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Design and multi-objective optimization of a CO_2 capture plant using deep eutectic solvents

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ABSTRACT

The United Nation's 2030 Agenda for Sustainable Development has called for taking of urgent action to combat climate change and its impacts, where CO_2 capture processes have gained relevance for achieving emission objectives. Traditionally, monoethanolamine (MEA) is used in post-combustion capture (PCC) as a solvent because of its high absorption capacity. However, the use of amines is related to several environmental problems. In this work a novel post-combustion carbon capture plant is designed in Aspen Plus, under a sustainable design scheme considering environmental and economic indexes, using novel green liquids: deep eutectic solvent (DES) choline chloride/urea (1:2). Four case studies are considered for the most used fossil fuels in the power plant: coal, natural gas, associated gas, and biogas. This work represents a base case for multi-objective optimization of the PCC process coupled with a power plant for combustion. An optimization problem was defined considering the following objective functions: minimization of the environmental impact (EcoIndicator 99), minimization of the total solvent recovery energy (TSRE) and greenhouse gas emissions (GHGE); the economic objectives were set to minimize the total annual cost of the plant (TAC) and maximize return over investment (ROI). A metaheuristic optimization method, differential evolution with tabu list was chosen, and Pareto fronts for the objective functions were obtained for all case studies. It was found that the PCC process for coal-based power generation exhibits the best overall performance among all evaluated fuels. A comparison with a similarly optimized MEA-based carbon capture process shows that the use of DES leads to a 171.8% reduction in environmental impact when treating flue gas from a coal-based power process. To showcase the feasibility of the DES as a green solvent, an energy consumption of 6.62 MJ/kgCO_2 is needed, compared with 6.40 MJ/kgCO_2 for the MEA-based process.

1. Introduction

The high concentration and growing emissions of greenhouse gasses caused by anthropogenic activities have impacted natural and human systems through the increase of global average temperature among other effects (Chen et al., 2014). CO_2 is recognized as the main component of

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Nomenclature

Abbreviations

PCC	post-combustion carbon capture
MEA	monoethanolamine
DES	deep eutectic solvent
ChCl/urea	choline chloride/urea
EI99	eco-Indicator 99
TSRE	Total Solvent Recovery Energy
GHGE	Greenhouse Gas Emissions
TAC	Total Annual Cost
ROI	Return on Investment
CCS	Carbon Capture and Sequestration
IL	Ionic Liquid
NG	Natural Gas
AG	Associated Gas
BG	Biogas
C	Bituminous Coal
AC	Absorber Column
DC	Desorber Column
FT	Flash Tank

Variables

x_{H_2O}	water molar fraction present in the absorbent mixture
F_{DES}	molar feed flow of the absorbent mixture, kmol/h
T_{DES}	absorbent feed temperature, °C
N_{AC}	absorber column's total stages
N_{PS1}	absorber first packing section number of stages
N_{PS2}	absorber second packing number of stages
N_{DC}	desorber number of trays
N_{feed}	desorber feed stage
P_{AC}	absorber pressure, atm
P_{FT1}	Flash 1 pressure, atm
P_{FT2}	Flash 2 pressure, atm
P_{DC}	desorber pressure, atm
Ψ_{FT1}	Flash 1 vapor fraction
Ψ_{FT2}	Flash 2 vapor fraction
RR	distillate reflux ratio
D	distillate molar flow rate, kmol/h

greenhouse gasses (US EPA, O., 2015), and its emission to the atmosphere is mainly attributed to the burning of fossil fuel in the industrial, transport, electricity, and heat generation sectors. Worldwide commitments to limit global warming to well below 2°C, compared to pre-industrial levels, require transforming the development trajectories towards sustainability. The United Nation's 2030 Agenda for Sustainable Development has called for taking urgent action to combat climate change and its impacts, mainly through Goals 7, 9, 12, and 13 (Transforming our World: The 2030 Agenda for Sustainable Development, 2015), citing examples of the efforts companies can make to contribute by decarbonizing their operations and supply chains through continuously improving energy efficiency, reducing the carbon footprint of their products, services, and processes, and setting ambitious emissions reductions targets in line with climate science, as well as scaling up investment in the development of innovative low-carbon products and services.

Technologies that aim to mitigate the amount of emitted CO_2 into the atmosphere, particularly in traditional energy generation processes, have been proposed (Pires et al., 2011). One set of these technologies is known as CO_2 capture and storage (CCS) processes, which involves capturing CO_2 from emission points from fossil fuels or biomass, industrial facilities, or directly from the air. The CO_2 is transported and compressed through pipelines or by sea transport from the point of capture to the point of use or storage. Captured CO_2 can be used as feedstock to create products; on the one hand, it is possible to permanently store CO_2 in subway geological formations. Another applicability is Enhanced Oil Recovery, where CO_2 injection into partially depleted oilfields forces out additional volumes of oil, with CO_2 being residually trapped and stored (Al-Shargabi et al., 2022). Post-combustion carbon capture (PCC) is the process commonly used in thermal power plants to separate carbon dioxide from flue gasses and is one of the most used CCS technologies due to its ability to capture the CO_2 from gasses in the 3–15 vol% concentration range (Han et al., 2014) and to be adapted as a complementary process in existing thermal power plants (Yu et al., 2012). The capture is achieved by chemical or physical absorption using some amine, conventionally a 30% aqueous solution of monoethanolamine (MEA), as the absorbing liquid. MEA as an absorbent substance offers many advantages, such as high reactivity with CO_2, low cost, high absorption capacity, reasonable thermal stability, and resistance to thermal degradation, although the problem of high energy consumption to regenerate the sorbent persists as roughly 60% of the energy required comes from this step (Wu et al., 2014).

Several studies regarding sustainable design and optimization of carbon capture plants are reported in the literature using MEA as the absorbing agent. Romero-García et al. (2022) optimized a carbon capture plant by using a metaheuristic optimization method, coupled with a power plant, considering environmental, economic, and controllability metrics. They showed that the capture process can be economically viable and that the search for optimal design parameters and variables leads to designs that minimize environmental impact, improve the economic performance, and better the controllability of the PCC process. Allahyarzadeh et al. (2021) optimized the configuration of a carbon capture plant to reduce heating and cooling demands, and power consumption. They showed that an optimum operating condition (by a stochastic optimization method) produced a considerable reduction in the energy consumption of processing plants compared with conventional operating conditions at no additional cost. Despite efforts to minimize energy consumption and environmental impact, the capture process with amines has a huge drawback. The emission of MEA and other amines into the environment is not negligible, as potentially toxic emissions of nitrosamines and nitramines have been detected (Luis, 2016). Condensation nuclei in flue gas dominates the generation of amine aerosols resulting in heavy amine losses. MEA emission is the main contributor to solvent loss, accounting for approximately 67% of solvent lost (Morken et al., 2017) or 1.1 kg MEA/tonne CO_2 captured. Morken et al. (2017) report a value of total losses of 1.6 ± 0.1 kg MEA/tonne CO_2 captured, and that losses can occur by MEA emissions via the absorber and the stripper, by oxidative and thermal degradation, losses due to leakage and reclaimer waste. Solvent degradation due to oxidative and thermal degradation in the presence of SO_2 accounts for 15 – 25% of total solvent losses of the system (Raksajati et al., 2018). Although SO_2 removal is a prerequisite

