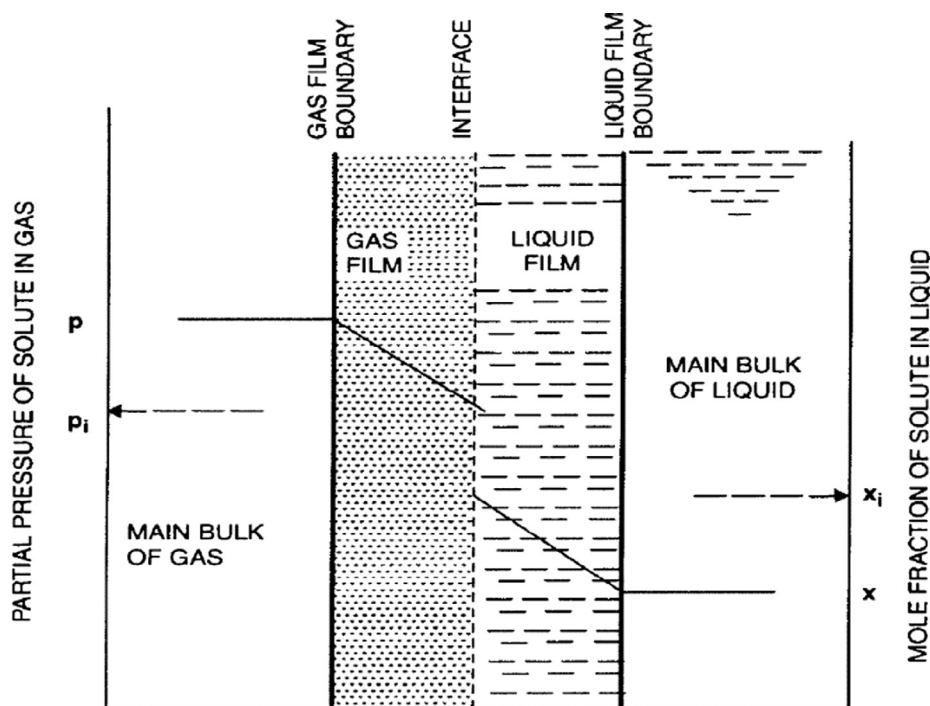


Fig. 4. Two-Film Theory [41].

Table 2
Scalar properties of [bpy][BF₄] [17,32].

Parameters	Unit	Value
T _b	K	697.9
P _c	bar	25.8
ΔH _f ⁰	kJ/mol	−1356.3
ΔH _c ⁰	kJ/mol	−5451

Temperature dependent properties of [bpy][BF₄] such as heat capacity, molar volume, surface tension, thermal conductivity were obtained using the following equations [11]:

Vapour pressure

$$\ln P_i^v = C_{1i} + \frac{C_{2i}}{T + C_{3i}} \quad (7)$$

Heat capacity

$$C_{pi} = C'_{1i} + C'_{2i}T + C'_{3i}T^2 \quad (8)$$

Molar Volume

$$V_m^l = \frac{RT_{ci}[Z_i^{*,RA}(1 + d_i(1-T_r))^{1+(1-T_r)^2}]}{P_{ci}} \quad (9)$$

Viscosity

$$\ln \eta_i = A_i + B_i/T + C_i \ln T \quad (10)$$

Surface tension

$$\sigma_i = C''_{1i}(1-T/T_{ci})^{(C''_{2i}+C''_{3i}T_{ri}+C''_{4i}T_{ri}^2+C''_{5i}T_{ri}^3)} \quad (11)$$

Thermal conductivity

$$\lambda_i = D_i + D_{ii}T + D_{iii}T^2 \quad (12)$$

The Liquid heat capacity is a basic thermodynamic property used for specifying the amount of heat needed to change a liquid temperature by a given amount while the molar volume is a transport property used to describe the volume occupied by one mole of the component at a given temperature and pressure. Given that ionic liquids are well known as a non-volatile liquid whose vapour pressure is difficult to observe [11]. Equation coefficients for (8)–(12) were estimated using data obtained from literature [13,15,17,36] on Aspen Plus® simulation software.

3.2.2.2. Phase equilibria modelling. Generally, the phase equilibrium of the CO₂-H₂O-[bpy][BF₄]-MEA system was based on ELECNRTL model. The electrolyte and interaction parameters of MEA and other components are available in ASPEN properties databank except the pyridinium based IL. The solubility of N₂ in [bpy][BF₄] was neglected [43]. The phase equilibrium relationship for CO₂ - [bpy][BF₄] system was modelled as follows:

$$\varphi_i^V \gamma_i^V P = x_i \gamma_i^* H_{ij} \quad (13)$$

$$\gamma_i^* = \left(\frac{\gamma_i}{\gamma_i^\infty} \right) \quad (14)$$

where γ_i^∞ is the infinite dilution activity coefficient of component i in the mixture. Due to the low vapour pressure of ILs, it is assumed that there will be no IL in the gaseous phase thus, the Henry's law constant of component i is defined as:

$$H_{ij} = \frac{\varphi_i^V P}{x_i \gamma_i^*} \quad (15)$$

where H_{ij} , P , x_i , γ_i^* and φ_i^V are Henry constant, total pressure, mole fraction of component i in liquid phase, activity coefficient of component i in liquid phase and the fugacity coefficient in the vapour phase respectively. Redlich-Kwong (R-K) equation of state was used to obtain

the fugacity coefficient in vapour phase as follows:

$$\ln \varphi = Z - 1 - \ln(Z - bp/RT) - \left(\frac{a/R^2 T^{2.5}}{b/RT} \right) \ln(1 + bp/ZRT) \quad (16)$$

$$Z = pV/RT \quad (17)$$

$$p = \frac{RT}{V-b} - \frac{a}{T^{0.5}V(V+b)} \quad (18)$$

$$a = 0.42748 \frac{R^2 T_c^{2.5}}{P_c} \quad (19)$$

$$b = 0.08664 \frac{RT_c}{P_c} \quad (20)$$

where φ is the fugacity coefficient, Z is the compressibility factor, R is the gas constant, a and b are equation of state constants. T_c , P_c , V are the Critical temperature, critical pressure and molar volume respectively. The Henry's constants of component i in mixture j were obtained by using the temperature dependent henry constants equation shown below [11]:

$$\ln H_{ij} = a_{ij} + b_{ij}/T + c_{ij} \ln T + d_{ij} T \quad (21)$$

where $a_{ij} - d_{ij}$ are the Henry constant binary interaction parameters. The liquid activity coefficient of CO₂ in the mixture was modelled by the NRTL using (22):

$$\ln \gamma_i = \frac{\sum_{j=1}^{\delta} x_j x_{ji} G_{ji}}{\sum_{k=1}^{\delta} x_k G_{ki}} + \sum_{j=1}^{\delta} \left(\frac{x_j G_{ij}}{\sum_{k=1}^{\delta} x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_{m=1}^{\delta} x_m \tau_{mj} G_{mj}}{\sum_{k=1}^{\delta} x_k G_{kj}} \right) \right) \quad (22)$$

$$G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$$

$$\tau_{ij} = \alpha_{ij} + b_{ij}/T + e_{ij} \ln T + f_{ij} T$$

$$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15)$$

$$\tau_{ii} = 0; G_{ii} = 1; c_{ij} = 0.3$$

where a_{ij} , b_{ij} , c_{ij} , d_{ij} , e_{ij} and f_{ij} are the binary interaction parameter, δ is the number of components and x is the mole fraction. The parameters of Henry constants and NRTL binary interaction parameters between CO₂ and [bpy][BF₄] generated by Huang et al. [11] were inputted in ASPEN Plus® simulation software. The parameters have been validated in Huang et al. [11].

For the H₂O-[bpy][BF₄]-MEA system, VLE calculation was carried out based on the modified Raoult's law as follows:

$$y_i P = x_i \gamma_i^V P_i^V \quad (23)$$

Based on the assumption that the vapour mole fraction of [bpy][BF₄] is negligible, (23) is simplified into the following equations for both H₂O-[bpy][BF₄] and H₂O-[bpy][BF₄]-MEA;

$$p = x_a \gamma_a P_a^V \quad (24)$$

$$p = x_a \gamma_a P_a^V + x_c \gamma_c P_c^V \quad (25)$$

where subscripts "a" and "c" denotes H₂O and MEA respectively [9] obtained the binary parameters of [bpy][BF₄]-H₂O and [bpy][BF₄]-MEA system from experimental data based on (24) and (25) in combination with NRTL model (22). These binary parameters obtained were used in this study.

3.3. Process simulation

Acid gas sweetening process models using aqueous MEA solvent and aqueous [bpy][BF₄]-MEA solvent were developed in Aspen Plus®. The composition of the solvents for each process are shown in Table 3. The Equilibrium based approach was basically adopted to estimate the column sizes. Under rate based approach, Bravo et al. [44] correlation

Table 3
Components and composition.

MEA		
H ₂ O	wt%	70
MEA	wt%	30
IL-MEA		
H ₂ O	wt%	40
MEA	wt%	30
[Bpy][BF ₄]	wt%	30

Table 4
Base specifications of each Unit Operation.

Unit Operation Specification		Unit
Absorber		
Theoretical stages number	20	
Column height	6	meter
Top stage pressure	6860	kPa
Packing Type	FLEXIPAC	
Packing dimension	250Y	
Packing material	Metal	
Flash tank		
Pressure	620	kPa
Heat Exchanger		
Hot/Cold outlet temperature approach	5	°C
Hot side pressure drop	0	kPa
Stripper		
Number of stages	20	
Condenser	Partial-vapour	
Top stage pressure	170	kPa
Column pressure drop	0.1	kPa
Column height	6	meter
Packing Type	FLEXIPAC	
Packing dimension	250Y	
Packing material	Metal	
Cooler		
Temperature	38	°C
Pump		
Discharge pressure	6860	kPa

was used to estimate the mass transfer coefficient and Interfacial area while the Chilton and Colburn correlation was used to estimate the heat transfer coefficients. Equipment specifications used in the process

simulation are detailed in Table 4. The model topology is given in Fig. 5.

