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Techno-economic feasibility of ionic liquids-based CO₂ chemical capture processes

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ABSTRACT

A techno-economic assessment of Ionic Liquids (ILs)-based post-combustion, biogas and pre-combustion CO₂ chemical capture processes was carried out using Aspen Plus and Aspen Process Economic Analyzer (APEA). This cost estimation procedure is newly integrated to our COSMO-based/Aspen Plus methodology used to design the chemical absorption processes with 90% of CO₂ capture. The equipment investment and variable operating cost were analyzed relating to the process operating conditions and the IL performance. The total annualized cost was used as the index to economically evaluate the processes at three CO₂ treatment capacities and employing three different ILs: [P₂₂₂₈][CNPyrr], [P₆₆₆₁₄][CNPyrr] and [Bmim][acetate]. It benefits from economy of scale as well as it is directly related to both IL enthalpy of reaction and process gap capacity, being [P₂₂₂₈][CNPyrr] -which has the most exothermic reaction and highest gap capacity- the solvent achieving the lowest costs. Current results indicate that operating at vacuum pressure to better regenerate the IL entails a remarkable cost penalty. Hence, both capital (CAPEX) and operational expenses (OPEX) could be reduced to achieve a total cost of 81.32 \$/t_{CO2} for [P₂₂₂₈][CNPyrr] in post-combustion CO₂ capture when regenerating the IL at atmospheric pressure and 121.5 °C. Three IL pricing basis were considered when calculating the solvent cost. A conservative IL scaled up price of 50 \$/kg only increments around 5% the total annualized cost of the process.

1. Introduction

The demand of fossil fuels for energy production carries an enormous release of CO₂ into the atmosphere, which is an aggravating of global greenhouse effect causing global warming and climate change [1,2]. It was estimated that more than 33 thousand million metric tons of CO₂ are emitted in the global atmosphere every year [1], so the prevention of harmful effects of CO₂ release in the atmosphere is needed. Carbon capture technology (i.e., pre-combustion, oxy-combustion or post-combustion) is widely developed to reduce CO₂ emissions in power and industrial plants [2,3]. CO₂ separation has been used for decades in natural gas sweetening process at large scale [2,4]. At the present time, biomethane is becoming a promising alternative to natural gas since it comes from raw biogas, so the high CO₂ (15–50 mol%) content and other impurities must be removed to obtain the enriched methane [5–7]. Technologies based on amine scrubbing using monoethanolamine (MEA), diethanolamine (DEA) and methyldiethanolamine (MDA) as absorbents, performed efficiently for CO₂ capture through the formation of carbamate and carbonate [8–10]. Considering the available amine solvents for CO₂ capture, 30% of MEA in water solution is pondered as industrial benchmark due to its great properties [11]. The CO₂ absorption capacity of MEA is about 2 mol of MEA per each mol of CO₂ at 25 °C and atmospheric pressure

[12]. However, the chemical reaction involves a large CO₂ enthalpy of reaction which implies high-energy consumption in the regeneration process [13]. By incorporating a CO₂ capture unit into an existing power plant using conventional amine scrubbing, this would lower the energy yield around 25–40% [14]. The technical challenge in regard to amine scrubbing remains at the insufficient carbon capture capacity, high absorbent volatility, equipment corrosion and high energy requirements [15]. Regarding the economy of the process, many studies estimated the cost of the MEA-based post-combustion CO₂ capture process in the range of 51–147 \$/t_{CO2} [13,16–19]; others reported 173 \$/t_{CO2} for biogas upgrading [20] and 27 \$/t_{CO2} for natural gas CO₂ removal [21].

Recent works have been focused on the development of new stable solvents with less energy requirement in its regeneration stage. In this sense, Ionic Liquids (ILs) have revealed that present a significant impact for CO₂ capture due to their unique characteristics. Mainly, ILs are able to absorb CO₂ and other acid gases demanding less energy in the regeneration step than conventional amine-based solvents [10,15,22–27], although vacuum is usually required [15,20,25,28]. However, their current intense solvent demand and price may make these systems not economical comparable with conventional solvents [13,19,20,23,29]. The U.S. Department of Energy established a cost target of 40 \$/t_{CO2} for new generation solvents [23,26].

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Regarding the techno-economic evaluation of CO₂ absorption processes with ILs, J. de Riva et al. [23] estimated a variable operating cost of 83 \$/t_{CO2} for post-combustion CO₂ capture using 1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]-imide ([Emim][NTf₂]) whereas the lowest total cost achieved by M. Mota-Martinez et al. [19] using an IL physical absorbent is 90 \$/t_{CO2} with 1-ethyl-3-methylimidazolium dicyanamide ([Emim][DCN]); more than 175 \$/t_{CO2} employing [Emim][NTf₂]. P. García-Gutiérrez et al. [20] reported a techno-economic assessment for [Emim][NTf₂], 1-Hexyl-3-methylimidazolium bis[(trifluoromethyl)-sulfonyl]imide ([Hmim][NTf₂]) and trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)-sulfonyl]imide ([P₆₆₆₁₄][NTf₂]) as physical absorbents for biogas upgrading, placing [Emim][NTf₂] as the most economical alternative with a total cost of \$271 per metric ton of captured CO₂. Y. Ma et al. [15] also registered costs for 1-butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]-imide ([Bmim][NTf₂]). T. E. Akinola et al. [21] used a mixture of 1-butylpyridinium tetrafluoroborate, [Bpy][BF₄], MEA and H₂O (30/30/40 wt%) for natural gas CO₂ removal, finding an optimistic cost (25 \$/t_{CO2}) to achieve an energy and cost-efficient capture process. Y. Huang et al. [18] also studied the economy of [Bpy][BF₄]-MEA based processes to capture CO₂ from flue gas, reducing the cost of the conventional MEA-based process from \$70 to \$60–\$62.5 per metric ton of CO₂. M. B. Shiflett et al. [16] presented a process equilibrium-based simulation for 1-butyl-3-methylimidazolium acetate, [Bmim][acetate], which chemically absorbs CO₂, reporting a total cost of 140 \$/t_{CO2}. H. Zhai et al. [26] published a cost of 62.4 \$/t_{CO2} for [P₆₆₆₁₄][CNPyrr] using a 2011 price basis which greatly benefits from economy of scale. The huge size of the absorption and stripping columns might question about the technical viability of the post-combustion capture process.

Several analyses have been carried out using amine solutions, mixtures of amines with IL or ILs with CO₂ physical absorption, but to the best of our knowledge, a systematic study using different ILs with CO₂ chemical absorption has not been conducted. Therefore, the aim of the present paper is to evaluate the techno-economic feasibility of using ILs in three different CO₂ chemical capture process configurations (post-combustion, biogas, and pre-combustion). We propose a rigorous and systematic procedure from equipment selection to cost estimation. Aspen Plus and Aspen Process Economic Analyzer were used to simulate CO₂ capture processes and estimate their costs, respectively. The capital investment and the operating cost were analyzed attending to the operating conditions, and IL properties in order to not only identify the cost penalties of the process but also clarify the wanted IL characteristics in terms of economic criteria for the three different configurations. Three CO₂ treatment capacities: 1 kmol/h (pilot plant [15]), 10 kmol/h (small biogas upgrading plant [28]) and 100 kmol/h (industrial scale [23]) were studied. To do so, three ILs chemical absorbents: triethyl(octyl)phosphonium 2-cyanopyrrole ([P₂₂₂₈][CNPyrr]), trihexyl(tetradecyl)phosphonium 2-cyanopyrrole ([P₆₆₆₁₄][CNPyrr]) and 1-butyl-3-methylimidazolium acetate ([Bmim][acetate]) were studied as they were found to be the ILs with the highest performance for CO₂ capture among other IL chemical absorbents in a previous work [25]. A wide IL pricing range of values from 500 to 5 \$/kg was examined to quantify the impact in the process total cost that using IL means. This analysis methodically evaluates for the first time the economy of different IL-based CO₂ chemical capture processes and guide future ab-

sorbent and process optimizations to propose a techno-economically viable industrial alternative able to replace the conventional amine plants.