for PCC, as this technology is designed to treat the outlet gas of a flue gas desulphurization unit (Sifat and Haseli, 2019), MEA may require SO_x concentrations of about 10 ppm to keep solvent consumption and make up costs at reasonable values. SO_2 concentration in flue gasses is typically around 300–6000 ppm, and commercial SO_2-removal plants remove up to 98%– 99%. An optimal SO_2 content for the gasses before the PCC process is a cost trade-off between SO_2 removal costs and solvent make up costs, therefore amine degradation due to the presence of SO_2 is expected in the carbon capture process. Wu et al. (2014) describe the main drawbacks of the use of amines, such as degradation due to the presence of O_2 and SO_2 and the severe corrosion rate of process equipment.

Due to some of the disadvantages that liquid amine absorption processes exhibit, such as low contact area between gas and liquid, low CO_2 loading, and severe absorbent corrosion, alternatives to the use of liquid amine solution have been proposed. Solid adsorption process may be an alternative to achieve the CO_2 capture purpose (Hasan et al., 2012), although some existing problems including high operational cost, low CO_2 adsorption capacities at low pressures and the negative impact of water vapor and other gases limit their practical application (Ünveren et al., 2017). Oxycombustion is an alternative considered one of the most promising combustion methods with low pollutant emissions, with several studies confirming oxy-fuel combustion as a suitable technology for pulverized coal in electric power plants. However, these results refer to a limited type of coal, and further research is needed for a broad type fuels (Raho et al., 2022).

As a result, the search for a sustainable alternative to amines and research on applicability of green solvents to replace amines as absorbing agents has gained relevance in recent years (Adeyemi et al., 2017). According to Luis (2016) the search for a solvent that substitutes the use of MEA requires that the former should not degrade, should operate at flue gas conditions, and would require less energy for its regeneration. It is, therefore, necessary to look for a solvent that has: High CO_2 capture capacity, low energy for regeneration, high absorption/desorption rates and regeneration at lower temperatures, low volatility and better stability, and lower degradation and corrosion. Additionally, in thermal power plants, fuel composition variations lead to changes in the flue gas composition, particularly in the carbon content. Operational flexibility is required for thermal power plants. Therefore, the capacity of the solvent used for the PCC process for treating flue gases of different compositions must be determined.

One of the relatively recent alternatives to the use of amines has been ionic liquids (ILs) selective towards CO_2 absorption (Hasib-ur-Rahman et al., 2010). These are green solvents with melting points below 100 °C, that possess vaporization resistance and thermal stability. However, their high production cost and the potential toxicity of most of the synthesized ILs limit their industrial application (Krishnan et al., 2020), so the search for a green solvent with a reasonable cost is not concluded. The design of PCC processes using ILs as an absorbent agent have been reported in literature. For example, a techno-economic analysis and dynamics of a pilot-scale carbon capture plant has previously been investigated (Valencia-Marquez et al., 2015). The results show that the IL-based plant features lower energy demand compared to traditional MEA-based plants. Seo et al. (2020) developed a rigorous simulation and design optimization based on the minimization of the total annualized cost. A comparison to a similarly optimized amine-based PCC system suggests that the IL absorbent can be economically competitive with amine absorbents, as long as the cost of the solvent decreases.

In recent years, research has developed around another category of green solvents called deep eutectic solvents (DES) with selective absorption capacity towards CO_2. This is a two-component mixture that has a lower melting point than either of its two constituent components and is typically obtained by mixing a quaternary ammonium halide salt, a hydrogen-bond acceptor (HBA), with a hydrogen-bond donor (HBD) molecule (García et al., 2015). Deep eutectic solvents are alternatives to ILs, as they maintain the benefits of the latter while minimizing the disadvantages (Krishnan et al., 2020). They usually offer superior biodegradability and are less combustible than ILs and have been shown as nontoxic (Marchel et al., 2022). DESs can be obtained from biodegradable sources and compounds commonly found in industry and the cost of deep eutectic liquids is potentially lower than that of ionic liquids. Marcus (2019) describes the extensive use of several DESs for the extraction and separation of diverse substances. In biodiesel and biomass processes, DESs have been applied to separate glycerol from biodiesel, and as pretreatment agents of cellulose. The applicability of DESs as absorbing agents for organic volatile compounds has been previously demonstrated (Moura et al., 2017).

The capacity of several DESs to selectively and efficiently absorb and desorb CO_2 has been reported in the literature (Zhang et al., 2018). Several studies have been carried out to determine the solubility of gases in choline chloride based DESs, and properties, such as Henry's law constant, have been reported. Their high solubility indicates that these solvents are better CO_2 solubilizers than similar IL counterparts (Sarmad et al., 2017). The eutectic combination of choline chloride (vitamin B4 precursor) with urea (a common fertilizer), forms a liquid solvent named choline chloride/urea (ChCl/urea). When ChCl/urea is prepared with a 1:2 molar ratio, it exhibits the highest CO_2 solubility among a series of screened HBDs and HBAs (García et al., 2015). The feasibility of using aqueous ChCl/urea (1:2) as an absorbing agent for CO_2 has been previously explored. Ma et al. (2018) modeled the DES in an Aspen Plus simulation software by fitting thermophysical experimental data to the models embedded in Aspen Plus. Through the simulation and evaluation of a biogas upgrading process, they highlight aqueous ChCl/urea (1:2) as a promising solvent for this application. Wang et al. (2020) simulated a PCC process from the flue gas of coal-fired power plants using ChCl/urea (1:2), demonstrating its potential to achieve a high CO_2 capture ratio, however, this process lacks an environmental assessment and its sustainability is yet to be evaluated. Luo et al. (2021) simulated an industrial-scale PCC capture plant from the flue gas of a coal-fired power plant, evaluating the life cycle environmental sustainability of the process, and confirming the advantages of the non-toxic nature of some DESs. Their findings also show that energy consumption and solvent loss of the DES during solvent regeneration is lower than those of MEA. They also show that the DES is inferior to MEA in terms of solvent flow and overall energy consumption.

However, to the best of the authors' knowledge, an optimization of the ChCl/urea (1:2)-based process under a sustainability scheme has not yet been developed. In other words, no study has been conducted to analyze the impact of post-combustion absorption process design variables and

their effect on the sustainability of the process. In order to align with the UN's 2030 sustainable development goals, new processes that aim to mitigate an environmental problem must be developed under a sustainability scheme to ensure that the DES-based carbon capture process represents a viable solution. Previous work on simulation of a PCC process using DESs evaluates the solvent's capacity to treat flue gasses from a coal-fired power plant (Wang et al., 2020; Luo et al., 2021).

