



# Aspen plus supported design of pre-combustion CO<sub>2</sub> capture processes based on ionic liquids

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## ABSTRACT

H<sub>2</sub> production processes from steam methane reforming and combined cycle power plants require carbon dioxide removal from raw synthesis gas to obtain a useful H<sub>2</sub>-rich product stream. In this work, a wide variety of operating configurations were techno-economically evaluated in Aspen Plus commercial process simulator to improve the efficiency and costs of the pre-combustion CO<sub>2</sub> capture process based on chemical absorption using [P<sub>2228</sub>][CN<sub>4</sub>Pyr] ionic liquid. Multiple absorption (from 30 °C to 70 °C) and regeneration (between 90 °C and 120 °C) temperatures were tested along with four different regenerating pressures: 0.1, 0.25, 0.5 and 1 bar. Energy and solvent consumptions and capital and operating costs were calculated for nine configurations using the COSMO-based/Aspen methodology combined with Aspen Economic Analyzer tool. The most promising results were obtained when regenerating the IL at 1 bar and at elevated absorption and regeneration temperatures, due to the higher operating and equipment costs associated with vacuum and the greater utilities cost related to heat transfer when the gap between both temperatures grows. The minimum cost achieved was 64.1\$/t<sub>CO2</sub> considering an IL scaled up price of 50 \$/kg, but it could even be further less than 40 \$/t<sub>CO2</sub> goal for new generation solvents, when only direct costs were considered.

## 1. Introduction

Carbon capture and storage (CCS) is expected to play a crucial role in many decarbonization scenarios not only to reduce carbon dioxide (CO<sub>2</sub>) emissions from power generation but also to accelerate the use of hydrogen (H<sub>2</sub>) as feedstock, fuel or energy carrier, since pre-combustion carbon capture may contribute to meet both goals [1,2].

Pre-combustion capture route coupled to power plants has the main advantage of enabling the co-production of power and H<sub>2</sub> by reforming or gasification of fossil fuels [1,3]. In fact, most of the world's H<sub>2</sub> production is generated from steam methane reforming (SMR) of natural gas and from coal gasification, so this capture technique is also applicable to these systems [4–6]. The representative scheme of a H<sub>2</sub> plant using SMR, or a coal gasification (IGCC) or natural gas (NGCC) combined cycle starts with a reformer or gasifier in which the synthesis gas (syngas) is produced, followed by a water gas shift reformer (WGS) wherein syngas carbon monoxide reacts with water steam to produce CO<sub>2</sub> and more H<sub>2</sub>. The resulting product stream is sent to the acid gas removal section, containing a CO<sub>2</sub> separation system, which generates the H<sub>2</sub>-rich syngas [2,3].

CO<sub>2</sub> removal in these industrial pre-combustion processes is regularly accomplished by absorption processes [1,7]. It consists of a scrubber in which a liquid solvent physically or chemically absorbs CO<sub>2</sub> from syngas, with a regeneration column to desorb the CO<sub>2</sub> to be latter compressed and transported and recirculated the lean solvent to the absorber. The syngas stream typically enters the separation stage at 20–70 bar of pressure with a CO<sub>2</sub> concentration in the range of 15–60% by volume [1,7,8]. Physical absorbents such as Selexol® or Rectisol® are commonly applied at relatively high pre-combustion CO<sub>2</sub> partial pressure (IGCC plants) because under proper operating conditions, they can entail less heating duty in comparison with chemical solvents since there is not any chemical reaction involved, but requiring a higher solvent flow rate and thus increasing the electricity consumption [1,7,9]. In contrast, at natural gas steam reforming moderate CO<sub>2</sub> partial pressures (NGCC and H<sub>2</sub> plants), the application of chemical absorption using amine-based solutions is also becoming standard practice due to their higher absorption capacities at lower pressure [1,10]. Several works are focused on introducing chemical absorption-based processes (often using MEA or MDEA) into power plants (IGCC and NGCC) or H<sub>2</sub> production systems [11–15] and optimizing the process configuration and

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operating conditions to develop versatile low-energy and cost-effective CO<sub>2</sub> removal technologies for these pre-combustion capture purposes [16–18]. Regardless of the technology, energy and solvent requirements are crucial aspects to design new low-cost alternatives. In this sense, Ionic Liquids (ILs) were reported to have favorable CO<sub>2</sub> capture properties for pre-combustion applications [2,19]. First tested ILs were those presenting physical absorption, but their uncompetitive mass absorption capacities and higher viscosities compared to current organic solvents meant worse results in terms of energy, solvent rate, and costs [20–22]. Then, promising results for pre-combustion processes using ILs capable of chemically absorbing CO<sub>2</sub> were found in previous works [23,24]. Aprotic heterocyclic anion-based ILs (AHA-ILs), particularly triethyl (octyl)phosphonium 2-cyanopyrrole ([P<sub>2228</sub>][CNPyr]) [25,26], exhibited outstanding energy and solvent demand values compared to MEA-based pre-combustion processes in the techno-economic analysis carried out, minimizing operating and investment costs and even revealing further improvement margin [23,24].