2. Simulation and cost estimation methodology

2.1. Component definition and property method specification

The post-combustion, biogas and pre-combustion CO₂ capture processes were modeled using Aspen Plus v10 commercial process simulator. The three ILs and their reaction products were introduced as pseudo-components into the simulator following a successful multiscale COSMO-based/Aspen Plus methodology, supported with experimental data and described in detail in prior works of our group [30]. As summary, quantum chemical structure optimizations and COSMO-RS calculations of the ILs and their reaction products were performed to fully specify the COSMOSAC property method for Aspen Plus simulations (in code 1, COSMOSAC method by Sandler et al. [31]). The experimental temperature dependent ILs viscosity data was added into the Aspen Properties to better describe the CO₂ mass transfer kinetics [30]. To define the chemical absorption of CO₂ in the selected ILs using Aspen Plus, CO₂-ILs experimental absorption isotherms were successfully fitted to a thermodynamic model in which the physical absorption is described by Henry's Law and the chemical equilibrium reaction considers the right stoichiometry of reaction depending on the IL (1:1 mechanism for AHA-ILs and 2:1 mechanism for [Bmim][acetate]) as explained elsewhere [25]. Hence, CO₂ was defined as Henry component into Aspen Properties and Aspen Plus Reactive-Distillation equilibrium reaction type was utilized to introduce CO₂-ILs chemical reactions [25]. Table 1 collects the ILs physical and chemical properties estimated by this COSMO-based/Aspen Plus approach. The thermodynamic, chemical reaction and kinetic parameters used to define the CO₂-ILs systems in Aspen Plus simulations are reported in Table S2 of Supplementary Material.

2.2. Stream model and process design

The inlet gas stream for post-combustion, biogas and pre-combustion processes was defined according to the operating conditions summarized in Table 2. The compositions were simplified to two major constituents (CO₂ plus N₂, CH₄ or H₂), so other typical compounds such as sulfur dioxide or water are not considered in this study.

The scheme of the ILs-based CO₂ capture process is shown in Fig. 1. The gas stream to be treated (S-01) enters in the absorption column (T-100) at the inlet conditions summed up in Table 2 where takes place the absorption of 90% of the CO₂ fed when contacting the recirculated IL from the regeneration column (S-07) at adiabatic operating conditions. The CO₂ cleaned gas (S-02) exits the absorber through the top meanwhile in bottom the saturated absorbent stream (S-03) leaves the tower to be pressurized (P-100) to reach the regeneration column (T-101), which operates under vacuum pressure conditions (E-100 and C-100). This configuration does not present a preheating step, so the column forced circulation (P-101) reboiler (E-101) supplies the heating needed to achieve the IL regeneration. This type of reboiler was considered because of the ILs high viscosity [32–35]. The CO₂ captured leaves the column after its desorption (S-04) and the IL regenerated (S-

Table 1

ILs estimated physical properties, CO₂-ILs Henry's (K_H), reaction equilibrium (K_{eq}) constants and enthalpy of reaction (ΔH_R) at 40 °C.

	MW (g/mol)	ρ (g/cm ³)	μ (cP)	K_H (bar)	K_{eq}	ΔH_R (kJ/mol)
[P ₂₂₂₈][CNPyrr]	322.47	0.94	163.45	66.97	1389.84	47.72
[P ₆₆₆₁₄][CNPyrr]	574.95	0.90	166.42	39.33	421.61	39.77
[Bmim][acetate]	198.26	1.03	179.79	93.14	65.56	35.12

Table 2
Inlet gas streams characteristics.

	Post-combustion	Biogas	Pre-combustion
Temperature (°C)	40	40	40
Pressure (bar)	1	3.2	32.7
CO ₂ molar flow (kmol/h)	1–100	1–100	1–100
Composition (%mol)	x _{CO₂}	13	38
	x _{N₂}	87	–
	x _{CH₄}	–	62
	x _{H₂}	–	60

05) is pressurized (P-102) and cooled (E-102) before it is recirculated to the absorption column (T-100).

2.3. CO₂ absorption unit

The CO₂ absorption unit was modeled as a packed column (T-100 in Fig. 1) using the RADFRAC rigorous model implemented in Aspen Plus v10. Calculations were performed in Rate-based mode to consider the CO₂ mass transfer kinetic process. Aspen Plus Reactive-Distillation equilibrium reaction type was utilized to define the chemical reaction between each IL and CO₂ as it can be enabled in RADFRAC column model. The K_{eq} equation is specified with the parameters (see Table S2 of Supplementary Material) estimated from the experimental isotherms as explained before [25]. The reaction occurs in the liquid phase and the equilibrium constant basis is the mole fraction.

The proposed gas streams for pre-combustion, biogas and post-combustion CO₂ capture are reported in Table 2. These gas streams were fed to the absorption column at 40 °C and different CO₂ partial pressures (0.13–13 bar) depending on the treatment process. The absorber operates at the corresponding inlet stream total pressure and adiabatic operating conditions, employing the necessary IL flow rate to achieve a 90% of CO₂ recovery for each system. Three CO₂ constant flows from 1 to 100 kmol/h were considered to study the plant size influence in process costs.

The column was discretized by 10 stages, it consisted of a 15 m of packing height for the biggest scale (100 kmol/h of CO₂) and the diameter needed to keep a fractional capacity of 80% in all cases, which was calculated by Column Internals' Interactive sizing tool. The resulting pressure drop across the column was also considered. When operating with lower gas flow rates, the column height was reduced to maintain the height to diameter ratio. The Flexipac 700Y structured packing was selected for the absorber.

2.4. ILs regeneration unit

The ILs regeneration unit consists of a stripping column (T-101 in Fig. 1) in which its forced circulation (P-101) reboiler (E-101) supports the sensible heat to get the regeneration temperature, the energy required to generate the vapor stripping stream (mainly CO₂ desorbed) and the energy needed to reverse the chemical reaction between CO₂ and each IL. It operates at 100 °C and 0.1 bar of vacuum pressure in order to avoid ILs thermal decomposition [36], so a vacuum unit was joined. Aspen Plus isentropic compressor model (C-100) estimates the vacuum energy by emulating the pressure drop from 1 to 0.1 bar directly to the vapor after cooling it to 35 °C (E-100). The saturated IL stream (S-03) leaving the absorber (T-100) does not suffer any preheating that involves energy saving before entering the regeneration column (T-101) meanwhile the regenerated IL is not only pressurized to reach the top of the absorption column (P-102) but also cooled to 40 °C (E-102). The RADFRAC rigorous column model calculating in Rate-Based mode 6 computation stages- and including the Reactive-Distillation reaction was utilized to simulate the regeneration column. Column Internals type of packing is Flexipac 700Y, the Interactive sizing option determined the column diameter for a fractional capacity of 80% and the right height was fixed to preserve a height to diameter ratio equal to 5 [37] in all cases.