In this work, the solvent's capacity to treat gasses from different fuels is researched. The fuels considered consist of some of the most commonly used for energy generation in thermal power plants, namely coal, natural gas and associated gas. Because of the recent relevance of biofuels, combustion of biogas is also studied. Furthermore, the PCC process proposed by (Wang et al., 2020), which focuses on maximizing CO_2 recovery by means of a sensitivity analysis, represents a base-case for further development of DES-based carbon capture processes. In the present work, consideration for several design variables is included for the optimization to further elucidate the effects of several operational and design parameters in the performance of the process.

Choline chloride/urea (1:2) is selected as the DES of choice for this work because of its high solubility of CO_2, thermal stability, non-toxicity (Marchel et al., 2022), and availability of experimental data that allows for the modelling of the DES in a chemical process simulation environment. Evaluation of the performance of ChCl/urea (1:2) as an absorbing agent in a PCC process designed under a sustainability scheme, and considering the use of several fuels will help to further the understanding of its applicability as a green solvent. Indices that evaluate the PCC process' environmental impact, the ratio of the CO_2 emitted for solvent regeneration and the CO_2 captured, and economic indices will help to evaluate the sustainability of the proposed process.

This work focuses on the design and optimization of a carbon capture plant using novel green DES aqueous ChCl/urea (1:2), under a sustainability scheme, as a first in the reported literature. The capacity of the DES to treat flue gasses with different CO_2 concentrations needs to be studied, as traditional power plants require flexibility in terms of the composition of the fuel used for energy generation, and the associated changes in CO_2 concentration for the flue gases. The impact of the design variables on environmental and economic metrics is analyzed. Furthermore, the PCC process' capacity for treating flue gases with different CO_2 concentrations is studied under this sustainability scheme. Four case studies, considering the use of Natural Gas (NG), Associated Gas (AG), Biogas (BG), and bituminous Coal (C), are studied to determine the DES's capacity to treat flue gas with different compositions.

2. Case study

The study case presented in this work evaluates the scenario of a power plant coupled with a post-combustion CO_2 capture process. The simulation of the DES-based process is conducted using Aspen Plus. The process can be explained in a two-step process, first the power plant and second the CO_2 capture process (Fig. 1).

2.1. Combustion

A vast amount of literature deals with the issues of simulating gas turbine and energy systems, given the complexity of the models (Couper et al., 2005). For simulating the flue gas composition, thermodynamic properties, and energy output for the combustion turbine, in this work a simplified model of the thermal power plant is considered, based on the proposal of Luyben (2013) to model the combustion process in Aspen Plus, considering temperature constraints for the combustor when using air as the oxygen source. Important outputs of the combustion process needed to evaluate the performance of the PCC plant can be determined by use of this simplified model, such as power output for the combustion turbine, and temperature and pressure conditions for the flue gas stack. They propose that a multi-stage compression setup reduces total compressor work and achieves a reduction of the required airflow to maintain fixed combustor temperature, which has a constrained value due to limitations because of the materials of construction (Luyben, 2013). Because of the non-polar nature of the components found in the air and fuel mixture, its physical properties are simulated using Peng-Robinson thermodynamic model. An Aspen RGibbs chemical-equilibrium reactor model is used for the combustor.

The power plant consists in a two-stage air compressor scheme, a traditional steam-generating boiler, and a combustion turbine. The case study considers a fuel feed flow of 1000 kmol/h, for NG, BG, and AG. Associated gas refers to the natural gas found in association with oil within the reservoir. For bituminous coal (C), a flue gas flow of the same order of magnitude as those obtained for the combustion of the gasses is considered. The composition of the flue gas for each of the fuels used in the case studies is presented in Table 1.

2.2. Carbon capture process

The capture plant design consists of an absorber/desorber system with intermediate vapor-liquid separators (Fig. 1). The flue gas from the boiler enters through the bottom of the packed absorber column (AC), which contains two structured-packing sections. The solvent is fed at the top of the column and consists of aqueous ChCl/urea (1:2). Although it's possible to find DESs with a higher CO_2 absorption rate reported in literature (García et al., 2015; Luo et al., 2021), experimental and theoretical data regarding the properties of ChCl/urea (1:2) aqueous solutions are more widely available, and its theoretical application for the PCC process has been previously been demonstrated (Ma et al., 2018; Wang et al., 2020). In the AC, Gas-liquid contact drives CO_2 to the liquid stream, although considerable amounts of N_2 and O_2 are absorbed as well via physical absorption. The enriched solvent (DES_{rich}) exits the absorption column at the bottom and enters a solvent regeneration stage, where improved CO_2 purity is achieved by reducing DES_{rich} pressure in vapor-liquid separators (FT-1 and FT-2), although too low pressure will cause excessive CO_2 desorption and affect the CO_2 capture rate (Wang et al., 2020). DES_{rich} finally enters the desorption column (DC), where CO_2 is obtained as a product at the top, whilst regenerated solvent exits at the bottom of the tower and is recirculated to the top of the absorption column. In Luo et al. (2021) a PCC process with two regeneration steps is proposed, where pressure is reduced from 44.41 to 9.87, and finally to 0.20 atm. This sequential separation allows N_2 and O_2 to separate gradually from DES_{rich}, while simultaneously maintaining a low CO_2 desorption rate. Vacuum separation operations have an impact on the economic and environmental indices considered in this work (Luyben, 2022). To achieve both high CO_2 purity and CO_2 capture rate,