Therefore, the main objective of this work is to improve the efficiency and reduce capital and operating costs of a [P<sub>2228</sub>][CNPyr]-based pre-combustion CO<sub>2</sub> capture process consisting of commercial packed absorption and stripping regeneration columns. For this purpose, an Aspen Plus supported techno-economic evaluation of multiple pre-combustion process configurations based on Rate-based simulations and cost estimations was accomplished using the COSMO-based/Aspen methodology [24,27–29]. A simplified syngas stream from coal gasification used on preceding works was again considered to contrast earlier results at equal inlet conditions [9,23,24]. Accordingly, 80 operating configurations, corresponding to different temperatures (90 – 120 °C) and pressures (0.1 – 1 bar) for the IL regeneration, as well as its absorber inlet temperature (30 – 70 °C), were analyzed in terms of solvent rate, energy demands and utilities costs and compared to conventional systems values and previous studies. Finally, total costs including the equipment investment were calculated for 9 representative configurations to reveal the most suitable operating conditions that minimize the overall expense of the CO<sub>2</sub> capture process in comparison with previous results.

## 2. Computational methodology

### 2.1. Component definition and property method specification

Aspen Plus v11 simulations of the pre-combustion CO<sub>2</sub> capture processes required [P<sub>2228</sub>][CNPyr] and its reaction product to be introduced as pseudo-components following our successful multiscale COSMO-based/Aspen Plus methodology [23,24,30]. The quantum chemical structure optimizations performed at B-P86/TZVP level together with COSMO-RS calculations of molecular weight, boiling point, density, molecular volume and the sigma-profile were used to specify the COSMOSAC property method of the Aspen Plus simulations (in code 1, COSMOSAC method by Sandler et al. [31]). CO<sub>2</sub>–[P<sub>2228</sub>][CNPyr] experimental isotherms at different temperatures were successfully fitted to a thermodynamic model (Eq. (1)), which combines the physical absorption described by Henry's Law and the chemical equilibrium reaction considering 1:1 stoichiometry between the IL and the CO<sub>2</sub> as explained elsewhere [23,24,27].

$$z = \frac{P_{CO_2}}{K_H - P_{CO_2}} + \frac{K_{eq} \cdot P_{CO_2} \cdot C}{K_H + K_{eq} \cdot P_{CO_2}} \quad (1)$$

where  $z$  is the molar ratio of CO<sub>2</sub> absorbed per mol of IL,  $P_{CO_2}$  is the CO<sub>2</sub> partial pressure in bar,  $K_H$  is the CO<sub>2</sub> Henry's law constant in the IL in bar,  $K_{eq}$  is the reaction equilibrium constant and  $C$  is an empirical ratio representing the [P<sub>2228</sub>][CNPyr] available to react with the CO<sub>2</sub> molecule whose value is fixed to 0.92 as reported in previous literature [25].

Therefore, the utilization of this model entailed defining CO<sub>2</sub> as Henry component into Aspen Properties and selecting Aspen Plus

Reactive-Distillation equilibrium reaction type.  $K_H$  and  $K_{eq}$  values fitting the experimental isotherms must be incorporated using Aspen Plus built-in temperature dependence expressions. The validation of this thermodynamic model to describe CO<sub>2</sub> absorption can be found in a preceding study [23]. H<sub>2</sub> solubility in IL is suggested to be negligible based on COSMO-RS Henry's Law constant calculations (507 bar for H<sub>2</sub> vs. 67 bar for CO<sub>2</sub> at 40 °C). The experimental temperature dependent [P<sub>2228</sub>][CNPyr] viscosity data were also introduced to better describe the CO<sub>2</sub> mass transfer kinetics [23,24]. As AHA-IL, its viscosity remains unchanged after reacting with CO<sub>2</sub> [32,33]. Figure S1 represents experimentally measured [25] and Aspen-predicted temperature dependent [P<sub>2228</sub>][CNPyr] viscosity values. Thermodynamic properties, chemical reaction and kinetic parameters used to define the CO<sub>2</sub>-IL system in Aspen Plus simulations are summarized in Table S1 of [Supplementary Material](#).

### 2.2. Process scheme

The pre-combustion CO<sub>2</sub> capture process depicted in Fig. 1 treats a 250 kmol/h inlet gas stream (S-01) composed of CO<sub>2</sub>/H<sub>2</sub> (40/60 %mol). It enters the absorption column (T-100) at 40 °C and 32.7 bar where contacts the IL recirculated from the regeneration column (S-07) which absorbs the 90% of the CO<sub>2</sub> fed at adiabatic operating conditions, obtaining a H<sub>2</sub>-rich stream with a purity of 94 %mol (S-02). The exhausted IL (S-03) leaves the absorber to be regenerated in a stripping column (T-101), which operates from atmospheric to vacuum pressure (E-100 and C-100) and different temperature controlled by a forced circulation (P-101) reboiler (E-101) depending on the configuration. The captured CO<sub>2</sub> exits the stripper after its desorption (S-08) and the IL regenerated (S-05) is pressurized (P-102) and cooled down (E-102) before being recirculated to the absorption column (T-100).

### 2.3. CO<sub>2</sub> capture process simulation and cost estimation

The CO<sub>2</sub> absorption (T-100 in Fig. 1) and IL regeneration (T-101 in Fig. 1) packed columns were modeled using Aspen Plus's RADFRAC rigorous column model. Rate-based mode calculations were performed to consider the CO<sub>2</sub> mass transfer kinetic process and Aspen Plus's Reactive-Distillation equilibrium reaction was employed to describe the chemical reaction between CO<sub>2</sub> and [P<sub>2228</sub>][CNPyr] occurring inside [23,24,29]. The absorber was discretized by 10 computation stages whereas 6 stages were applied for the stripper. Both columns were set to be 10 m of packing height with a variable diameter to maintain a fractional capacity of 80%, utilizing Flexipac 700Y structured packing type.