Both process models were simulated to achieve 1 mol% of CO₂ at the absorber gas outlet and 95 wt% CO₂ concentration recovered from the stripper by manipulating the lean solvent flowrate and reflux ratio.

3.3.1. Energy performance

The specific (reboiler) heat duty is a critical parameter to measure performance in the CO₂ removal process. The specific heat duty measures heat required in the reboiler to remove 1 tonne of CO₂. In this study, the energy consumption from the energy utilizing equipment (pump and reboiler) were considered to measure the energy performance of both MEA and [Bpy][BF₄]-MEA based process. For the reboiler, it is assumed that steam is supplied from the steam boiler at a pressure of 3 bar to achieve reboiler temperature specification (120 °C).

3.3.2. Cost analysis

The cost of CO₂ removed for both process, which depends on the annual capital and operational cost, was estimated based on the breakdown adopted in [11,45]. The equipment size selection and costing was carried out using Aspen Process Economic analyzer software, based on the first quarter of 2013 chemical engineering plant cost index (CEPCI). The annual capital cost (ACC) is calculated as:

$$ACC = \frac{TCC}{((1 + r)^n - 1)/r(1 + r)^n} \quad (26)$$

where TCC is the total capital cost with an interest rate (r) and project lifetime (n) of 20% and 30 years respectively. A breakdown of the total capital and operational cost (fixed and variable cost) components following [11,45,46] is detailed in Table 5. The cost of MEA and pyridinium based ionic liquid solvents adopted for this study was 0.93 GBP/kg (1.25 USD/kg) and 4.88 GBP/kg (6.6 USD/kg) respectively [11,46].

3.3.3. Process analysis

Analysis on the impact of pyridinium based ionic liquid concentration on the energy and cost performance of hybrid solvent-based process was carried out. The mass fraction of [bpy][BF₄] in the hybrid solvent was varied while keeping the mass fraction of MEA constant. For each case considered, the process was simulated to achieve 1 mol% of CO₂ at the absorber gas outlet and 95 wt% CO₂ concentration recovered from the stripper at minimum energy consumption.

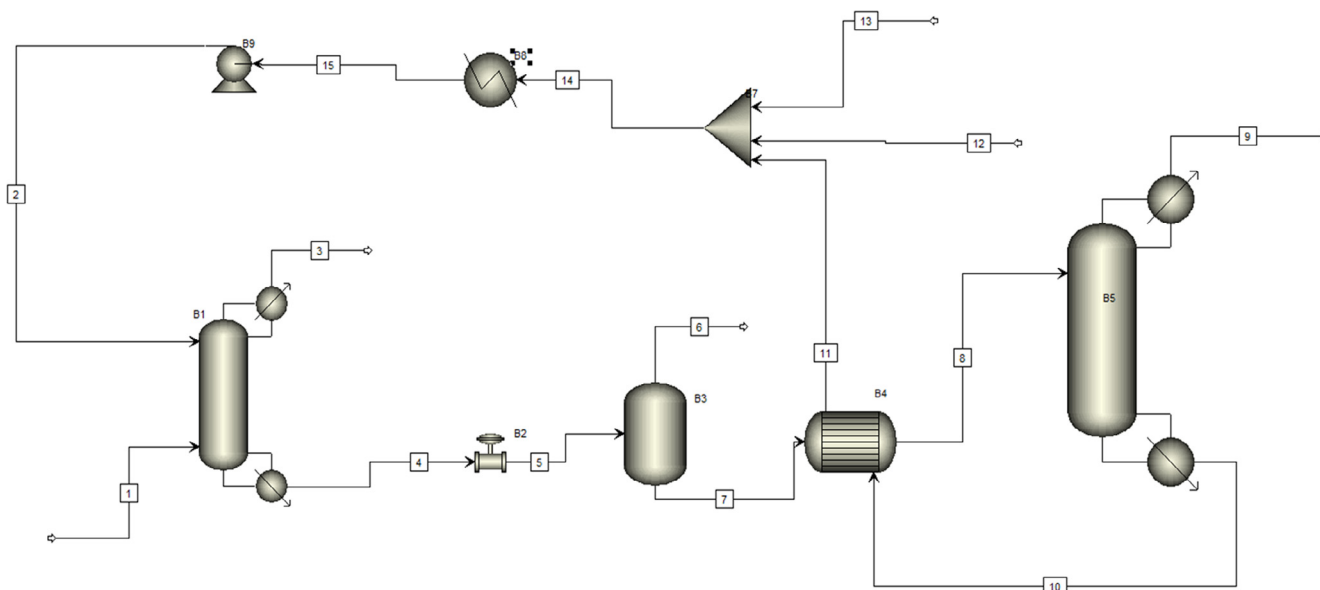
**Fig. 5.** Process model topology in ASPEN Plus®.

Table 5
Cost estimation breakdown.