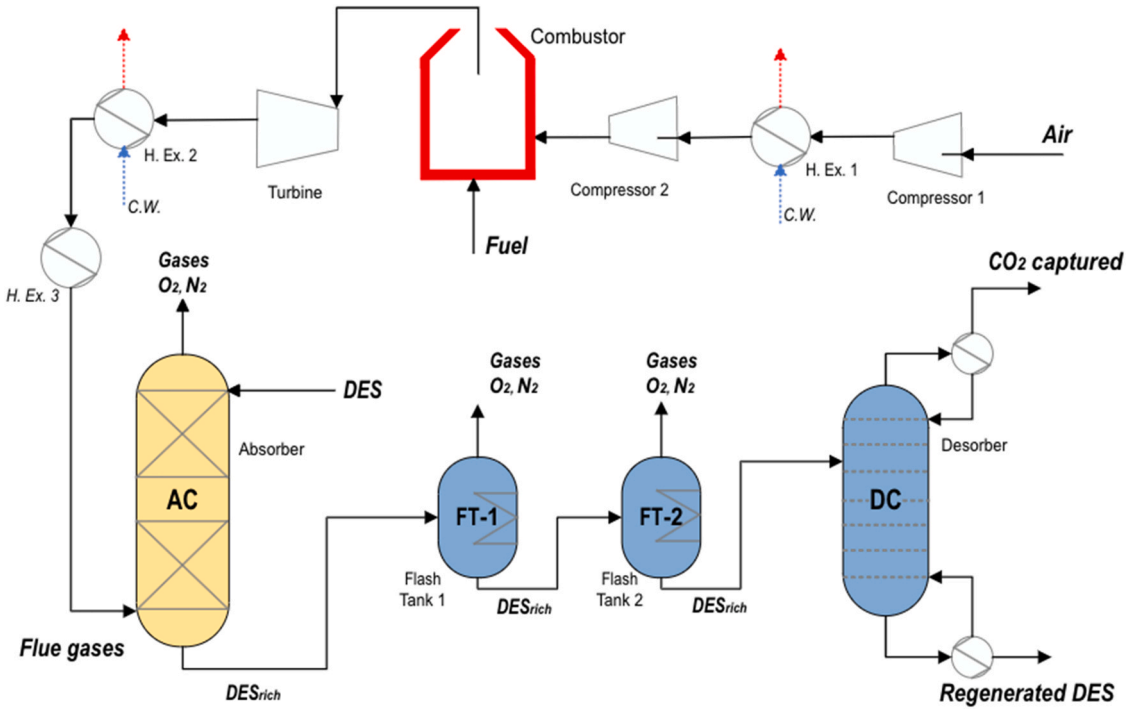

Fig. 1 – Combustion and PCC processes. Flue gasses from the combustor are fed to the Absorber (AC) where gas-liquid contact occurs with the solvent (DES). The enriched solvent (DES_{rich}) enters the regeneration scheme, where temperature and pressure changes occur in Flash Tank 1 (FT-1) and Flash Tank 2 (FT-2). Finally, in the Desorber (DC) the CO_2 captured is separated from the regenerated DES.

Table 1 – Flue gas composition in mole fraction.

Fuel	CO_2	N_2	O_2	H_2O
Natural Gas	0.049	0.752	0.102	0.097
Associated Gas	0.042	0.758	0.119	0.081
Biogas	0.054	0.747	0.110	0.088
Coal	0.124	0.766	0.030	0.080

while allowing operation above atmospheric pressure, a solvent regeneration scheme consisting of two isothermal flash tanks and a desorption column is proposed in this work.

All of the involved components were input into the simulation software from an already existing software database, while the DES molecule must be defined. Following a similar methodology as proposed by Wang et al. (2020), the ChCl/urea (1:2) molecule is modeled in Aspen Plus using group contribution methods. The critical properties of the DES were taken from Mirza et al. (2015). For the temperature-dependent properties proposed reliable parameters based on experimental data were fitted to the models embedded in Aspen Plus, as described by Ma et al. (2018). The phase equilibria include gas solubility in the solvent and vapor-liquid equilibrium for the solvent itself. For the physical absorption, an equilibrium-based approach is considered. ChCl/urea (1:2), due to its low vapor pressure, is assumed to only exist in the liquid phase. The Non-Random Two Liquid (NRTL) thermodynamic model was used to calculate the activity coefficient in the liquid phase, as the absorbing agent is reportedly a polar solvent (Pandey et al., 2013). The Peng-Robinson (PR) thermodynamic model was used to calculate the fugacity coefficient for the gaseous components, with parameters taken from Aspen databank. The solubility of gas (i) in the solvent is calculated from fugacity (φ_i^v) and Henry constant (H_i). The gas solubility's phase equilibrium in a solvent that consists in more than one pure absorbent, as is the case for aqueous ChCl/urea, can be expressed as:

$$py_i\varphi_i^v = H_{i,mix}x_i\gamma_i^* \quad (1)$$

Where p is the system pressure, y_i is the mole fraction in the vapor phase, φ_i^v is the fugacity coefficient in the vapor phase, $H_{i,mix}$ is Henry's constant of gas (i) in the mixed solvent, x_i is the mole fraction in the liquid phase, γ_i^* is the unsymmetric activity coefficient in the liquid phase. $H_{i,mix}$ was calculated from Henry's constant of gas (i) in the pure absorbents. The Henry coefficient is taken from Ma et al. (2018).

3. Sustainable design indicators

The design of a sustainable process under the framework of sustainable development has the purpose of minimizing environmental, economic, and social impacts. Several indicators exist to measure the level of sustainability in chemical process design, among them the environmental metrics proposed by Jiménez-González et al. (2012) represent clear mathematical definitions to evaluate the greenness of a process. A more complete evaluation of the sustainability of the process includes economic indicators, as well as environmental ones. In this work, a set of metrics is selected from life cycle assessment methodology (Eco-indicator 99 to evaluate environmental impact), green indices (greenhouse gas emissions and total solvent recovery energy), and economic evaluation (total annual cost and return on investment).

3.1. *Economic indices*

The economic evaluation is addressed by the total annual cost (TAC) of the carbon capture plant, and by return on

investment (ROI) as a measure of the overall economic viability of the capture process adjacent to an electrical power plant. The total annual cost involves the annualization of investment cost for major equipment over a 10-year payback period. Operating costs are equivalent to utility costs, and the plant is assumed to run 8500 h/year. The module costing technique outlined by Turton et al. (2009) was used. The TAC approximation is described in Eq. (2). As an objective function for the optimal designs, small values of TAC are preferred.

$$TAC = \frac{\sum_{i=1}^{n} C_{TM,i}}{r} + \sum_{j=1}^{n} C_{ut,j} \quad (2)$$

Where $C_{TM,i}$ is the capital cost of major process equipment in US dollars ($), r represents the payback period in years (yr.), and $C_{ut,j}$ is the cost of utilities in US dollars per year ($/yr.). The TAC is indicated in US dollars per year ($/yr.).

The return on investment is a financial indicator that measures investment profitability. For this work, ROI is used to determine if the capture plant equipment cost and operation are economically viable, considering the profit obtained from energy generation in the adjacent power plant, and considering the potential use of the captured CO_2 as a product. The ROI calculation is based on the annual revenue, the annual production costs, and the total capital investment, and it's stated as a percentage per year (%/yr.) (see Eq. (3)) (Gutiérrez, 2003; Seider et al., 2016).

$$ROI = \frac{P}{I} \quad (3)$$

Where (I) represents the total investment of the process, and P is the net profit in US dollars ($). A process is considered profitable when the ROI is bigger than the bank's annual rate for an investment of an annual term.