2.5. Pumps

The discharge pressures of the circulation pumps P-100 and P-102 shown in Fig. 1 were calculated using the pipeline model implemented in Aspen Plus. In order to do that, the length considered was equal to

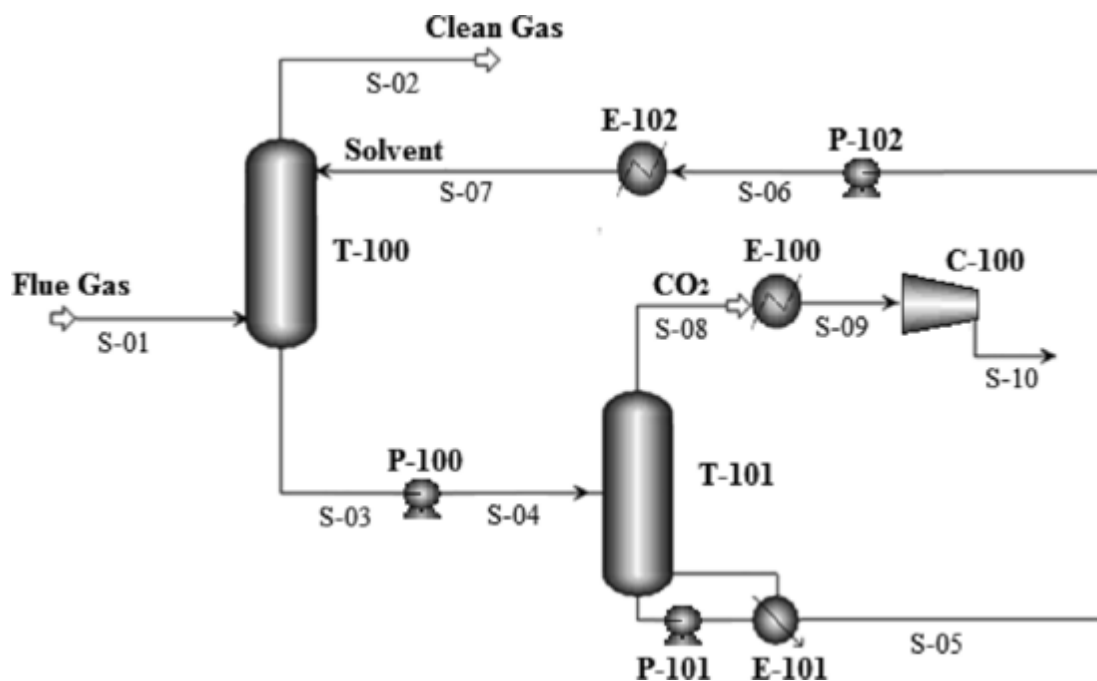


Fig. 1. ILs-based CO₂ chemical absorption process diagram.

the height of the column in which the fluid is discharged, a pipe diameter to maintain a fluid velocity below 0.6 m/s [38] and an angle of 90° were specified. Gear's model integration method and Beggs-Brill frictional and hold up correlations selected by default were utilized. The outlet pressure and temperature conditions were fixed. S-03 pressure (S-01 pressure, see Table 2) and temperature were used for P-100 meanwhile S-05 temperature (100 °C) and S-07 pressure (S-03 pressure plus absorber pressure drop) were used for P-102. The forced circulation reboiler pump (P-100) is not a simulation block so it is only considered for the economic analysis.

2.6. Cost estimation

The main objectives of this work are the preliminary estimation and analysis of the IL-based CO₂ capture process costs associated to plant erection (capital cost) and operation (operational cost) at post-combustion, biogas and pre-combustion operating conditions.

On the one hand, the capital expenses (CAPEX) components (direct and indirect costs) are reported in Table 3. The capital direct cost (CDC) represents the investment necessary for the purchase and installation of all the equipment assembling the unit operations of the process (see Fig. 1). The equipment selection (mapping), sizing and costing was carried out using Aspen Process Economic Analyzer (APEA) v10, which employs a 2016 pricing basis and it is integrated in Aspen Plus v10. Template US_IP was applied. The mapping and sizing of the equipment is required to create the volumetric model that APEA uses to estimate the cost. Both absorption (T-100) and regeneration columns (T-101) were mapped as single diameter packed towers, all pumps (P-

100, P-101 and P-102) were considered reciprocating positive displacement plunger pumps due to the high ILs viscosity [37], the vacuum compressor (C-100) was mapped as a reciprocating compressor [37], coolers (E-100 and E-102) were shell and tube heat exchangers and the selected type of reboiler (E-101) was a horizontal thermosyphon as it is the best of the three available reboiler options to deal with viscous fluids (TEMAs BJM) [32–35]. Notice that the forced circulation reboiler (P-101 and E-101) is included in the proper P&ID configuration of the regeneration column RADFRAC model when mapping. APEA sizing step was specified using the simulation blocks results. The equipment cost was analyzed for post-combustion, biogas and pre-combustion processes (100 kmol/h of CO₂) employing [P₂₂₂₈][CNPyrr]. APEA investment analysis tool reports the CDC result involving not only the purchased equipment cost but also piping, civil, structural steel, instrumentation, electrical, insulation, paint and manpower costs associated to the in-plant installation, similar as it is done by methods based on the percentage of equipment cost [16,20,21,39] to estimate this cost (see Table S5-S9 of Supplementary Material). Capital indirect costs (CIC) such as engineering or contingency costs are also estimated by APEA and hence, considered in this study.

On the other hand, the operating expense (OPEX) was estimated based on the breakdown (variable and fixed costs) detailed in Table 3. The variable operational cost (VOC) was calculated as the sum of the costs of the electricity consumed by the pumps (P-100, P-101 and P-102) and the vacuum compressor of the process (C-100), the low pressure steam required in the regeneration column reboiler (E-101) and the cooling water used as refrigerant in the vacuum unit (E-100) and in the cooler prior to the absorption column (E-102) that reduces the recirculated IL temperature. The pumps and vacuum compressor power consumptions were calculated fixing a pumping/compression efficiency of 60% and a driver (electric motor) efficiency of 85% in Aspen Plus simulations according to heuristic rules [37]. The utilities Electricity, LP steam and Cooling Water and their energy prices implemented by default in Aspen Plus were assumed when calculating the OPEX. The electricity and thermal utilities prices are summarized in Table 3. The VOC was analyzed at post-combustion, biogas and pre-combustion operating conditions (100 kmol/h of CO₂) employing [P₂₂₂₈][CNPyrr]. Fixed operating cost (FOC) includes maintenance, supervision, operating labor, operating charges, plant overhead and administrative expenses [39].

Then, the total annualized cost (TAC) was calculated and used as the index to evaluate the economic performance of each process [13,19–21] at three plant capacity sizes (1, 10 and 100 kmol/h of CO₂ in S-01) and employing three different ILs without considering the IL cost yet:

$$TAC = CFR \cdot \sum_n^{units} CAPEX_n + \sum_m^{units} OPEX_m \quad (1)$$

where CFR is the capital recovery factor which is a function of an interest rate (*i*) and an annuity period (*a*):

$$CFR = \frac{i \cdot (1 + i)^a}{(1 + i)^a - 1} \quad (2)$$

In this work, an interest rate of 10% and an annuity period of 25 years were considered [13,19]. The process was supposed to be operating continuously 8000 h/year [20,40].

Finally, the solvent cost was introduced into the TAC. An IL pricing range from 500 to 5 \$/kg were considered, particularly attending to three representative scenarios: laboratory manufacture (500 \$/kg) [22,28], scaled production (50 \$/kg) [16,19,20,23,28,41] and amines (5 \$/kg) pricing basis [16,18,21,28,41]. The solvent cost was estimated attending to both absorption (T-100) and regeneration (T-101) column liquid hold up [23], which is the amount of IL in the

Table 3
Assumptions for capital (CAPEX) and operational (OPEX) costs estimation.