Capital Cost Breakdown	(%) of Equipment Cost (EC)
Installed Cost	10% of EC
Instrumentation and Control	20% of EC
Piping	30% of EC
Electrical	5% of EC
Building and building Services	10% of EC
Yard Improvements	10% of EC
Land	5% of EC
Miscellaneous	2% of EC
Direct Cost (DC)	Sum of the above
Engineering and Supervision (E&S)	15% of DC
Contingency (C)	11% of DC
Procurement Cost (PC)	2% of DC
Indirect Cost (IDC)	E&S + C + PC
Fixed Capital Cost (FCC)	DC + IDC
Working Capital (WC)	15% of FCC
Start-up Cost (SC)	1% of FCC
Initial Solvent Cost (ISC)	Solvent circulation × cost
TCC	FCC + WC + SC + ISC
Operating Cost Breakdown	
Steam Utility Cost (£/GJ)	1.63
Cooling water Utility Cost (£/GJ)	0.157
Electricity Utility Cost (£/kWhr)	0.057
Make-up water Cost (£/kg)	0.00037
Make-up MEA Cost (£/kg)	0.925
Make-up IL Cost (£/kg)	4.884
Miscellaneous operating cost	2% of VOC
VOC	Sum of the above cost
FOC	Sum of the below cost
Local Tax (LT)	1% of FCC
Insurance	1% of FCC
Maintenance (M)	3% of FCC
Operating Labour (OL)	£ 26.64 per hr
Lab Costs	20% of OL
Supervision	20% of OL
Plant Overheads	50% of OL
Operating Supplies	15% of M
Admin Cost	15% of OL
Distribution and Marketing	0.5% of OC
R&D Cost	5% of OC
Operating Cost (OC)	VOC + FOC

Table 6
Scalar property parameters of [bpy][BF₄].

Property	Unit	
T _c	°C	723.81
DHVLB	J/kmol	6.54E+07
V _B	m ³ /kmol	0.23
RKTZRA		0.22
VLSTD	m ³ /kmol	0.18
V _c	m ³ /kmol	0.82
Z _c		0.26
P _c	bar	25.8

4. Physiochemical property validation of [bpy][BF₄]

Scalar properties and the coefficients of temperature dependent properties of [bpy][BF₄] estimated using Aspen Plus® simulation software are listed in Tables 6 and 7. The temperature dependent properties estimated by Aspen Plus® gave a good prediction when compared with

Table 7
Temperature dependent parameter for [bpy][BF₄].

Liquid Viscosity (N-sec/m ²)	
A _i	−2.435E+03
B _i	1.618E+05
C _i	3.380E+02
Liquid Surface Tension (N/m)	
C _{1i}	7.040E+01
C _{2i}	8.819E+01
C _{3i}	−4.431E+02
C _{4i}	9.597E+02
C _{5i}	−7.821E+02
Liquid thermal conductivity (W/m-K)	
D _i	1.292E+01
D _{ii}	2.453E+04
D _{iii}	3.949E−08
D _{iiii}	−2.020E−09
D _{iiiii}	2.441E−12
Liquid heat Capacity (J/kmol-K)	
C _{1i}	−2.435E+03
C _{2i}	1.617E+05
C _{3i}	3.380E+02

the experimental data retrieved from literature as shown in Fig. 6.

5. Performance comparison of MEA and [bpy][BF₄]-MEA process

Performance evaluation of both MEA-based and [bpy][BF₄]-MEA-based process was based on the following performance index: energy performance, mass transfer within the absorber, make-up solvent required, cooling water and CO₂ removal cost. The summary of results for both process simulation is shown in Table 8.

5.1. Energy performance

The specific heat duty of MEA and [bpy][BF₄]-MEA process was evaluated by varying CO₂ lean loading to achieve the minimum specific heat duty. The CO₂ loading with minimum specific heat duty for both process were compared. Fig. 7 shows the specific reboiler heat duty plot as a function of CO₂ loading. It can be seen that the specific heat duty decreases with increasing CO₂ loading until it gets to its minimum, and then a steady rise in the specific heat duty is observed as CO₂ loading is increased further. This is because at low CO₂ loading, the heat duty is mainly governed by the latent heat of vaporization. The latent heat reduces as the CO₂ loading is increased until it is constant. The sensible heat begins to have a dominant effect on the heat duty due to the increase in the solvent circulation flowrate. The minimum specific heat duty was attained at a CO₂ loading of 0.18 for MEA process and 0.11 for [bpy][BF₄]-MEA based process.

It was observed that the specific heat duty required for [bpy][BF₄]-MEA based process (3.80GJ/tonne) is less than that required for a MEA based process (4.5GJ/tonne). This is attributed to reduction of latent heat and heat capacity of the hybrid solvent in a reboiler. The reduced latent heat is as a result of reduced concentration of water to vaporize in the hybrid ([bpy][BF₄]-MEA) solvent. The presence of [bpy][BF₄] in the hybrid solvent reduces the heat capacity despite an increase in the solvent circulation flowrate.