3.2. Green indices

The Eco-Indicator 99 (EI99) consists of a quantitative life cycle analysis evaluated from beginning to end and is one of the most widely used environmental impact estimation methods (Curzons et al., 2001). This methodology takes into account: raw material origin in the process, processing, and degradation (Goedkoop and Spriensma, 2001). Mathematically, EI99 can be expressed as shown in Eq. (4) (Klemes, 2015).

$$EI99 = \sum_{i} \sum_{j} \omega \cdot C_i \cdot \alpha_j \quad (4)$$

The standard unit of expression for EI99 in all categories is point per year (Pt/yr.) or millipoint per year (mPt/yr.). From Eq. (4) ω represents the damage weight factor (Pt/kg), C_i represents the impact value of each i category and α is the value for the j subcategory (kg/yr.). The method analyzes three different damage categories: human health, ecosystem quality, and resources. The evaluated subcategories are the steel necessary for major equipment, electricity for pumping and compressing, cooling water, steam needed for heating, and inlet and outlet material streams for reactants and products, including ChCl/urea (1:2) and water used for the carbon capture. Smaller values of EI99 are preferable, as they represent a lower environmental impact based on the categories measured. The data relating to the materials, energy, etc. was taken from Ecoinvent database 3.7.

Curzons et al. (2001) provide a list of green indicators that represent sustainability metrics for process and product design. Those that have been identified as relevant to the process of carbon capture by absorption-desorption with a solvent are mentioned below.

The fundamental purpose of the carbon capture plant design is to reduce emissions from fossil fuel combustion, so it is necessary to use an index to compare carbon dioxide emissions (as a byproduct of generating steam) with CO_2 captured. The green indicator associated with the CO_2 emitted in the desorption column reboiler is defined with Eq. (5):

$$GHGE = \frac{CO_2 \text{ emitted for solvent regeneration [kg]}}{CO_2 \text{ captured [kg]}} \quad (5)$$

A carbon capture process with GHGE index values close to zero represents a design that minimizes CO_2 emission for solvent regeneration purposes. On the other extreme, a design with a GHGE index > 1 emits more CO_2 than it captures.

The green metric related to calculating total solvent recovery energy per kg of CO_2 captured is defined by Eq. (6):

$$TSRE = \frac{\text{Total solvent recovery energy [MJ]}}{CO_2 \text{ captured [kg]}} \quad (6)$$

Low TSRE (MJ/kg) index values are desirable, as minimizing solvent recovery energy is directly related to reducing operational costs, environmental impact, and GHGE.

4. Formulation of the multiobjective optimization problem of design

The PCC process design is an appropriate case to be optimized, considering the objective functions described in the previous section. The design parameters involved in the process directly impact the economic and environmental performance of the process. To develop a design with high CO_2 recovery, low environmental impact, low cost, and high return on investment, optimization strategies are important tools to help find the best combination of design parameters and process variables. The sustainable design of the capture process is complex given the number of decision variables involved and more variables than equations can be defined. Variables such as the conditions of the DES represent a set of parameters that affect the overall performance of the system. For example, optimal conditions must be determined for the water:ChCl/urea ratio, feed temperature, and DES molar flow to comply with process requirements and achieve a sustainable design based on the considered indices. ChCl/urea is reported in the literature to have a very high viscosity (Yadav and Pandey, 2014), which drives up pumping costs. The addition of water to ChCl/urea diminishes the viscosity but decreases CO_2 solubility (Xie et al., 2014), which leads to a higher amount of absorbent needed to achieve capture. The solvent mass flow has an impact on overall costs, mainly through regeneration energy required in the reboiler, which is reported extensively as the main cost of the process (Luo et al., 2021; Wang et al., 2020). Additionally, the existence of design variables such as the absorber and desorber total stages leads to the inclusion of multiple types of variables. The Radfrac module in Aspen plus, used to model the columns, considers the calculation of phase equilibrium along with the complete set of MESH equations (MESH = material balance, phase equilibrium, summation, and heat balance equations for each stage). This represents a non-linear and multivariable problem, where the objective function used as optimization criterion is

generally non-convex with several local optimums (Vazquez–Castillo et al., 2009).

Although a deterministic global optimization provides a theoretical guarantee of finding the global solution to an optimization problem, for solving non-convex and large-scale optimization problems, the application of deterministic methods may not lead to a straightforward solution within a reasonable time lapse due to the complexity of the problem (Lin et al., 2012). Moreover, the use of rigorous non-linear thermodynamic models that are non-convex, and the inclusion of integer variables further increases the difficulty of solving the model by use of these methods (Vazquez–Castillo et al., 2009). Srinivas and Rangaiah (2007) stated that stochastic global optimization methods such as Genetic Algorithms (GA) have been reported as useful strategies for the optimal design of separation schemes. Genetic algorithms are robust and can handle both MESH equations and phase equilibrium calculations with complete models. This study uses the multi-objective meta-heuristic optimization algorithm differential evolution and tabu-list (MODE-TL). Several works regarding its application to process design and optimization have been reported in the literature in the field of chemical engineering design and control. Rangaiah and Sharma (2017) simulated an amine absorption process in Aspen HYSYS, and then optimized using differential evolution with tabu list, for two objectives: capital and operating costs. Sánchez-Ramírez et al. (2022) optimized a process based on liquid-liquid extraction to purify methyl ethyl ketone that involved several distillation columns simulated in Aspen Plus. Using MODE-TL they were able to propose a sustainable process considering simultaneous environmental and economic objectives. Singh and Rangaiah (2019) optimized a hybrid separation process for bioethanol recovery and dehydration considering double-effect distillation and vapor-liquid separators. The use of MODE-TL resulted in Pareto-optimal solutions for the process designs that minimize fixed capital investment and annual operating cost. This algorithm allows the comparison of multiple solutions in terms of the objective functions, described in the previous section.

The hybrid stochastic algorithm known as Differential Evolution with Tabu List (DETL) is selected for the case study considered in this research work. DETL is a stochastic global search technique where the search for the global optimum is carried out in all feasible regions through an iterative procedure. The method was proposed by Srinivas and Rangaiah (2007). It has been shown to have several advantages compared to other optimization methods. For example, DETL has faster convergence, smaller computational efforts, and less computational time to solve non-linear and non-convex problems than other methods like genetic algorithms or simulated annealing (Vazquez–Castillo et al., 2009). Another advantage of DETL is its ability to memorize previously tested solutions, thus avoiding the evaluation of previous solutions. This ability reduces the computational time needed to obtain the optimal solution (Segovia-Hernández and Gómez-Castro, 2017). Recent implementations of this algorithm for the optimization of multiple chemical processes can be found in other works that prove its robustness, practicality, and flexibility to provide optimal designs for these processes. Sharma et al. (2016) have showcased the application of multi-objective differential evolution with Tabu List for an amine absorption plant that contains gas-liquid absorption and separation operations, using an absorption column, a flash tank, and a desorption column. Romero-García et al. applied DETL for the optimization of a PCC process using MEA, considering environmental, economic, and controllability indices. Alcocer-García et al. (2019) used DETL for the multi-objective optimization for the purification of levulinic acid by use of Radfrac distillation columns, involving economic and environmental objectives.