CAPEX	
Process equipment (columns, heat exchangers, pumps and compressor)	
Plant general equipment	
Equipment setting	
Piping	
Civil	
Steel	
Instrumentation	
Electrical	
Insulation	
Paint	
Capital direct cost (CDC)	Sum of the above
Engineering, design & procurement cost	
Other project costs: construction indirects, taxes, contract fee, general & administrative overheads, etc.	
Contingency	
Capital indirect cost (CIC)	Sum of the above
Fixed capital cost (FCC)	CDC + CIC
Working capital (WKC)	10% of FCC
Initial IL cost	Mass of solvent (kg) · cost (\$/kg)
Total CAPEX	Sum of the above
OPEX	
Electricity	0.0775 \$/kWh
Low Pressure Steam (125 °C, 2.3 bar)	1.90·10 ⁻⁶ \$/kJ
Cooling Water (20 °C)	2.12·10 ⁻⁷ \$/kJ
Make-up IL cost	10%-mass of solvent (kg) · cost (\$/kg)
Variable operating cost (VOC)	Sum of the above
Maintenance (M)	2% of FCC
Operating labor (OL)	2 operators · 20 \$/h
Supervision (S)	1 supervisor · 35 \$/h
Operating charges (OCH)	25% of OL + S
Plant overhead (PO)	50% of OL + S + M
General & administrative costs	8% of VOC + OL + S + M + OCH + PO
Fixed operating cost (FOC)	Sum of the above
Total OPEX	VOC + FOC

packing surface. This column liquid hold up is calculated by the RAD-FRAC Column Internals hydraulics in Aspen Plus simulations. The obtained total volume multiplied by the average density of the liquid inside each column gives the mass of IL in the packing section. It might be also a little quantity of IL in columns liquid distributors and other accessories which is pondered to be an extra 15% in each packed tower. A 10% of the IL is assumed to be circulating through the overall process when calculating the total IL needed [23]. This IL cost is considered an initial investment (see Table 3). As the three ILs used in this work are supposed to be low volatile and chemically stable under the operating conditions of this study, only a 10% of the IL is replaced annually and computed as an operating cost [19] (see Table 3).

3. Results

3.1. Technical evaluation

As starting point for this work, Table 4 shows the performance evaluation of the ILs-based capture processes: energy demand, solvent required and columns size carried out previously by our group [25]. It summarizes results for the post-combustion, biogas and pre-combustion systems simulations using [P₂₂₂₈][CNPyrr], [P₆₆₆₁₄][CNPyrr] and [Bmim][acetate] absorbents to capture 3.96 t/h of CO₂.

[P₂₂₂₈][CNPyrr] has the lowest IL and energy needs as well as the smallest columns because its major CO₂ gas solubility and higher exothermic reaction (see Table 1). This implies an increase in the liquid temperature along the absorption column that improves mass transfer rates (due to viscosity reduction), meaning lower solvent requirement in the absorber and consequently lower energy demand in the IL regeneration stage. This effect is even higher when operating at higher CO₂ partial pressures (see Fig. S1 of Supplementary Material). This synergistic effect is reflected in the process gap capacity, which is the CO₂ loading difference between the absorber inlet (S-07, lean solvent) and outlet (S-03, rich solvent). Thus, this term includes a penalty on the neat absorption capacity considering the incomplete regeneration of the solvent, making this parameter a more realistic approach to the IL performance at process scale [25]. Higher values of this parameter are associated to both fewer IL and energy requirements as can be seen in Table 4. The IL required is lower than those reported for IL physical absorbents [23,29] and there is not solvent loss like when using amines solutions. An analysis on the different contributions to energy consumption concludes that the thermal heat invested in these processes using [P₂₂₂₈][CNPyrr] is similar to MEA-based post-combustion process (4.2 GJ/t_{CO2}, [42]), but much inferior than amine-based natural gas (4.5 GJ/t_{CO2}, MEA [21]) and pre-combustion (3.7 GJ/t_{CO2}, MDEA [43]) processes. Regarding the cooling demand, it is 18% higher than MEA-based post-combustion system [18], although it is significantly lower than amines-based pre-combustion process (2.1 GJ/t_{CO2} [43]). However, the electricity power consumption of the IL-based

systems (0.3–0.4 GJ/t_{CO2}) is similar compared to amines at post-combustion operating conditions (0.4 GJ/t_{CO2} [18]) but much higher when compared at higher CO₂ partial pressures (0.1 GJ/t_{CO2} in both natural gas [21] and pre-combustion [43]). Finally, all the columns height to diameter ratios (H/D) are in the industrial range [37].

3.2. Economic analysis

The calculated VOC components: refrigeration, steam and electrical costs of the CO₂ capture process utilizing [P₂₂₂₈][CNPyrr] to treat 100 kmol/h of CO₂ in post-combustion, biogas and pre-combustion operating conditions are shown in Fig. 2. The VOC (without the IL cost) goes from 0.46 M\$/year (14.62 \$/t_{CO2}) in post-combustion to 0.35 M\$/year (10.93 \$/t_{CO2}) in biogas and 0.33 M\$/year (10.56 \$/t_{CO2}) in pre-combustion, so it decreases with the raise in CO₂ partial pressure owing to the explained synergistic effect.

As represented in Fig. 2, the vacuum compressor implies great part of the VOC cost in the three systems (0.21 M\$/year) and is independent of the case studied as the regenerating pressure is equal for them. The rest of the VOC components can be related with the operating pressure at the absorber. Pressure increases the CO₂-IL solubility besides the heat of reaction warms up the solvent, improving the CO₂ absorption mass transfer kinetics by reducing IL viscosity. This combination implies that the absorber requires a smaller solvent flow that leaves it at higher temperature when increasing the CO₂ partial pressure (see Fig. S1 of Supplementary Material). This effect reduces the reboiler steam consumption (E-101) and the cooling water needed to refrigerate the recirculated IL (E-102). Thus, the LP steam and cooling water costs decrease while increasing CO₂ partial pressure from 0.21 M\$/year to 0.07 M\$/year and from 0.02 M\$/year to 0.01 M\$/year, respectively, as can be seen in Fig. 2. The synergistic effect makes the VOC going from a fifty-fifty ratio between utilities (0.23 M\$/year) and electricity (0.24 M\$/year) in post-combustion to be dominated by the electrical cost (0.22 M\$/year, 64%) in biogas and pre-combustion (0.25 M\$/year, 76%) operating conditions. In general, the electrical cost associated to pumping is not significant, increasing to its maximum at pre-combustion case (0.04 M\$/year) due to the high operating pressure. The calculated VOC is comparable to the sum of steam, water, and electricity costs of other IL-based biogas (0.5 M\$/year) [20] or MEA-based natural gas (12.45 \$/t_{CO2}) [21] systems, but it is notably lower than other IL-based post-combustion CO₂ capture processes [16,19] (for example, [emim][NTf₂]: 83 \$/t_{CO2} [23]). The VOC of each process is disclosed in Tables S5-S9 of Supplementary Material.

Fig. 3 depicts the estimated equipment cost at post-combustion, biogas and pre-combustion operating conditions, using [P₂₂₂₈][CNPyrr] to treat 100 kmol/h of CO₂. The total equipment investment is \$3.45 in post-combustion, \$2.95 million in biogas and \$2.89 million in pre-combustion. These equipment costs are in reasonable agreement with those

Table 4
Summary of solvent, energy and sizing results of the evaluated processes [25].