The energy consumption for each process is shown in Fig. 8. This takes into consideration pump duty in addition to the specific heat duty. It can be seen from Fig. 8 that the reboiler accounts for the largest share of energy consumed in both MEA and [bpy][BF₄]-MEA process. From

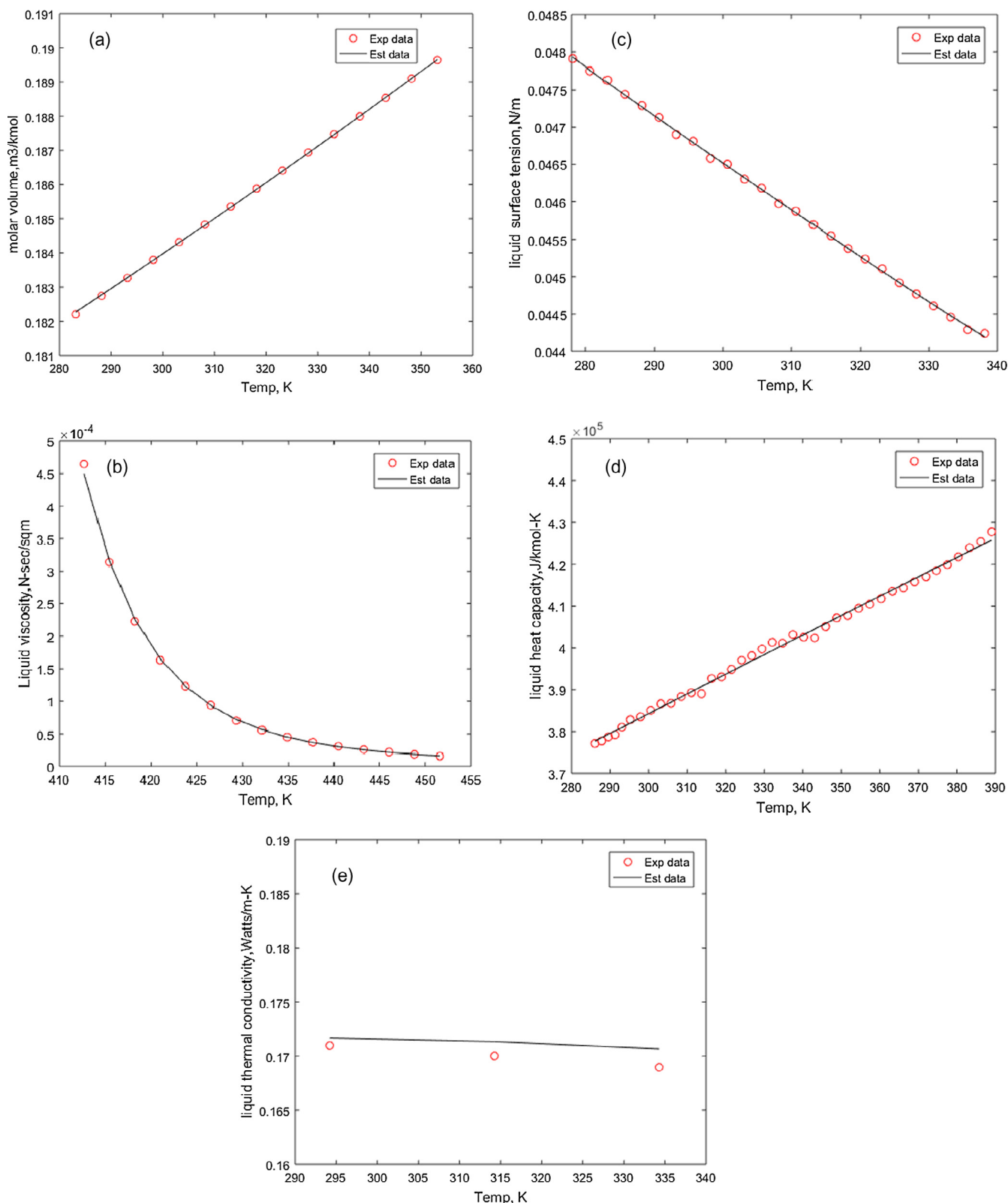


Fig. 6. Temperature dependent properties prediction for [bpy][BF₄] using Aspen Plus (a) molar volume (b) liquid viscosity (c) liquid surface tension (d) liquid heat capacity (e) liquid thermal conductivity; circles and lines denoted experimental data from literature and estimated data [13,15,17,36] respectively.