The optimal design of the PCC process means minimizing the objective functions based on the sustainable metrics considered: TAC, -ROI, EI99, TSRE, and GHGE. The process is restricted to satisfy the CO_2 recovery rate and purity constraints. A general mathematical expression for the objective function and the decision variables involved in the optimization procedure is shown in Eq. (7).

$$\min[TAC, -ROI, EI99, TSRE, GHGE] = f(x_{H_2O}, F_{DES}, T_{DES}, N_{AC}, N_{PS1}, N_{PS2}, P_{AC}, P_{FT1}, \Psi_{FT1}, P_{FT2}, \Psi_{FT2}, RR, D, N_{DC}, N_{feed}, P_{DC}) \quad (7)$$

$$\text{s. t. } a_{i,f} \geq b_{i,f}, \text{ and } w_{i,f} \geq u_{i,f} \quad (8)$$

where x_{H_2O} is the water molar fraction present in the absorbent mixture, consisting of water and ChCl/urea (1:2), F_{DES} (Fig. 1) represents the molar feed flow of the absorbent mixture fed into the absorption column, whilst T_{DES} is the absorbent feed temperature. N_{AC}, $N_{PS1}$and N_{PS2} are the absorber column's total stages, the first packing section number of stages, and the second packing number of stages, respectively. P_{AC} is the absorber's top-stage pressure. P_{FT1}, P_{FT2}, Ψ_{FT1} and Ψ_{FT2} are the pressures and vapor fractions for the first and second flash drums, respectively. For the variables related to the desorption column, RR is the reflux ratio, D is the molar distillate rate. N_{DC}, N_{feed} and P_{DC} are the number of trays, feed stage, and condenser pressure, respectively. The objective function is restricted to satisfy the recovery of at least 95% of the CO_2 produced during the combustion and also to achieve a purity of 95%mol of CO_2. Where $a_{i,f}$ represents the CO_2 recovered in the desorber column and $b_{i,f}$ represents 95% of the CO_2 produced during the combustion. As well $w_{i,f}$ represents the purity achieved at the desorber column and $u_{i,f}$ represents the purity expected of at least 95% mol of CO_2.

Two types of variables are used to define the capture plant coupled with the simplified power plant: discrete and continuous. A sensitivity analysis in Aspen Plus, as well as considerations of design heuristics, lead to the definition of search bounds for the relevant decision variables, such as minimum and maximum column pressure and number of maximum stages. The list of variables used in this study, along with the search bounds, is given in Table 2.

The optimization method has been implemented using a hybrid platform that interconnects the Aspen Plus simulation with Excel through Visual Basic. The numerical method, coded in Visual Basic, generates vectors that consist of variable design inputs (F_{air}, x_{H_2O}, F_{DES}, T_{DES}, *etc*). Through dynamic data exchange, the inputs are fed to the process model, where the rigorous simulation is implemented in Aspen Plus. In the absorber column (AC) the model considers the complete set of MESH equations, and isothermal operation is defined. Vapor-liquid equilibrium is defined for the ChCl/urea (1:2) - O_2 and the ChCl/urea (1:2) - N_2 systems via NRTL binary interaction parameters, and gaseous components are described with the PR equation of state. The solubility of CO_2 in the DES is described by Eq. (1). The flash tanks

Table 2 – Decision variables and search range for multi-objective optimization.

Symbol	Variable Type	Lower value	Upper value	Units
x_{H2O}	Continuous	0.625	0.921	—
F_{DES}	Continuous	5000	125,000	kmol h^{-1}
T_{DES}	Continuous	40	60	°C
N_{AC}	Discrete	20	100	—
N_{PS1}	Discrete	2	$(N_{AC} - 1)$	—
N_{PS2}	Discrete	$(N_{AC} + 1)$	N_{AC}	—
P_{AC}	Continuous	1	14	atm
P_{FT1}	Continuous	1	6	atm
Ψ_{FT1}	Continuous	0	1	—
P_{FT2}	Continuous	1	6	atm
Ψ_{FT2}	Continuous	0	1	—
RR	Continuous	0.1	5	—
D	Continuous	1000	1200	kmol h^{-1}
N_{DC}	Discrete	10	30	—
N_{feed}	Discrete	2	29	—
P_{DC}	Continuous	1	14	atm

are modeled as single liquid-vapor separation stage, with a vapor outlet and a single liquid outlet. Finally, a rigorous simulation of the desorption column (DC), or stripper, considers the complete set of MESH equations. The outputs of the process model (flows, thermal loads, temperatures, etc.) are fed back to Excel, where the optimization algorithm evaluates the objective functions and proposes new values of input vectors based on their performance. According to the evolutionary nature of the algorithm, the process begins to iterate. For this work, the parameters used for DETL consisted of 120 individuals, 600 maximum generation number. The values of tabu list of 50% of individuals, tabu radius of 1×10^{-4} and 0.9 and 0.3 crossover probability and mutation factor were taken based on the recommended values for these parameters by Sharma and Rangaiah (2010). All case studies were rigorously modeled using the process simulator Aspen plus v8.8, considering PR thermodynamic model for the combustion process, and NRTL-PR for the PCC process.

5. Results and discussion

This section provides the multi-objective optimization results of the PCC process coupled with a power generation plant, considering economic and environmental indices, for the four case studies considered. The Pareto diagrams obtained for all four cases studies are presented in Fig. 2 as two-dimensional representations. The solutions found in the Pareto front may be used in decision-making regarding which fuel results in a PCC that is more economically viable, less environmentally hazardous, and provides a higher return on investment. Each of the points represents a PCC design that meets the CO_2 purity and recovery desired.

The Pareto front's forms in Fig. 2 for EI99 and TAC exhibit a trend of competing for objective functions. This behavior indicates that the selection of a design with the lowest EI99 causes the TAC to increase, hence the solutions that offer the best trade-offs between the two objectives are those located in the curve zone of the Pareto chart. When a gas is used as fuel a tendency can be observed, where for a decrease in flue gas CO_2 content, designs with lower cost and environmental impact are obtained. Thus, the best tradeoff between EI99 and TAC corresponds to AG > NG > BG. However, the Pareto front for coal shows optimal designs with a considerably more favorable tradeoff than when any of the gasses are used for combustion. The Coal PCC process manages to capture CO_2 at a significantly higher rate, which boosts performance indices.

An optimal design is selected for each case study and is indicated in each Pareto front (denoted as OP in Fig. 2), considering the Utopian point method. Design variables, operation conditions, and performance indices from each optimal design are presented in Table 3. To analyze the results for each design, it's important to consider the CO_2 content of the flue gasses for each fuel considered. The combustion of Natural Gas, Coal, Biogas, and Associated Gas produces a flue gas with 4.9%, 12.4%, 5.43% and 4.17%mol of CO_2 content. The burning of Coal produces the highest carbon-containing combustion vapor, followed by those obtained from Biogas and Natural Gas.