Ionic liquid		[P ₂₂₂₈] [CNPyrr]			[P ₆₆₆₁₄] [CNPyrr]			[Bmim] [acetate]		
		Post-C	Biogas	Pre-C	Post-C	Biogas	Pre-C	Post-C	Biogas	Pre-C
IL flow rate (t/h)		96.9	49.9	31.5	167.6	76.2	45.0	184.6	84.0	43.2
Gap capacity (mol/kg)		0.94	1.82	2.88	0.54	1.18	2.01	0.49	1.09	2.11
Electricity (GJ/t _{CO2})		0.3	0.3	0.4	0.4	0.3	0.4	0.4	0.3	0.4
Thermal heat (GJ/t _{CO2})		3.5	1.8	1.2	6.0	2.7	1.6	6.8	3.1	1.6
Refrigeration (GJ/t _{CO2})		3.5	1.8	1.2	6.0	2.8	1.7	6.8	3.1	1.7
Abs. column dimensions (m)	H	15	15	15	15	15	15	15	15	15
	D	2.7	1.4	1.0	3.0	1.6	1.2	2.9	1.5	1.1
Reg. column dimensions (m)	HD	10.5	8.0	1.2	12.2	9.0	8.2	12	8.6	7.5
		2.1	1.6	1.4	2.4	1.8	1.6	2.4	1.7	1.5

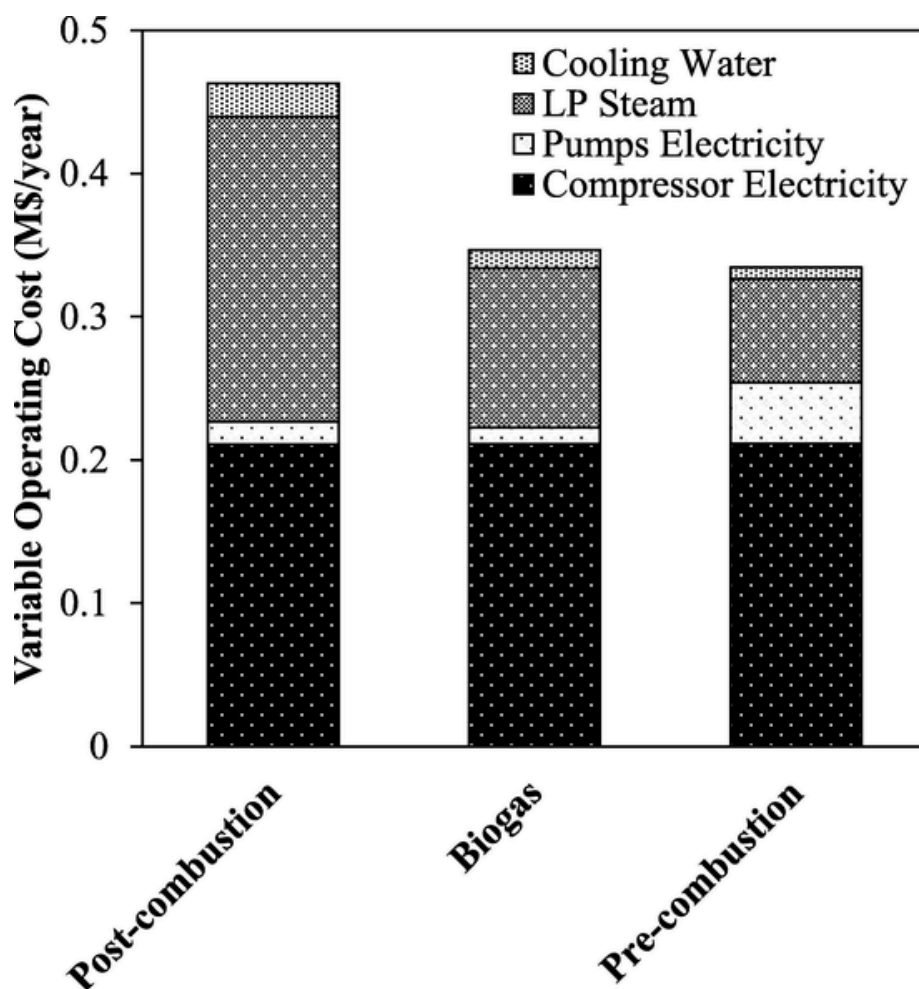


Fig. 2. VOC breakdown for the $[P_{2228}][CNPy]$ -based process depending on the operating conditions (100 kmol/h CO_2). Make-up IL cost is not represented.

calculated in the literature for IL-based post-combustion CO_2 capture (\$5.88 million [23]) or biogas upgrading (\$2.17–\$2.25 million [20]) processes with a similar gas mass treatment capacity (2–3 t/h of capture CO_2). The equipment cost of each process is reported in detail in Tables S3 and S4 of Supplementary Material.

As can be observed in Fig. 3, the cost of the vacuum compressor (C-100) represents the major side (greater than 70%, 2.48 M\$) of the lump-sum of the equipment cost and it is the same for the three processes, since the gas molar flows are very similar and temperature (35 °C) and pressure change (0.1–1 bar) are fixed in the compression stage. Regarding to the absorption (T-100) and regeneration (T-101) packed columns, the second most important percentage in all cases, they are more expensive in post-combustion (0.82 M\$) than biogas (0.36 M\$) and pre-combustion (0.27 M\$) operating conditions because the higher amount of IL required increments the column size [25]. A similar trend is found for the heat exchangers cost too (from 0.08 M\$ in post-combustion to 0.05 M\$ in pre-combustion). The heat transfer area decreases not only because of the less solvent flow rate at higher CO_2 partial pressure but also due to the synergistic effect caused by the enthalpy of reaction in the absorber that reduces the reboiler energy demand, since higher temperature is achieved [25]. Hence, the total equipment cost is reduced when increasing the CO_2 partial pressure. The pumps purchased cost represents a minor part of the process total equipment cost ($\leq 3\%$) in the three processes like heat exchangers, although the high operating pressure in pre-combustion increments 30% their cost as shown in Fig. 3.

The capital and operating expenses per metric ton of captured CO_2 for three plant sizes (1, 10 and 100 kmol/h of CO_2) of the post-combustion, biogas and pre-combustion processes employing $[P_{2228}][CNPy]$ are summarized in Table 5. The total annualized cost (TAC) is the sum of the annualized CAPEX and OPEX, as explained before (Eq. 1).

As can be seen in Table 5, the bigger the plant is, the cheaper the process is per ton of captured CO_2 [40,44]. For example, in post-combustion TAC goes from 5820.19 \$/t CO_2 treating 1 kmol/h (pilot plant [15]) of CO_2 to 643.69 \$/t CO_2 for 10 kmol/h (small biogas upgrading plant [28]) and 104.05 \$/t CO_2 for 100 kmol/h (industrial scale [23]). The same difference can be appreciated in Table 5 for biogas and pre-combustion systems. This effect is known as economy of scale, which is the inverse relationship between per-unit fixed cost and the quantity produced [44] or treated in this case. The greater the quantity treated, the lower the cost per ton of CO_2 . When operating with lower flow rates, both capital direct (CDC) and indirect (CIC) costs drastically increase because electrical or instrumentation direct costs besides others indirect costs such as engineering and contingency expenses do not suffer a major reduction in million dollars (see Tables S5–S9 of Supplementary Material). The capital indirect cost plus the working capital imply around the 50% or more of the total capital expenses (CAPEX), being analogous in the three CO_2 capture systems. CAPEX represents the 30–40% of the TAC, which means that OPEX is the 60–70% remaining (see Fig. S2 of Supplementary Material). Table 5 shows that the main part ($\geq 76\%$, see Fig. S2) of the operational expenses (OPEX) is the fixed operating cost (FOC). FOC cost per metric ton of CO_2 also declines when scaling up the size of the plant because operat-