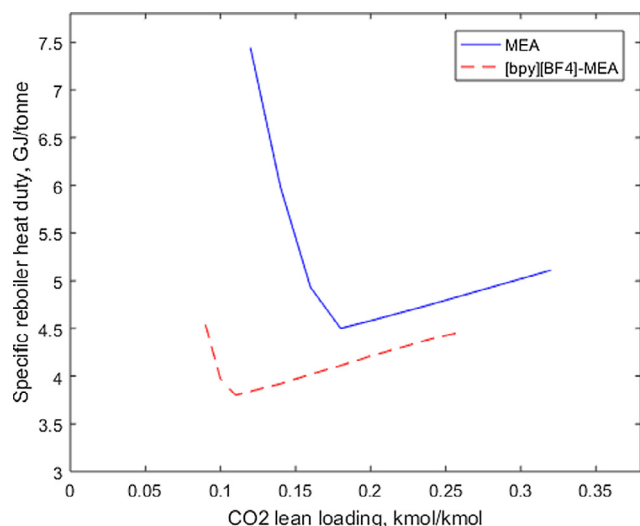
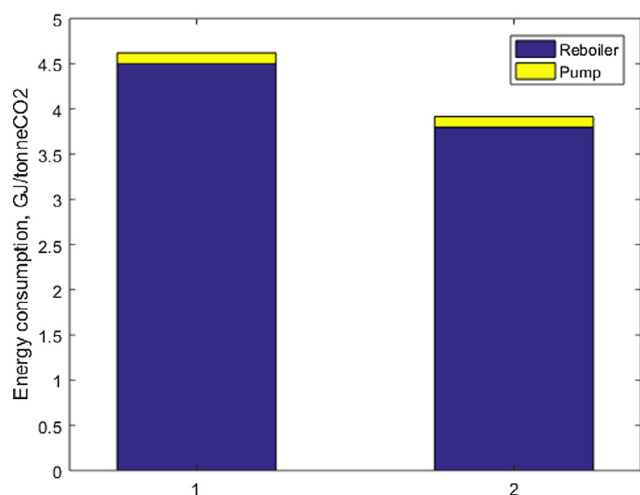
Table 8, the pump duty required for the hybrid process is slightly similar compared to the MEA based process. This is because solvent circulation flowrate required for [bpy][BF₄]-MEA based process is similar compared to the MEA based process with a percentage difference

of 5.54%. The [bpy][BF₄]-MEA based process is shown to be more energy saving in the reboiler by 15% than the conventional MEA based process.

Table 8

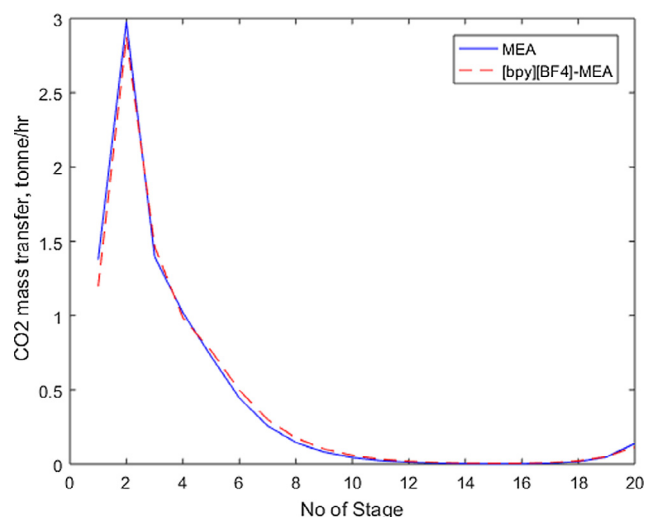
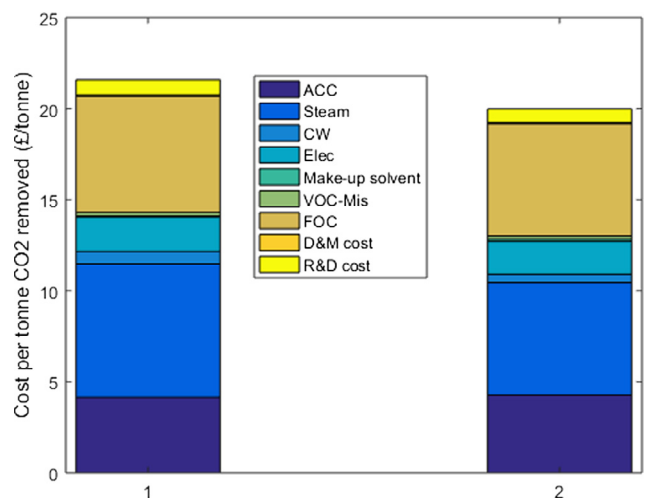
Key parameters result summary.

Process Parameters	Unit	MEA	[bpy][BF ₄]-MEA
lean solvent flowrate	kg/hr	122,931	129,737
L/G	kg/kg	4.37	4.61
CO ₂ lean loading	kmol CO ₂ /kmol solvent	0.18	0.11
CO ₂ Rich loading	kmol CO ₂ /kmol solvent	0.59	0.42
rich solvent temperature	°C	80	76
Reboiler temperature	°C	120	126
Specific heat duty	GJ/tonne CO ₂	4.50	3.80
Pump Duty	GJ/tonne CO ₂	0.12	0.11
Cooling Water	tonne/hr	1958.59	1398.71
Make-up Solvent	kg/tonne CO ₂	33.28	32.91

**Fig. 7.** Effect of CO₂ lean loading on the specific reboiler heat duty requirement of MEA and [bpy][BF₄]-MEA.**Fig. 8.** Energy Consumption for MEA (1) and [bpy][BF₄]-MEA (2) based process.