The optimization results reveal that the Coal process provides the lowest energy usage per unit of CO_2 captured when compared with each of the gaseous fuels, with a TSRE and GHGE which are 12.3%, 27.7%, and 31.7% lower than AG, NG, and BG respectively. The energy savings are also reflected in the value of TAC for Coal (12.0%, 27.3%, and 32.4% lower per tonne of CO_2 captured, compared with AG, NG, and BG respectively). In terms of environmental impact, the Coal process presents a value of EcoPoints/tonne CO_2 that is 21.9%, 56.1%, and 72.8% lower than AG, NG, and BG respectively. The coal process also exhibits the highest ROI (56.94%, 47.17%, and 2146.25% higher than AG, NG, and BG respectively), and the best overall performance considering all environmental and economic indices simultaneously.

The performance of the proposed PCC process seems to benefit greatly from the considerably higher CO_2 content in the flue gasses from coal combustion. Although an opposite trend can be observed when using gaseous fuels, where AG shows the best performance despite having the lower CO_2 content, followed by NG and BG. This behavior seems to indicate that at low CO_2 content in the treated gases, the process is inefficient energy-wise and has a higher environmental burden as carbon content increases. A tipping point for this behavior is reached when treating a considerably higher CO_2 content for the coal flue gases (153%, 197%, and 128% higher CO_2 molar content when compared with each of the gaseous fuels NG, AG, and BG). From Table 3, the impact of some variables on the performance indices can be observed. The total heating duty directly affects TAC, ROI,

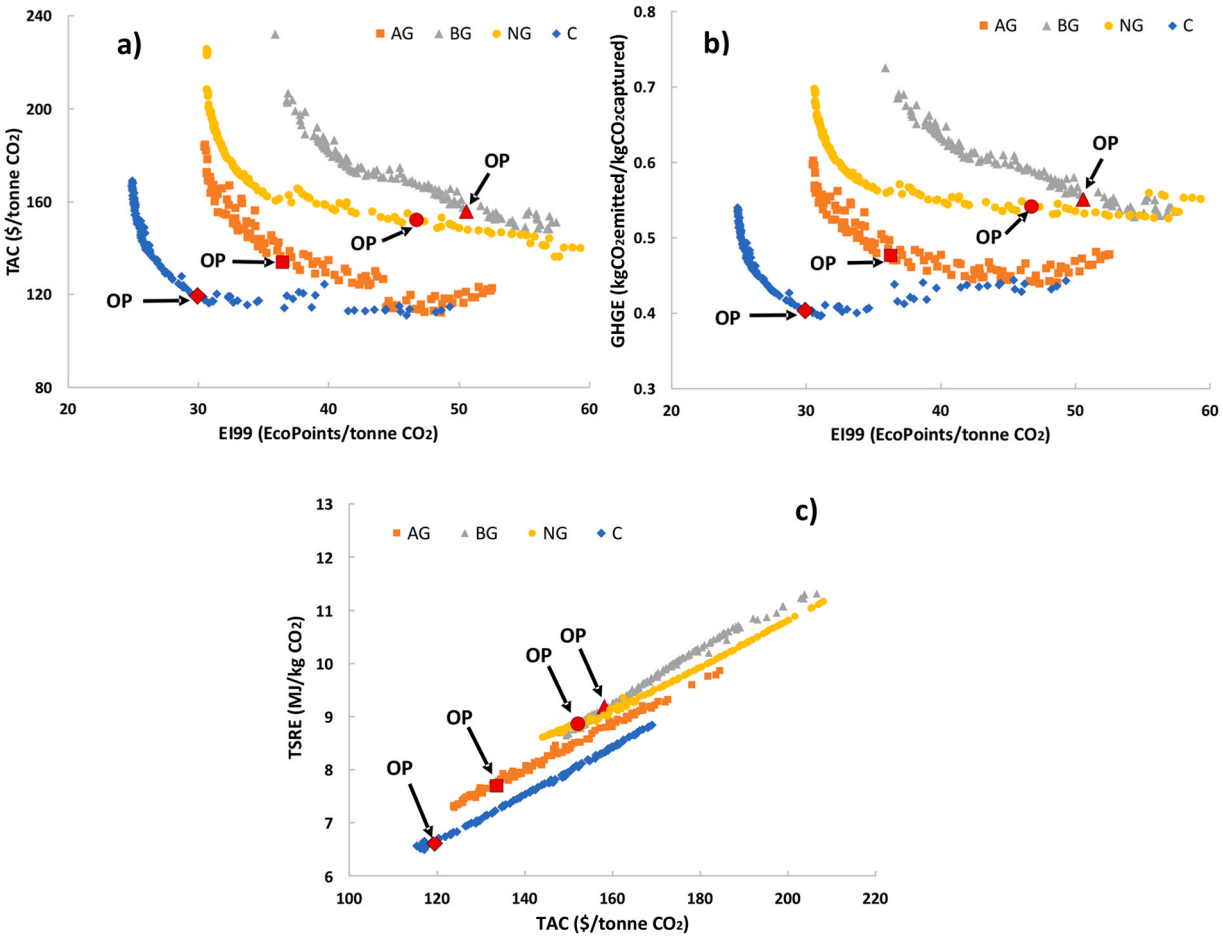

Fig. 2 – Two-dimensional Pareto fronts for a) EI99 vs TAC per tonne of CO_2 captured, b) EI99 per tonne of CO_2 vs GHGE, and c) TAC per tonne of CO_2 captured vs TSRE.

TSRE, and GHGE, and is one of the main categories impacting in the EI99. The heating duty usage increases with increasing CO_2 content for the different flue gases. The AG process reveals the lowest energy used (13.3% lower than NG and 16.2% lower than BG). Overall, the Coal process provides the lowest energy usage per unit of CO_2 captured, with a TSRE and GHGE which is 16.2%, 34.0%, and 38.7% lower than AG, NG, and BG respectively. The energy savings are also reflected in the value of TAC for the Coal PCC process (8.2%, 15.5%, and 16.2% lower per tonne of CO_2 captured, compared with AG, NG, and BG respectively). In terms of environmental impact, the Coal process presents a value that is 20.1%, 15.7%, and 30.2% lower per tonne of CO_2 captured when compared with AG, NG, and BG, respectively. In terms of the DES's composition, it can be observed that higher water to ChCl/urea proportion diminishes CO_2 absorption capacity, increasing the need for total solvent flow. This causes the regeneration energy requirements to increase, as observed in the TSRE values. As a consequence, GHGE also increases, and from the Pareto chart trends in Fig. 2, the environmental impact decreases. A higher ChCl/urea concentration in the DES will increase environmental impact and pumping costs considerably due to higher viscosity of a poorly diluted absorbent. As well, the reflux ratio is directly related to the energy requirements. A higher reflux ratio causes energy requirements for the capture to increase.