To select the suitable operating conditions that enhance the CO<sub>2</sub> capture process economy, a wide range of configurations were evaluated. Temperatures from 30 to 70 °C (E-102 outlet values) for the IL enrolling the absorption (S-07), in which 90% of the inlet CO<sub>2</sub> is

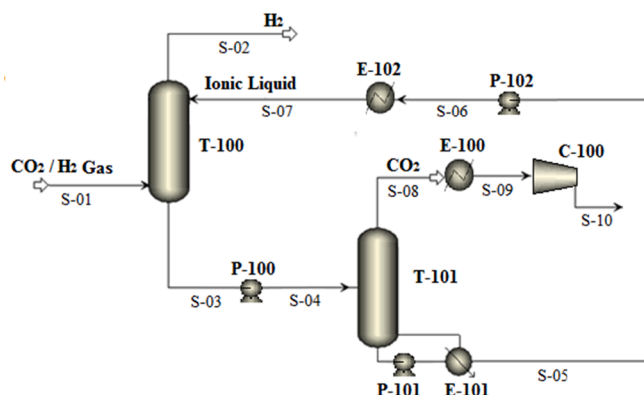


Fig. 1. [P<sub>2228</sub>][CNPyr]-based pre-combustion CO<sub>2</sub> chemical absorption process scheme.

captured at 32.7 bar and adiabatic conditions, were tested. Regarding the regeneration step, not only multiple temperatures between 90 and 120 °C for the forced circulation (P-101) reboiler (E-101) were considered but also 0.1, 0.25, 0.5 and 1 bar of pressure were analyzed [23,24]. The energy consumed when operating at vacuum pressure (0.1, 0.25 and 0.5 bar) was estimated by Aspen Plus's isentropic compressor model (C-100), emulating the pressure drop from 1 bar to the pressure corresponding directly to the vapor after cooling it to 35 °C (E-100). The pumping efforts (P-100, P-101 and P-102) were also calculated as explained elsewhere [24]. The vacuum compressor and pumps power demands were estimated using a pumping/compression efficiency of 60% and a driver efficiency of 85% according to heuristic rules [24,34]. In addition to the energy requirements, the IL consumption was determined to assess the efficiency of the CO<sub>2</sub> capture process depending on the chosen configuration.

Since the main objective of modifying the operating conditions is lowering both capital (CAPEX) and operating (OPEX) expenses of the CO<sub>2</sub> capture process, an economic evaluation was carried out. Aspen Process Economic Analyzer (APEA) v11 was applied to cost the equipment investment following the aforementioned mapping assumptions [24], whereas the variable operating cost (VOC) was calculated as the sum of the costs of the electricity required by pumps (P-100, P-101 and P-102) and the vacuum compressor (C-100), the medium-pressure steam (MP steam) consumed by the reboiler (E-101) and the cooling water used as coolant by the vacuum unit (E-100) and the cooler prior to the absorption column (E-102). The prices implemented by default in Aspen

Plus ( $7.75 \cdot 10^{-2}$  \$/kWh for electricity,  $2.2 \cdot 10^{-6}$  \$/kJ for MP steam and  $2.12 \cdot 10^{-7}$  \$/kJ for cooling water) were assumed for these utilities. Both capital and operating indirect costs (CIC and FOC) were also determined following a methodology previously published [24]. The total annualized cost (TAC) was calculated as the sum of the annualized CAPEX (determined using a capital recovery factor which considers an interest rate of 10% and an annuity period of 25 years) and OPEX (supposing an operation time of 8000 h/year) [24]. Finally, the IL cost was included into the most favorable TAC values considering two different prices (50 and 500 \$/kg) due to the uncertainty about their future large-scale production price. Further details for cost estimation can be found in [Supplementary Material](#) and preceding works [24].

### 3. Results

Different scenarios were analyzed for regeneration stage by changing the operating pressure: 0.1, 0.25, 0.5 and 1 bar. For each pressure, absorption and regeneration temperatures were modified from 30 to 70 °C and between 90 and 120 °C, respectively. The IL flow rate was calculated to maintain a CO<sub>2</sub> capture of 90%, corresponding to a purity of 94% of H<sub>2</sub> at the absorber outlet, together with the total energy consumption and associated utilities costs. [Fig. 2](#) illustrates the resulting solvent requirements at each stripper working pressure and different operating temperatures.