5.2. Mass transfer

The mass transfer performance of both process was evaluated by plotting the mass transfer rate of CO₂ from the vapour phase to liquid phase in the absorber. As shown in Fig. 9, both process gave a similar mass transfer performance. Despite this, it was observed from Table 8 that the solvent circulation rate for the MEA based process is slightly reduced by 5.54% compared to the [bpy][BF₄]-MEA based process to

**Fig. 9.** CO₂ mass transfer rate (kmol/hr) in the Absorber for MEA and [bpy][BF₄]-MEA based process.**Fig. 10.** Breakdown of the Cost of CO₂ removed for (1) MEA-based process and (2) [bpy][BF₄]-MEA based process.**Table 9**Breakdown of the Cost of CO₂ removed for (1) MEA-based process and (2) [bpy][BF₄]-MEA based process.

Cost	MEA –based process (£/CO ₂ removed)	[bpy][BF ₄]-MEA based process (£/CO ₂ removed)
ACC	4.15	4.25
VOC steam	7.33	6.19
VOC water	0.67	0.45
VOC electricity	1.91	1.80
Make -up Solvent	0.04	0.13
VOC Miscellaneous	0.20	0.17
FOC	6.37	6.15
Distribution & market	0.08	0.07
R&D cost	0.83	0.75
Total	21.58	19.98

achieve the same CO₂ removal specification. This is attributed to the high viscosity, molecular weight and density of the [bpy][BF₄]-MEA solvent compared with MEA.

5.3. Make-up solvent

The make-up solvent is measured as the kg of solvent per tonne of

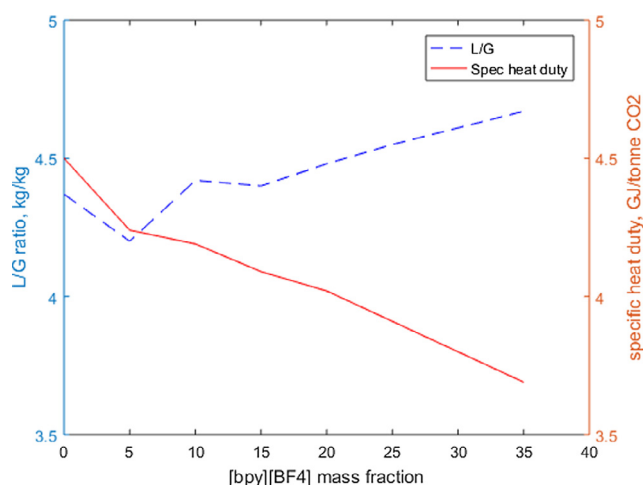


Fig. 11. Effect of [bpy][BF₄] mass fraction on L/G (kg/kg) (dashed line) and Specific heat duty (GJ/tonne CO₂) (straight line) in the [bpy][BF₄]-MEA based process.

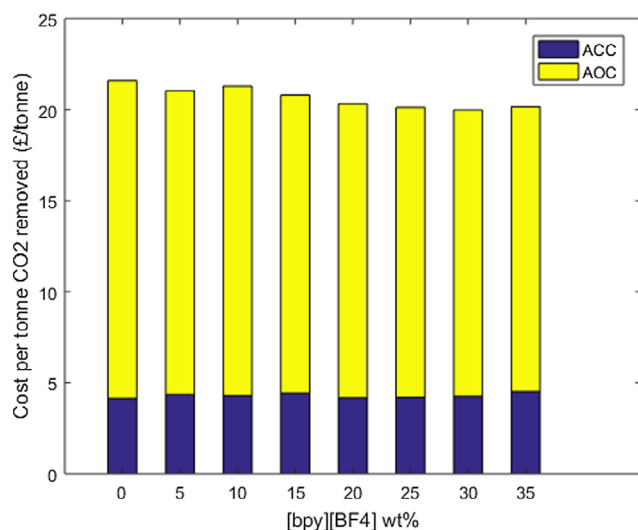


Fig. 12. Effect of [bpy][BF₄] mass percentage on the Cost of CO₂ removed.

CO₂ removed. From Table 8, the make-up solvent needed for the [bpy][BF₄]-MEA process is slightly lower than make-up needed for MEA process. The make-up solvent is composed of mainly MEA and H₂O. This is basically due to the low vapour pressure of [bpy][BF₄], which reduces degradation of the ionic liquid. Thus making make-up for [bpy][BF₄] negligible.

5.4. Cooling water

The cooling water required for [bpy][BF₄]-MEA based process and MEA based process takes into consideration the cooling water required in condenser and cooler. The [bpy][BF₄]-MEA process requires less cooling water required compared with MEA process. The reduced amount of water vaporized in the stripper reduces cooling water required in the condenser duty to achieve CO₂ purity specification. The cooling water required in the cooler is reduced for the [bpy][BF₄]-MEA based process due to the increased temperature of the inlet stream to the cooler.