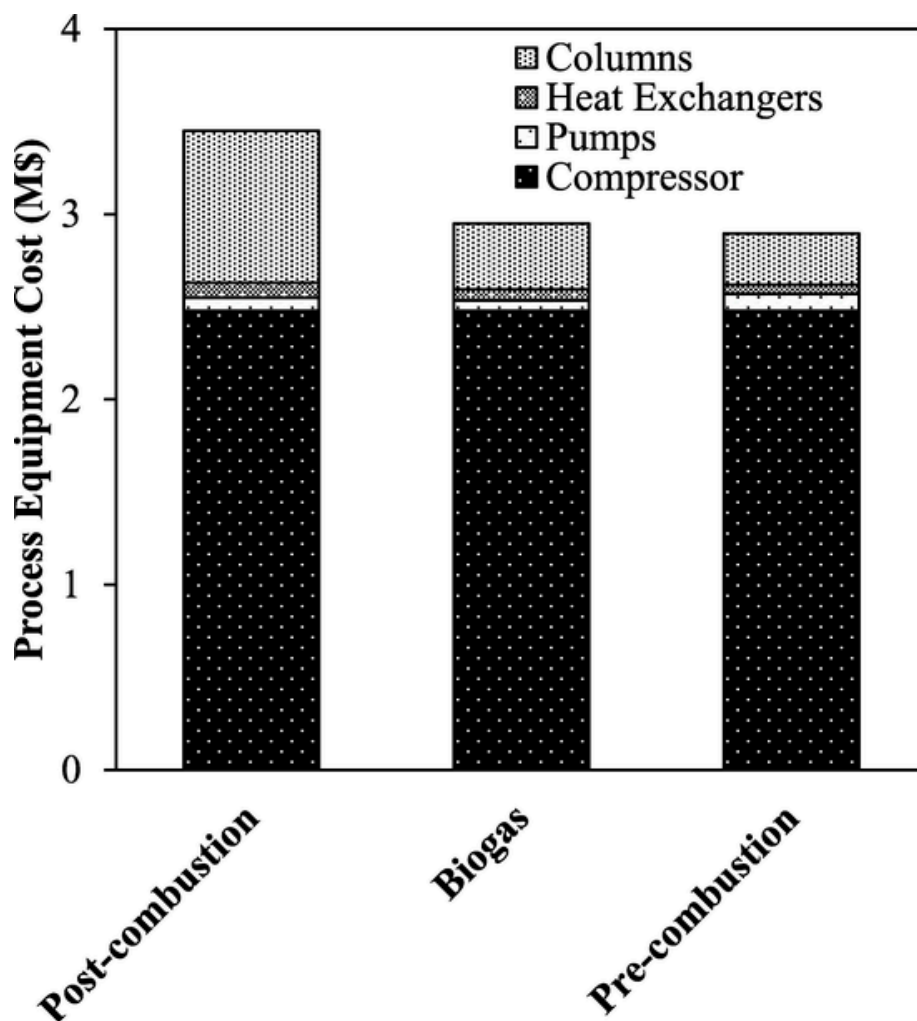


Fig. 3. Process equipment cost breakdown of each process employing $[P_{2228}][CNPyrr]$ and 100 kmol/h of CO_2 .

Table 5

Capital and operating expenses for different plant sizes (1–100 kmol/h CO_2) of the $[P_{2228}][CNPyrr]$ -based process depending on the operating conditions. Solvent cost is not added.

System		Post-combustion			Biogas			Pre-combustion		
CO_2 (kmol/h)		1	10	100	1	10	100	1	10	100
Cost (\$/t CO_2)	VOC	20.7	14.8	14.6	13.2	10.9	10.9	12.5	10.5	10.6
	FOC	4049.2	416.0	48.0	4047.6	414.4	46.6	4047.4	414.3	46.5
	OPEX	4069.9	430.9	62.7	4060.9	425.2	57.6	4060.0	424.8	57.0
	CDC	614.4	84.5	20.5	611.8	81.9	18.2	611.1	82.3	17.9
	CIC	976.8	109.0	17.1	976.2	106.9	15.7	976.3	106.6	15.6
	WKC	159.1	19.4	3.8	158.8	18.9	3.4	158.8	18.9	3.4
	CAPEX	1750.3	212.8	41.4	1746.8	207.7	37.2	1746.2	207.8	36.8
	TAC	5820.2	643.7	104.1	5807.7	632.9	94.8	5806.2	632.6	93.9

ing charges, plant overheads, supervision, operating labor, maintenance and administrative costs in M\$/year are identical or very similar for the three CO_2 treatment capacities (see Tables S5–S9 of Supplementary Material), meanwhile variable operating cost (VOC) seems independent of the effect of the economy of scale as they are directly related to the solvent circulation rate (see Table 5).

3.3. IL properties and cost

The TAC of the $[P_{2228}][CNPyrr]$ -based CO_2 capture processes was compared to those estimated using $[Bmim][acetate]$ and $[P_{66614}][CNPyrr]$ to analyze the influence of the properties of the ionic liquid on the costs of the CO_2 capture process. Fig. 4 shows the TAC divided in CAPEX and OPEX at post-combustion, biogas and pre-combustion operating conditions using $[Bmim][acetate]$, $[P_{66614}][CNPyrr]$ and $[P_{2228}][CNPyrr]$ to treat 100 kmol/h of CO_2 .

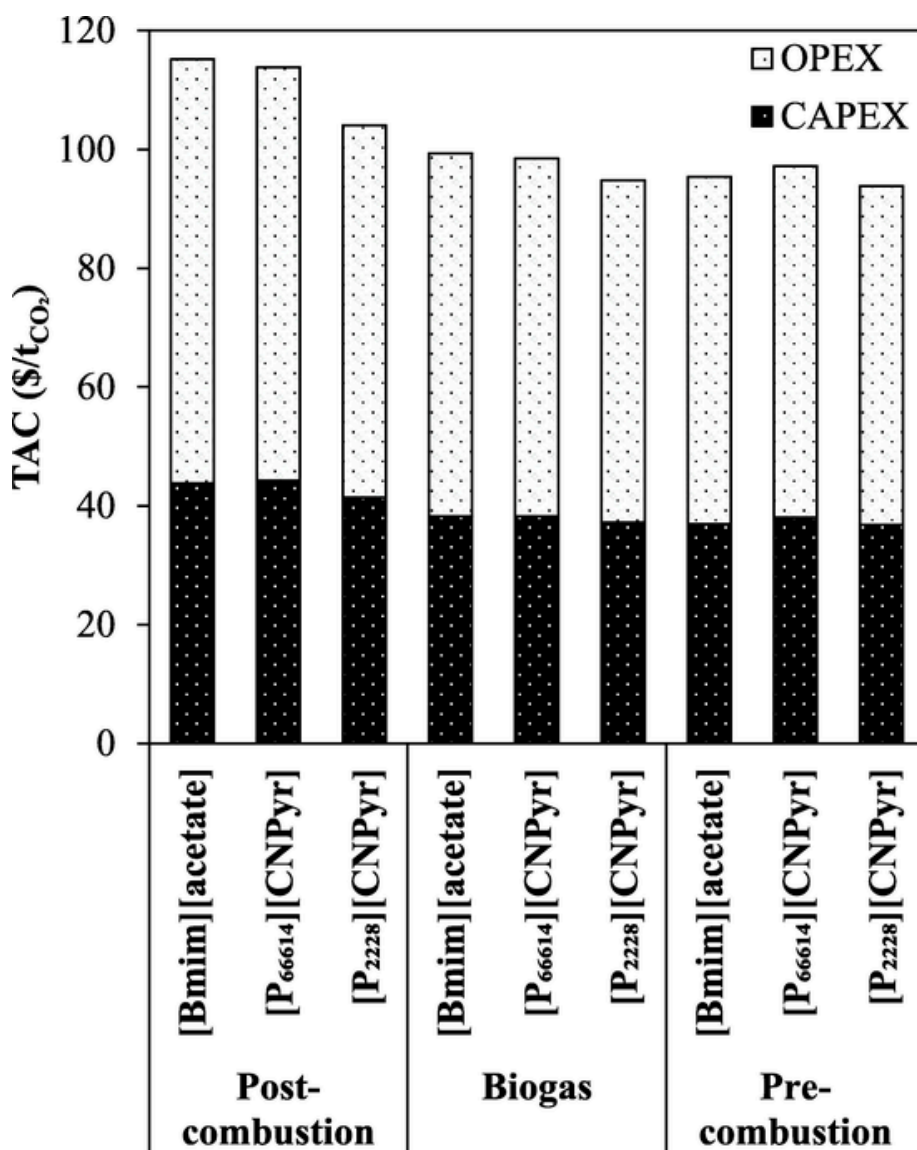


Fig. 4. TAC breakdown depending on the IL and the operating conditions (100 kmol/h CO₂). IL cost is not considered.