As can be seen in [Fig. 2](#), the IL mass flow required during absorption is strongly determined by its regenerating conditions. More severe

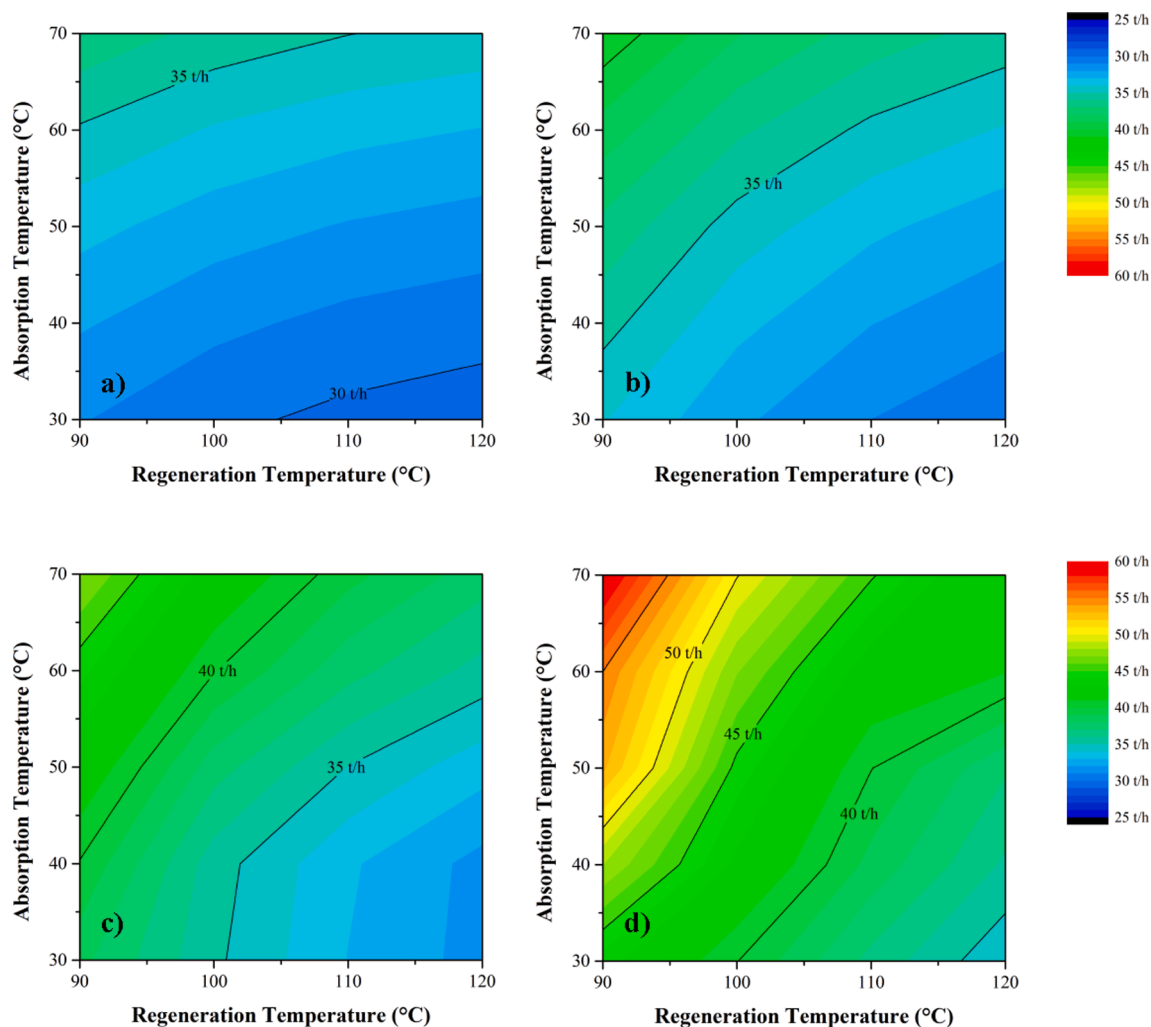


Fig. 2. IL consumption depending on the operating temperatures at 0.1 (a), 0.25 (b), 0.5 (c) and 1 bar (d) of regenerating pressure.

vacuum pressures (0.1 and 0.25 bar) facilitate the reversibility of the CO<sub>2</sub>-IL reaction, better regenerating the IL and leading to lower solvent consumptions. Similarly, higher reboiler temperatures (110–120 °C) achieve major IL regenerations, hence reducing the IL mass flow rate. However, as the stripper pressure increases, the absorber inlet temperature becomes more relevant. In Fig. 2d, it is clearly shown how the IL mass flow increases when operating at higher absorption temperatures because the absorption capacity is decreased. Therefore, the most favorable mass flow (29.4 t/h) is achieved with the configuration feeding the IL at 30 °C to the absorption column and regenerating it at 120 °C and 0.1 bar, 14% lower compared to 1 bar (34.2 t/h) of regenerating pressure. These operating conditions present higher IL performance and hence a lower amount of IL because they enhance the IL cyclic capacity [23], which is the difference of the IL load at the inlet (S-07) and outlet (S-03) of the absorber (see Figure S2 of Supplementary Material). Hence, CO<sub>2</sub> chemical absorption controls the process since mass transfer limitations are overcome by the IL viscosity reduction (see Figure S1) at absorption adiabatic conditions as demonstrated elsewhere [23]. Per ton of captured CO<sub>2</sub>, these obtained flow rate values are lower than those reported for IL physical absorbents or conventional organic solvents as Selexol® using bigger columns [20], but higher than MEA-based systems [13].