Regarding the solvent regeneration scheme proposed in this work via sequential separation using FT-1, FT-2, and DC, an improvement of operation parameters was achieved by the use of three sequential regeneration steps. Compared to the operation conditions proposed by previous PCC schemes using ChCl/urea (1:2) (Luo et al., 2021; Wang et al., 2020), the costly absorber column pressure (44.41 atm) is improved to a lower 13.62 atm, and vacuum pressure operation for the solvent regeneration in the flash tanks is avoided. Still, a high energy load destined for solvent regeneration is present, as evidenced by the GHGE values obtained for all case studies. Regarding solvent loss, it was found that only trace amounts of the DES are lost in the process, due to its high thermal stability. These results are in accordance with previous works reported. Wang et al. (2020) report 0.3 g/h solvent loss for the DES, while using 22,000 kg/h of solvent, accounting for a DES loss of 0.0001364%. Luo et al. (2021) report a solvent loss of 0.00083 kg/tonne CO_2 compared to a solvent loss of 0.178 kg/tonne CO_2 for the MEA-based process. It must be emphasized that the results showing the influence of operational parameters and design variables in the performance of the DES presented in this work, as well as the negligible solvent loss found, are based on the properties of the solvent obtained from group contribution methods and parameter estimates in the Aspen Plus simulation software. As more experimental data and reliable parameter estimation for the properties of the DES is available, the feasibility of the proposed process and the influence of the design variables will be more clearly determined.

The feasibility of the DES carbon capture process is analyzed by comparing with the reference solvent MEA. Results are compared with the PCC process optimized by Romero-

Table 3 – Design variables of optimal designs of the PCC process, considering 2D Pareto chart.

Design variable	NG	AG	BG	C
Absorbing agent				
Water molar fraction in DES	0.835	0.757	0.745	0.769
Feed DES molar flow rate, kmol h^{-1}	35,003.46	26,487.86	26,698.86	31,523.12
Temperature of solvent feed, °C	41.27	42.04	40.36	43.22
Absorber column (AC)				
Total absorber stages	49	60	73	66
Packed stages	20	32	47	50
Absorber top pressure, atm	13.79	13.81	13.73	13.74
Diameter, m	0.50	1.04	0.51	2.80
Height, m	29.87	36.58	44.50	38.41
Flash tank 1 (FT-1)				
Operation pressure, atm	2.51	4.44	4.45	2.51
Vapor fraction	0.023	0.026	0.028	0.026
Cooling duty, kW	40,201.13	38,977.38	42,087.77	71,637.95
Flash tank 2 (FT-2)				
Operation pressure, atm	2.22	3.74	2.27	4.99
Vapor fraction	9×10^{-4}	8×10^{-4}	2.4×10^{-3}	9×10^{-4}
Heating duty, kW	24,475.58	33,491.74	17,661.16	71,304.73
Desorber column (DC)				
Reflux ratio	0.1	0.1	0.1	0.1
Distillate rate, kmol h^{-1}	1018.09	1064.92	1018.14	1377.32
Number of stages	5	6	13	5
Feed stage	2	5	11	4
Top pressure, atm	1	1	1	1
Top temperature, °C	4.10	7.31	7.04	22.15
Bottom temperature, °C	95.68	96.52	107.08	89.50
Diameter, m	0.59	0.86	0.74	0.88
Height, m	1.83	2.44	6.70	1.83
Heating duty, kW	80,362.98	61,583.50	90,899.44	52,844.03
Molar flowrates of CO_2 streams				
Total CO_2 entering the PCC, kmol h^{-1}	1009.97	1054.20	985.22	1364.30
CO_2 product stream, kmol h^{-1}	968.15	1011.85	967.93	1314.73
Performance indices				
ROI, %/yr.	22.90	24.42	1.6	35.94
TAC, $/tonne CO_2	152.05	133.70	158.15	119.41
EI99, Eco-points/tonne CO_2	46.71	36.48	51.69	29.92
GHGE, tonneCO_2emit./tonneCO_2capt.	0.541	0.470	0.561	0.404
TSRE, GJ/tonne CO_2capt.	8.87	7.69	9.18	6.62

García et al. (2022) using a similar optimization scheme, considering economic, environmental, and controllability indices. In terms of environmental impact, Romero-García et al. (2022) determined the EI99 using the same impact categories. For the capture of carbon from coal flue gases, the DES-based process shows 63.2% reduction in EcoPoints/tonne CO_2, compared to MEA, highlighting the advantages of the non-toxic nature of the green solvent. Furthermore, the DES-based process shows an improvement in terms of sustainability compared to the MEA-based process when treating flue gasses from AG (28.2% decrease for the environmental impact). For NG no discernable benefit was found from the proposed DES-based process (2.65% decrease in environmental impact), and for BG the MEA-based process was found to have a 15.9% smaller environmental impact than the DES-based process. Romero-García et al. (2022) report a TSRE of 6.4 GJ/tonne CO_2 for the coal-fired power plant, using MEA. The energy used for solvent regeneration for the DES process is 3.44% higher than MEA for the coal-fired plant, although Romero-García et al. (2022) standardized recovery to 99% with 99%mol purity for the CO_2 captured. TSRE is considerably higher for the DES-based process for AG, NG and BG when comparing each fuel with the corresponding case in the MEA-based process (11.4%, 61.3%, and 33.0% higher). Benchmark cases for solvent regeneration with MEA have been reported at around 3.0 – 4.5 GJ/tonne CO_2 (Song et al., 2018). The higher solvent regeneration found by the methodology for sustainable process design used in Romero-García et al. (2022) is explained by the authors in terms of the tradeoff between the minimization of several objective functions, where the sole purpose of the sustainable process design is not minimizing solvent recovery, but rather a compromise between several objective functions is obtained in the Pareto-optimal solutions. For the DES-based process, a similar clarification must be made. The consideration of simultaneous environmental and economic vectors leads to a sustainable process design, in which further work might help improve the high solvent regeneration found.

These results show that, although more energy expensive, the DES-based process is more sustainable than the conventional PCC process when treating flue gasses from bituminous coal (C) and associated gas (AG) but shows no benefits from greater sustainability when treating flue gasses from natural gas (NG) and biogas (BG). It must be emphasized that the results showing the influence of operational parameters and design variables in the performance of the DES presented in this work, as well as the negligible solvent loss found, are based on the properties of the solvent obtained from group contribution methods and parameter estimates in the Aspen Plus simulation software. As more experimental

data and reliable parameter estimation for the properties of the DES is available, the feasibility of the proposed process and the influence of the design variables will be more clearly determined.

6. Conclusions

A novel PCC process is designed and optimized using DES ChCl/urea (1:2), under a sustainability scheme. The Multi-objective optimization considering simultaneous economic (TAC and ROI) and environmental (EI99, TSRE, and GHGE) objectives showed that the PCC process for CO_2 from the flue gas of a coal-fired power plant outperforms the use of all other fuels evaluated. The proposed process can achieve a 95% recovery rate and a 95%mol purity for CO_2 captured for all case studies considered. A comparison with a similarly optimized PCC MEA-based process indicates a considerably lower environmental impact for the DES-based carbon capture plant, and comparable energy consumption for solvent regeneration. Potential for further development of the process lies in considering industrial-scale combustion and PCC coupled process, safety, and controllability indices.

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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