As can be seen in Fig. 4, [P₂₂₂₈][CNPyr] -which is the IL having the most exothermic reaction- brings down the TAC of the three systems (104.05–94.79–93.86 \$/tCO₂) compared to [Bmim][acetate] (115.11–99.32–95.38 \$/tCO₂) and to [P₆₆₆₁₄][CNPyr] (113.82–98.48–97.18 \$/tCO₂), so on average [P₂₂₂₈][CNPyr] implies cheaper processes per metric ton of CO₂. Therefore, the solvent and energy demand decline caused by the higher enthalpy of reaction of [P₂₂₂₈][CNPyr] [25] improves the economy of the processes. The gap in cost between ILs is more appreciable in post-combustion ([P₂₂₂₈][CNPyr]-based process cost is reduced by 8.6% (9.78 \$/tCO₂) compared to [P₆₆₆₁₄][CNPyr] and 9.6% (11.06 \$/tCO₂) to [Bmim][acetate]) than in biogas or pre-combustion because of the higher difference in the amount of IL required (see Table 4). Fig. 4 shows the three ILs having similar CAPEX in the three systems (≈44 \$/tCO₂ in post-combustion, ≈38 \$/tCO₂ in biogas and ≈37 \$/tCO₂ in pre-combustion), relating the differences in cost to OPEX. Furthermore, the TAC values represented in Fig. 4 has the same trend that the process gap capacity presented in Table 4 (see Fig. S3 of Supplementary Material), being the IL ([P₂₂₂₈][CNPyr]) with the highest value (i.e. the highest CO₂ absorption capacity once the regeneration penalty is considered) the one presenting the lowest TAC in each CO₂ capture process. As consequence, optimizing the en-

thalpy of reaction to enhance the CO₂ chemical absorption capacity of the IL without increasing the regeneration cost is the step forward. Improving other properties like reducing viscosity would help to cut down the IL needs and researching in high thermally stable ILs to prevent their thermal decomposition is a must to evade vacuum pressures.

Finally, the solvent cost was introduced into the total annualized cost (TAC) considering multiple price scenarios for [P₂₂₂₈][CNPyr] (see Fig. S4 of Supplementary Material). Fig. 5 depicts the TAC values adding the IL cost in post-combustion, biogas and pre-combustion processes considering three representative prices: 500 (actual IL laboratory price), 50 (scaled production price) and 5 \$/kg (amines price).

Actual IL laboratory prices (500 \$/kg) significantly increase TAC in 49.6 \$/tCO₂, 20.6 \$/tCO₂ and 12.0 \$/tCO₂ at, respectively, post-combustion, biogas and pre-combustion operating conditions. Increment directly dependent on IL demand (see Table 4). However, if a scaled up-production price (50 \$/kg) is established for [P₂₂₂₈][CNPyr], the TAC of the proposed CO₂ capture process suffers a much minor appreciation of 4.96 \$/tCO₂ in post-combustion, 2.06 \$/tCO₂ in biogas and 1.20 \$/tCO₂ in pre-combustion meanwhile when the IL price is equalized to amines (5 \$/kg) the TAC rising is almost negligible (0.50 \$/tCO₂ in post-combustion, 0.21 \$/tCO₂ in biogas and 0.12 \$/tCO₂ in pre-combus-

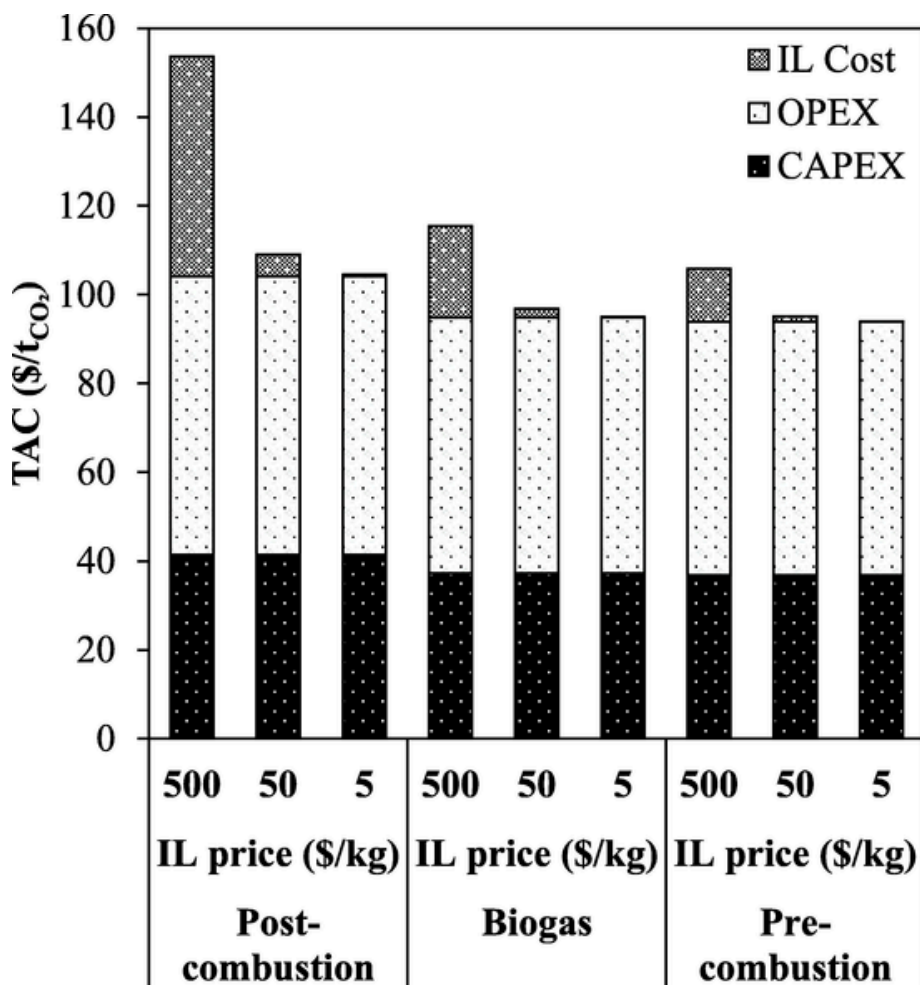


Fig. 5. Solvent cost incorporation into the TAC of the [P₂₂₂₈][CNPyrr]-based process depending on the operating conditions (100 kmol/h CO₂).

tion), although this price is unrealistic assuming nowadays IL synthesis methods. The linear trend of TAC with the IL price is clearly represented in Fig. S4 of Supplementary Material.