Fig. 3 represents the total energy demand at the studied ranges of operating pressures and temperatures. It can be observed that the energy needed at low regeneration pressure (0.1 and 0.25 bar, corresponding to Fig. 3a and 3b) is almost identical due to the similarity of mass flows values (see Fig. 2a and 2b). However, when gaining pressure (0.5 and 1

bar, Fig. 3c and 3d) the higher quantity of IL required (see Fig. 2c and 2d) slightly increases the energy requirements, since it is the variable controlling the thermal consumptions that dominates the total demand [23,24]. Heating and cooling duties of the exchangers involved are also affected by the gap in fluid inlet and outlet temperatures. In this sense, the major difference in the energy results of Fig. 3 is made by the absorption inlet and regeneration outlet temperatures in all cases. When the gap is reduced (IL leaves the reboiler at 90 °C and it is cooled to 70 °C to enter the absorption column), the energy demanded by the CO<sub>2</sub> capture process is decreased below 2.0 GJ/tCO<sub>2</sub>, whereas it is maximized (above 3.5 GJ/tCO<sub>2</sub>) when this temperature difference between both units is remarkable (IL regenerated at 120 °C and entering the absorber at 30 °C). Indeed, the heat required to reverse the CO<sub>2</sub>-IL reaction (0.8 – 0.9 GJ/tCO<sub>2</sub>) can represent a 40% of the total requirement for these low-energy demanding processes ( $\leq 2.0$  GJ/tCO<sub>2</sub>), corresponding to reboiler duty values  $\leq 1.0$  GJ/tCO<sub>2</sub>. Thus, there were found several operating configurations that not only reduced our previous energy results (2.8 GJ/tCO<sub>2</sub> [23,24]) using [P<sub>2228</sub>][CNPyrr] and achieved a reboiler duty similar to those reported for MDEA-based optimized processes ( $\approx 1.0$  GJ/tCO<sub>2</sub>) [10–12,16,17] but also whose total energy requirement is equal or even lower than the thermal heat consumed by MEA-based pre-combustion CO<sub>2</sub> capture processes (2.1 – 4.6 GJ/tCO<sub>2</sub>) [13,15,18]. However, physical absorbents based on organic solvents achieve lower energy demands at this particularly high CO<sub>2</sub> partial pressure [9].

Fig. 4 presents the estimated utilities cost (composed by refrigeration, steam and electrical costs) of the pre-combustion CO<sub>2</sub> capture process at the studied operating conditions. Clearly, the regeneration

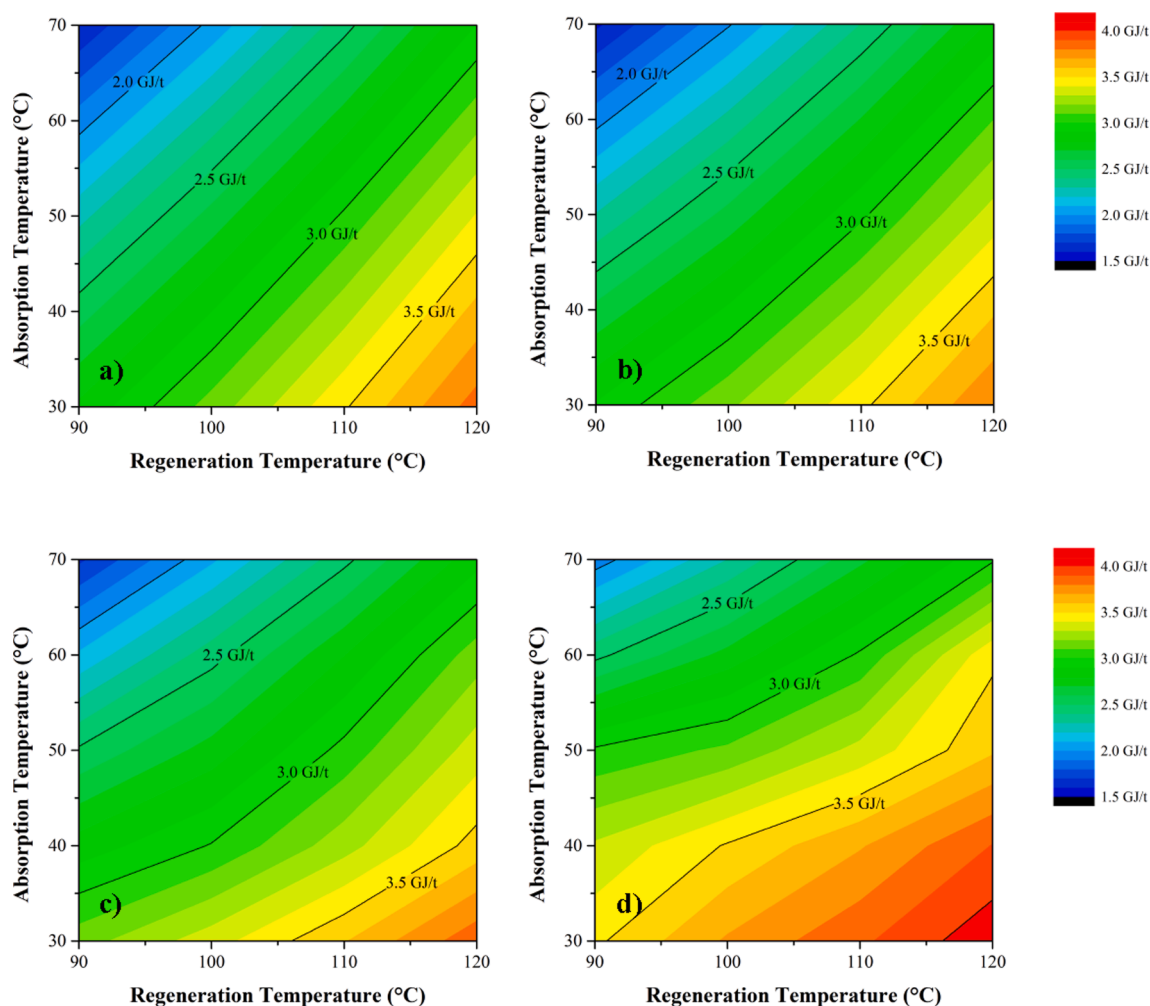


Fig. 3. Energy requirements depending on the operating temperatures at 0.1 (a), 0.25 (b), 0.5 (c) and 1 bar (d) of regenerating pressure.