5.5. Cost analysis

A breakdown of the cost of CO₂ removed is shown in Fig. 10. This includes the annual capital cost (ACC), which is a reflection of mainly

the equipment cost and initial solvent circulation cost, as well as the operating cost, which include variable operating cost (VOC) and fixed operating cost (FOC). The capital cost of the hybrid CO₂ removal process is higher than the MEA based process by 2.48%. This is due to the increase in initial solvent circulation rate and high cost of [bpy][BF₄]. It was also observed that steam cost mainly governs the process operating cost. From the study, the steam cost in the [bpy][BF₄]-MEA process was reduced by 15.55% compared with the MEA based process. Despite the increased solvent make-up cost for the [bpy][BF₄]-MEA based process, it was observed that the solvent make-up cost accounts for small percentage (0.18% and 0.67%) of the total cost of CO₂ removed for both process. The low steam cost is reflected on the reduced total cost of CO₂ removed in the [bpy][BF₄]-MEA based process (£19.98/tonne CO₂) compared with the MEA based process (£21.58/tonne CO₂). This showed an energy saving cost of £1.6/tonne CO₂ for [bpy][BF₄]-MEA based process. Based on the model result, 85,021 tonnes of CO₂ is capture annually. This implies that a savings of £136,033.06 is attained annually by adopting [bpy][BF₄]-MEA solvent, indicating that the hybrid solvent-based process is a cost-saving system. See Table 9 for details on the cost of CO₂ removed.

6. Effect of [bpy][BF₄] concentration

Fig. 11 shows a plot on the effect of [bpy][BF₄] Concentration on the L/G ratio of the absorber and reboiler heat duty. The L/G ratio and specific heat duty reflects the solvent circulation rate and the reboiler steam rate required to meet CO₂ removal specifications. The concentration of [bpy][BF₄] in the hybrid solvent was varied 0 wt% to 35 wt%. 0 wt% of [bpy][BF₄] represents the MEA based process. It was observed that an introduction of a small concentration (5 wt%) of [bpy][BF₄] slightly reduces the L/G ratio but a further [bpy][BF₄] concentration increase resulted to relatively steady rise in the L/G ratio. Also, the specific reboiler heat duty reduces as the concentration of [bpy][BF₄] is increased. This indicates that less amount of steam, which basically governs the CO₂ removal cost, is required in the reboiler to meet the CO₂ removal specification with increasing [bpy][BF₄] concentration. This is attributed to decreasing heat capacity of the hybrid solvent as with the presence of [bpy][BF₄] in hybrid solvent.

The plot in Fig. 12 shows the cost of CO₂ removed (as annual capital cost (ACC) and annual operating cost (AOC)) as a function of the concentration of [bpy][BF₄]. This is to investigate the concentration of [bpy][BF₄] required in the hybrid solvent to achieve the minimum cost of CO₂ removed. From Fig. 12, The minimum cost of CO₂ removed (£19.98/tonne CO₂) was attained at 30 wt% of [bpy][BF₄]. This is due to the reduced annual operating cost despite the increase in annual capital cost. It can be seen from Fig. 12 that after 30 wt% of [bpy][BF₄], the cost of CO₂ removed increases. This implies that the significance of capital cost to the cost of CO₂ removed increases because of the initial solvent cost increased despite the reduced operating cost.

7. Conclusion

Application of IL-MEA process for CO₂ capture from power plant flue gases has been [11]. Similar investigation has not been performed for CO₂ removal process in natural gas cleaning in operations. This study aims to fill the gap by providing a comparative study of conventional MEA and IL-MEA based process for natural gas sweetening through modelling and simulation. This study assesses the process and energy performance of the hybrid (IL-MEA) solvent, which can replace the conventional amine as the future solvent.

The physiochemical properties of IL ([bpy][BF₄]) used in this study were estimated using Aspen Plus®. The results were shown to agree well with the experimental data from literature. The [bpy][BF₄]-MEA based process with lean solvent composition of 30 wt% MEA, 30 wt% [bpy][BF₄] and 40.0 wt% H₂O showed an energy savings of 15% in the reboiler duty and a reduction of 7.44% in the cost of CO₂ avoidance

compared to the MEA (30 wt%) based process. Despite the reduced solvent circulation rate in the MEA based process and high cost of [bpy][BF₄], the hybrid solvent-based process proved to be more cost efficient. This is due to the reduced operating cost of the [bpy][BF₄]-MEA based process as result of the low utilities (majorly steam) cost. Further analysis on the effect of [bpy][BF₄] concentration on the process performance and cost of CO₂ removed was carried out. An increase in the concentration of [bpy][BF₄] resulted in a rise in L/G ratio (solvent circulation rate) and a reduction in the overall energy consumption. Also, the cost of CO₂ removed is reduced with increasing [bpy][BF₄] concentration. From the economic analysis, the 30 wt% concentration of [bpy][BF₄] in the [bpy][BF₄]-MEA based process achieved the minimal cost of CO₂ removed. Thus, [bpy][BF₄]-MEA based solvent was able to achieve an energy and cost-efficient capture process.

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