The resulting TAC values (109.01–95.06 \$/tCO₂, for 50\$/kg_{IL}) for this IL-based CO₂ chemical absorption process are higher than the U.S. Department of Energy's 40 \$/tCO₂ goal for new generation solvents [23,26] and also than some conventional MEA-based post-combustion CO₂ capture processes (≈ 50–70 \$/tCO₂ [13,18]). However, the obtained TACs correspond to a process configuration without any economic optimization at post-combustion, biogas and pre-combustion operating conditions. As reference, even without optimization, this configuration is competitive compared with those IL-based absorption systems proposed in the literature for post-combustion CO₂ capture (different ILs physical absorbents: 90–265 \$/tCO₂ [19]; [Bmim][acetate]: 140 \$/tCO₂ [16]) or biogas upgrading (271–277 \$/tCO₂ [20]) which considered lower scaled up IL prices (10–34 \$/kg). Zhai estimated cost of 62.4 \$/tCO₂ for a [P₆₆₆₁₄][CNPyrr]-based post-combustion CO₂ capture process greatly benefits from economy of scale [26] (94,980 kmol/h of gas flow rate).

3.4. Pre-optimization hypothesis

Attending to Figs. 1 and 2, which illustrate the equipment purchase and operational costs, optimizing the IL regeneration unit to avoid vacuum as well as energy integration would further reduce the TAC values of this work and make ILs a promising alternative to current amines solutions even from the economical point of view if their

production is promoted to industrial scale. Fig. 6 compares the TAC of both conventional MEA (30%) and [P₂₂₂₈][CNPyrr] based post-combustion CO₂ capture processes considering three different IL regeneration scenarios: IL Base Case operates at 100 °C and 0.1 bar of vacuum pressure, IL Case I increases the temperature to 160 °C but eliminates vacuum (1 bar) and IL Case II regenerates the IL at 121.5 °C and 1 bar (similar MEA regeneration conditions [45]). All processes treat 100 kmol/h CO₂. Excepting the IL Base Case, medium pressure steam is used to heat in the reboiler (2.20·10⁻⁶ \$/kJ). The costs of solvent and CO₂ compression are excluded.

Eliminating the need of vacuum (IL Case I) reduces cost from 104.05 \$/tCO₂ to 82.61 \$/tCO₂. If the regeneration column reboiler operates at the same 121.5 °C as in the MEA-based process (IL Case II), the cost slightly declines to 81.32 \$/tCO₂ because a higher amount of IL is demanded. These results reflect great optimization margin that the proposed IL-based CO₂ capture processes have, either improving the solvent properties or the process engineering in order to economically compete to current amines (MEA) plants (74.84 \$/tCO₂). The MEA-based capture cost of 74.84 \$/tCO₂ by this work is reasonable among the literature values (51–147 \$/tCO₂) [13,16–19].

4. Conclusions

Aspen Process Economic Analyzer (APEA) integrated with COSMO-based/Aspen Plus multiscale methodology was successfully applied to estimate the cost of post-combustion, biogas and pre-combustion CO₂ capture processes based on ILs chemical absorbents. The capital and operational expenses of the previously designed CO₂ capture process by

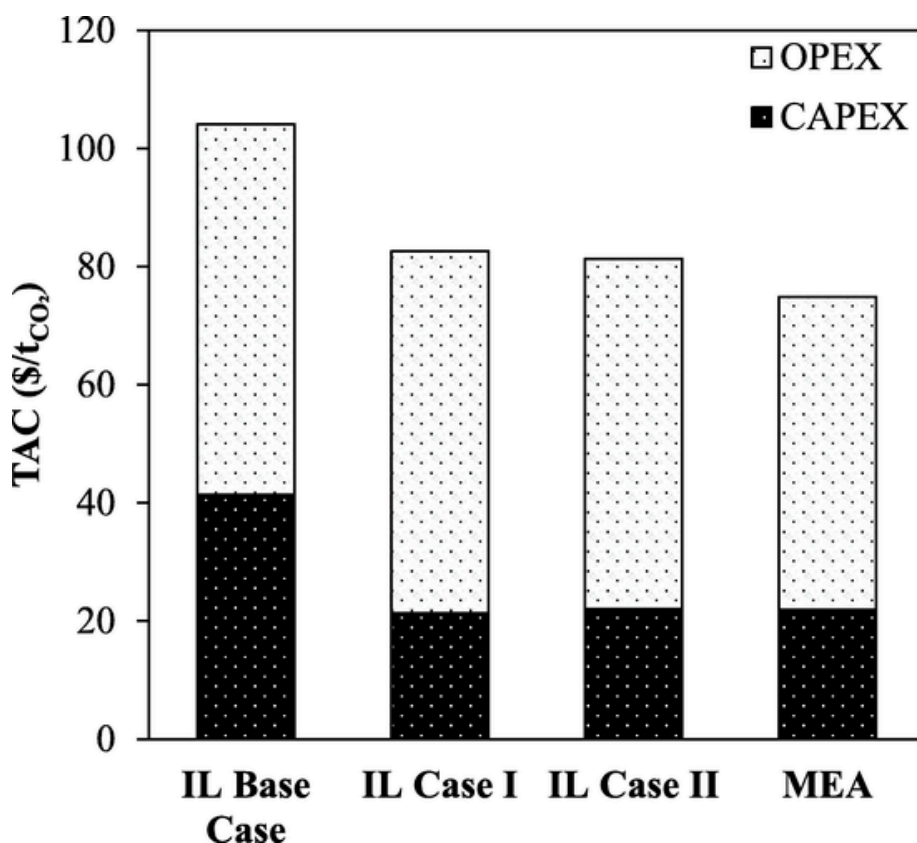


Fig. 6. Cost comparison between three [P₂₂₂₈][CN₂Pyr]-based process configurations and MEA-based CO₂ capture process at post-combustion operating conditions.

our group -composed of an adiabatic absorption column plus an IL regeneration at vacuum pressure- were analyzed. The influence of the plant size was also studied. It was detected that the cost of the CO₂ capture processes could greatly benefit from economy of scale, hence the lower total annualized cost per metric ton of CO₂ was obtained for the greatest studied CO₂ treatment capacity (100 kmol/h) in every process (post-combustion: 104.05 \$/tCO₂, biogas: 94.79 \$/tCO₂, pre-combustion: 93.86 \$/tCO₂, using [P₂₂₂₈][CN₂Pyr]). Purchased equipment cost and variable operating cost depends on the absorption operating conditions, being pre-combustion the most favorable scenario in cost terms. It was demonstrated that vacuum raise both capital and operational expenses of the IL regeneration step. In fact, once vacuum pressure is avoided the total annualized cost of the post-combustion CO₂ capture process descends from 104.05 \$/tCO₂ to 81.32 \$/tCO₂ when regenerating at atmospheric pressure and 121.5 °C. Optimizing the IL regeneration unit as well as energy integration are the step forward in process design to further reduce the cost values of this work.

IL properties had a clear effect over the operational cost of the process, especially in post-combustion when the difference in amount of solvent required between ILs is higher. Thus, the cost of the CO₂ capture processes was found to be related to the IL enthalpy of reaction and gap capacity. [P₂₂₂₈][CN₂Pyr] -which is the IL having both highest gap capacity and enthalpy of reaction- implies almost 10% cheaper processes per metric ton of CO₂. Researching in new less viscous and high thermally stable ILs is crucial to decrease the solvent demand and evade thermal decomposition when regenerating at high temperature. Moreover, the IL enthalpy of reaction might be optimized to both improve its CO₂ chemical absorption capacity and reduce the cost of regenerating the solvent. Multiple IL pricing scenarios were assumed, finding out that a scaled up price of 50\$/kg increases the [P₂₂₂₈][CN₂Pyr]-based base case process's total cost 4.96 \$/tCO₂ in post-combustion, 2.06 \$/tCO₂ in biogas and 1.20 \$/tCO₂ in pre-combustion when

capturing 3.96 t/h of CO₂, which only represents a maximum increment of 5%.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ccej.2020.127196>.

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