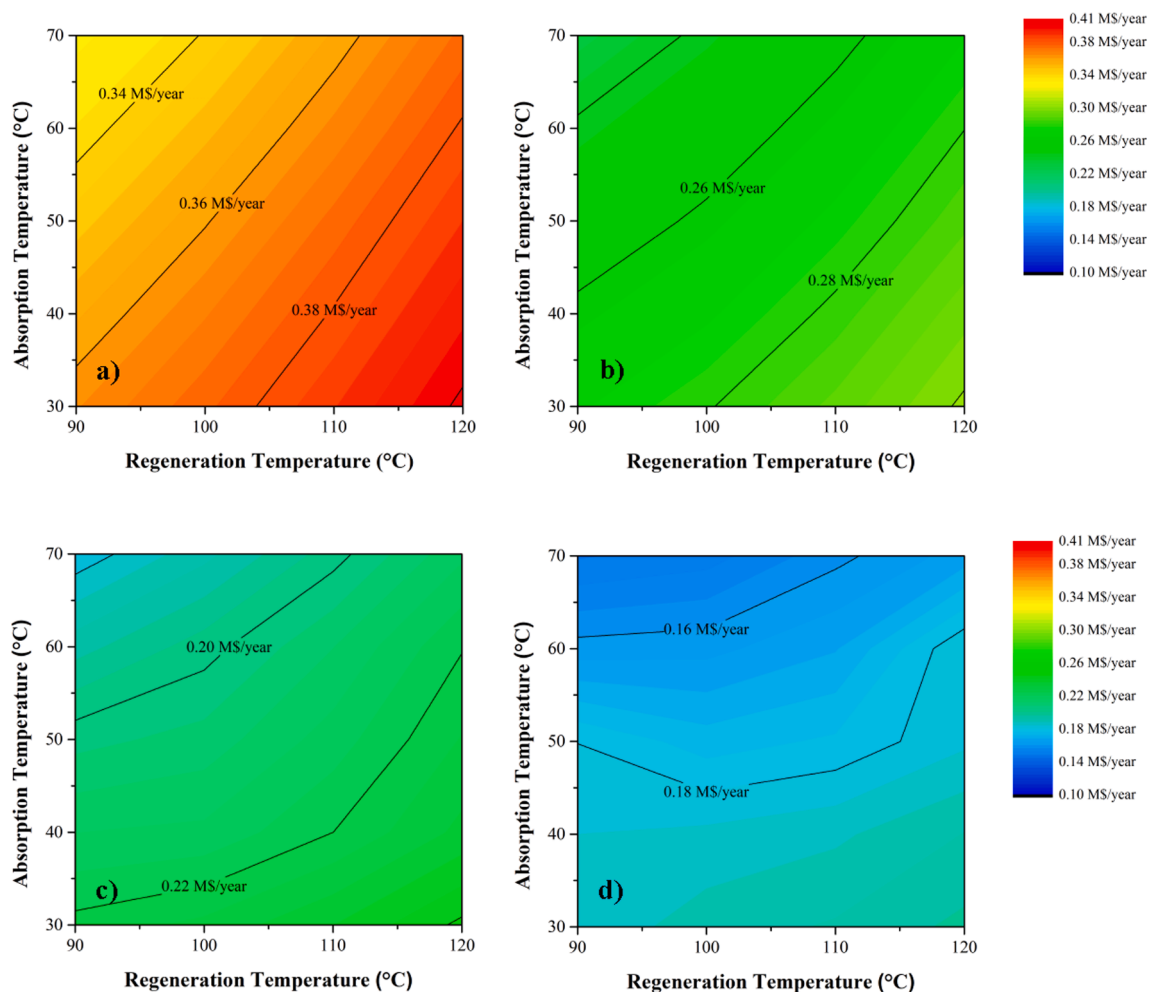


Fig. 4. Utilities costs depending on the operating temperatures at 0.1 (a), 0.25 (b), 0.5 (c) and 1 bar (d) of regenerating pressure.

pressure determines this cost, whereas operating temperatures play a secondary role. A great cost penalty is noticeable when regenerating [P<sub>2228</sub>][CNPy] at vacuum pressure compared to 1 bar [24]. The high price of electricity compared to MP steam ( $7.75 \cdot 10^{-2}$  \$/kWh or  $2.2 \cdot 10^{-5}$  \$/kJ vs.  $2.2 \cdot 10^{-6}$  \$/kJ) increases vacuum operating costs [24], that convert the less energy-demanding processes into more expensive ones. In fact, regenerating below 0.5 bar (Fig. 4a for 0.1 bar, Fig. 4b for 0.25 bar and Fig. 4c for 0.5 bar) makes no sense if trying to minimize costs, since solvent (see Fig. 2a, 2b and 2c) and energy consumptions were very similar (see Fig. 3a, 3b and 3c) as discussed before. Consequently, depressurizing from 32.7 to 1 bar is the most cost-effective regeneration method. And these utilities costs are further improved (below 0.16 M \$/year) by reducing both reboiler and absorber inlet temperatures at the expense of increasing IL consumption, but the increment it would bring in CAPEX has to be additionally considered [24].

In this regard, Fig. 5 shows the relationship between the IL mass flow and the variable operating cost (utilities cost) in the studied range of operating pressures and temperatures to illustrate the most suitable and representative configurations for complete economic evaluation (black symbols).

A classification of the data according to the regeneration pressure is clearly shown in Fig. 5. Black-colored symbols depict 9 representative cases of operating configurations, selected in this work to be economically evaluated using Aspen Economic Analyzer. Cases 1 and 9 are opposite to each other. Case 1 is selected due to its minimum utilities cost to reduce OPEX, although assuming a high IL demand that may increase equipment investment (CAPEX), whereas Case 9 represents the

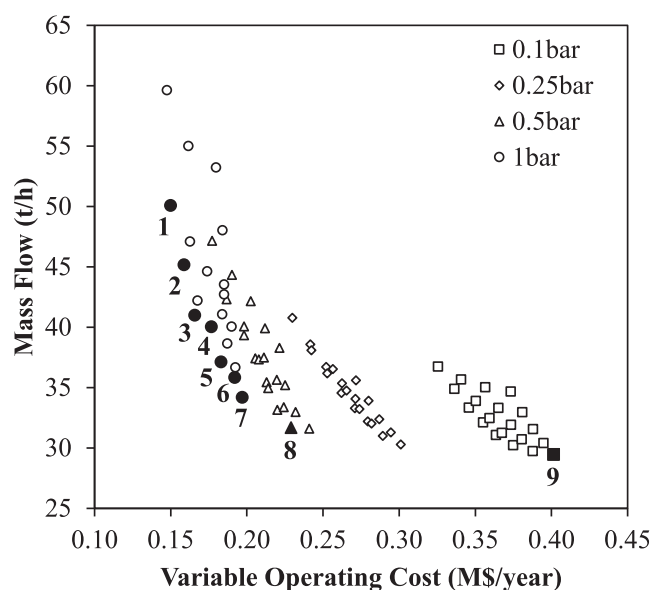


Fig. 5. Distribution of IL mass flow with the variable operating cost depending on the regenerating pressure. Black-colored symbols are the economically evaluated cases.



configuration with lowest IL mass flow, but greatest variable operating cost to assess the contrary issue. Cases from 2 to 8 maintain a significantly reduced utilities cost without excessively increasing the IL flow rate in comparison with the rest of configurations. Thereby, these designs are potentially candidates to achieve a compromise between low variable operating cost and low equipment investment affected by the quantity of IL. Table 1 reports the techno-economic results for all 9 selected cases, including CAPEX, OPEX and TAC estimations (IL cost excluded).

Regarding the data collected in Table 1, Cases 8 and 9 regenerating [P<sub>2228</sub>][CNPyrr] at vacuum pressure are the most expensive ones, whereas Cases from 1 to 7 achieved similar TAC values. In Cases 8 and 9 there is a significant gap in CAPEX (7 – 24 \$/t<sub>CO2</sub> more than in Cases 1–7) associated with the cost of the required vacuum unit, since the dimensions of the columns are similar to those of the rest of the cases, and in OPEX (3 – 15 \$/t<sub>CO2</sub> more), due to the extra electricity consumed [24]. Attending to Cases from 1 to 7, the difference in IL mass flow does not imply significant changes in the dimensions of the columns and hence in the direct capital costs (CDC) (6.2 – 6.5 \$/t<sub>CO2</sub>). Indirect capital costs (CIC and WKC) and fixed operating costs (FOC) are almost analogous in these cases that regenerate the IL at 1 bar too. The greatest contrast between these economically analyzed configurations is exhibited in the variable operating cost (VOC). Cases 1, 2 and 3 -presenting less energy consumption (below 3.0 GJ/t<sub>CO2</sub>)- achieve lower VOC (4.7 – 5.2 \$/t<sub>CO2</sub>), consolidating them as the most cost-effective configurations. Case 2 obtains a minimum total cost (TAC) of 62.7 \$/t<sub>CO2</sub> followed by Cases 1 and 3 with 62.9 \$/t<sub>CO2</sub> (excluding the cost of the IL), representing the optimum balance between VOC and CDC, namely, OPEX and CAPEX. Therefore, regenerating the IL at atmospheric pressure and working at temperatures that make the process nearly autothermic improve economic results. Including a price for the IL of 50 \$/kg, TAC for Cases 1, 2, and 3 rises less than 5% to 64.4 \$/t<sub>CO2</sub>, 64.1 \$/t<sub>CO2</sub>, and 64.2 \$/t<sub>CO2</sub>, respectively. On the contrary, if the price of the IL is as high as 500 \$/kg, a configuration with lower flows than Case 2 (76.7 \$/t<sub>CO2</sub>) results in slightly lower TAC, as case 3 (75.9 \$/t<sub>CO2</sub>).

Remarkably, these results (64.1 \$/t<sub>CO2</sub> of Case 2, as reference) represent a decrease of 31 \$/t<sub>CO2</sub> respect to previous TAC value (95.1 \$/t<sub>CO2</sub>) reported using the same [P<sub>2228</sub>][CNPyrr], equal 50 \$/kg IL price and pre-combustion stream [24]. If only plant equipment investment (CDC), IL cost (using the scaled-up price of 50 \$/kg) and the variable operating cost (VOC) are considered, the TAC of these three configurations descends to ≈ 12.7 – 12.8 \$/t<sub>CO2</sub>, values close to those reported for Selexol® pre-combustion processes (≈ 8 \$/t<sub>CO2</sub>) [20], and MEA-based natural gas sweetening systems (19.5 \$/t<sub>CO2</sub>, operating at similar CO<sub>2</sub> partial pressure) [35] that considered the same contributions for cost

estimation, and significantly below the U.S. Department of Energy's 40 \$/t<sub>CO2</sub> goal for new generation solvents [36], and the 20 \$/t<sub>CO2</sub> ambitious target of many US and European [37].

#### 4. Conclusions

Complete [P<sub>2228</sub>][CNPyrr]-based pre-combustion CO<sub>2</sub> chemical capture processes were modeled using our COSMO-based/Aspen methodology. A wide range of absorption (30 – 70 °C) and regeneration (90 – 120 °C) temperatures together with four different regeneration pressures (0.1, 0.25, 0.5 and 1 bar) were screened to evaluate the techno-economic feasibility of these multiple operating configurations and improve the economic results of previous publications. Solvent and energy requirements to reach a 90% of CO<sub>2</sub> capture corresponding to a hydrogen product with 94% purity from a 250 kmol/h flow gas stream with 40 %mol of H<sub>2</sub> and 60 %mol of CO<sub>2</sub> were calculated. It was found that operating at vacuum pressure reduced the IL mass flow in all cases (specially at 0.1 bar) and energy demand particularly when working at low absorption and regeneration temperatures (up to 50 °C and 110 °C). However, the high electricity price consumed by these vacuum regenerations became these configurations the highest operational costed processes. On the contrary, reducing the gap between absorption and regeneration temperatures allows decreasing both solvent and energy demands as well as utilities cost.

A total of 9 different configurations were economically evaluated using Aspen Economic Analyzer. Cases regenerating [P<sub>2228</sub>][CNPyrr] at 1 bar presented similar capital expenses, whereas those that regenerated the IL at vacuum pressure entailed higher investment in required equipment. Hence, the greatest difference between analyzed cases was found on the variable operating cost. A configuration in which the IL entered the absorber at 70 °C and whose regeneration took place at 110 °C and 1 bar achieved the minimum cost value of 64.1 \$/t<sub>CO2</sub>, considering a 50 \$/kg scale-up price for the IL. The results of this work confirm the techno-economic viability of the proposed IL-based pre-combustion CO<sub>2</sub> capture processes, but their sustainability may be studied through future life cycle analyses to close the full evaluation of these IL-based systems.

#### CRediT authorship contribution statement

**D. Hospital-Benito:** Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Visualization. **J. Lemus:** Conceptualization, Formal analysis, Writing – review & editing, Visualization, Supervision, Project administration. **C. Moya:** Conceptualization, Methodology, Formal analysis, Writing – review & editing, Visualization. **R. Santiago:**

**Table 1**

Summary of solvent, energy, sizing and economic results for the cases evaluated by APEA. IL cost is not included.

Case		1	2	3	4	5	6	7	8	9
Abs. temperature (°C)		70	70	70	50	50	40	30	40	30
Reg. temperature (°C)		100	110	120	110	120	120	120	120	120
Reg. pressure (bar)		1	1	1	1	1	1	1	0.5	0.1
IL mass flow (t/h)		50.1	45.2	41.0	40.0	37.1	35.8	34.2	31.7	29.4
Energy demand (GJ/t <sub>CO2</sub> )		2.3	2.7	3.0	3.3	3.6	3.9	4.1	3.5	3.8
Abs. column dimensions (m)	H	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
	D	1.2	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0
Reg. column dimensions (m)	H	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
	D	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.3	1.5
Cost (\$/t <sub>CO2</sub> )	VOC	4.7	5.0	5.2	5.6	5.8	6.1	6.2	7.2	12.7
	FOC	40.8	40.7	40.7	40.9	40.8	40.9	40.9	43.0	47.7
	OPEX	45.5	45.7	46.0	46.4	46.5	46.9	47.1	50.2	60.4
	CDC	6.5	6.3	6.3	6.4	6.2	6.4	6.4	10.4	20.4
	CIC	9.3	9.1	9.1	9.3	9.1	9.2	9.2	12.2	16.6
	WKC	1.6	1.5	1.5	1.6	1.5	1.6	1.6	2.3	3.7
	CAPEX	17.3	17.0	16.9	17.3	16.9	17.2	17.2	24.8	40.7
	TAC	62.9	62.7	62.9	63.7	63.4	64.1	64.3	75.1	101.1

Conceptualization, Writing – review & editing, Visualization. **C. Paramio:** Conceptualization, Writing – review & editing, Visualization. **J. Palomar:** Conceptualization, Formal analysis, Writing – review & editing, Visualization, Supervision, Project administration, Funding acquisition.

### 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.seppur.2022.120841>.

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