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Implementing CO_2 capture process in power plants: Optimization procedure and environmental impact

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ABSTRACT

Because of the current high concentrations of greenhouse gases in the atmosphere, global warming is one of the main challenges to solve in the 21st century. The present work evaluated the environmental impact of coupling an optimized CO_2 capture plant to an electric power generation plant. The use of four different fuels in the power plant was considered; biogas, coal, non-associated natural gas, and associated natural gas. Two operating scenarios were considered; in the first, the same fuel flow was considered for all the plants, and in the second, the same energy demand was specified. The design and simulation of the process plants were developed using the ASPEN Plus simulator, optimization using a stochastic technique named Differential Evolution with Tabu List, while the LCA was carried out with SimaPro software. The efficiency of the capture processes is directly related to the CO_2 concentration in the combustion gas and the absorbent flow for CO_2 capture. Note that both the energy used and the demand for the solvent in CO_2 capture are variables that significantly affect the environmental impact of the overall process, so it is necessary to determine the effect of selecting one fuel or another in the generation stage and capture of CO_2 such as energy requirements, design parameter in the downstream process, and so on. According to the results obtained, for the scenario with a constant flow, the best alternative for capture is the one that considers biogas as fuel. On the other hand, non-associated gas was the most promising alternative for the scenario with constant energy demand.

1. Introduction

Global warming is one of the major environmental problems that affect humans worldwide, caused by the constant emissions of greenhouse gases from the burning of fossil fuels (McCarthy et al., 2002; O'Neill and Oppenheimer, 2003). Moreover, the environmental effect of greenhouse gases considers that Carbon dioxide (CO_2) contributes 60% of the effects of global warming (Olajire, 2010). CO_2 is produced by several industrial processes such as the combustion of fossil fuels to produce electricity and in the transport sector. According to the International Energy Agency, from 37.1 GT of CO_2 produced in 2019, 35 GT belongs to the energetic sector. The remaining of the emissions were due to the transport sector and the rest from other sectors such as buildings, industry and so on. To set climate change, it is necessary to develop sus-

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tainable alternatives for electricity production, as well as alternatives to mitigate CO_2 emissions. Due to growing environmental problems, it is imperative to seek industrial processes in accordance with the Sustainable Development Goals – United Nations, that are not just sustainable but also ecofriendly.

Considering the aforementioned, the production of greenhouse gases due to electricity production is of relevant importance. In the USA the electricity production from coal and natural gas is within the three major categories jointly with nuclear energy and renewable energy sources to obtain electricity. Natural gas is used directly to produce steam or even to operate gas turbines to generate electricity due to its high thermal efficiency. On the other hand, coal was the second energy source, in the same sense as natural gas, coal is almost all used in coal-fired power plants which use a turbine to generate electricity. Currently, the options to reduce total CO_2 emissions can be summarized into three options: 1) enhance conversion efficiency; 2) use a low/carbon-free fuel, and 3) improve CO_2 capture. While it is expected that the energy produced by renewable sources will be able to cover the world energy demand, during this transition it is planned to continue using fossil sources. In this sense, to minimize the environmental footprint of fossil fuel combustion, several efforts have been carried out to improve the efficiency of the current processes. As well, the implementation of Carbon capture and storage (CCS) technologies exhibited promising results in reducing global warming and climate change.

The capture of CO_2 in post-combustion involves the separation of CO_2 from a gas stream produced by the combustion of some fuel. A typical chemical absorption process consists of an absorber and a separator where the absorbent is regenerated. In a chemical absorption process for CO_2 capture, the gas effluent enters the bottom of an absorber and comes into contact in countercurrent with a CO_2 absorber. After the absorption process, the gas effluent enters a separator for thermal regeneration. After regeneration, the CO_2 burner is returned to the absorber for reuse. The pure CO_2 is released from the separator to be subsequently compressed and transported. In recent years, different studies have focused on implementing new green solvents that can be used for the CO_2 capture process and thus reduce the environmental footprint of the use of solvents and, therefore CO_2 emissions. For instance, Haider et al. (2021) report the use of phosphonium based deep eutectic solvents for CO_2 capture process, ensuring the use of green solvents. As well, Silva-Beard et al. (2021) propose the implementation of mixtures of ionic liquids, improving the processing features. These solvents are non-corrosive, non-toxic, and have favorable physiochemical properties such as negligible volatility, high thermal stability (Armand et al., 2009). According to the Global CCS Institute, despite the efforts in the search for new solvents or new technologies for CO_2 capture that minimize the environmental footprint, these new technologies are not scalable at an industrial level, due to the high costs of implementation and operation. Moreover, the use of monoethanolamine (MEA) as a solvent in the capture of CO_2 continues being widely used at industrial and pilot level (Global CCS Institute, 2019). Some examples of carbon capture using chemical absorption with MEA at industrial level are shown in Table 1.

Besides that, its thermodynamic properties are widely known, facilitating the process modeling. Therefore, the CO_2 capture process using MEA can be used as a reference point for a rigorous analysis of the process variables that directly impact energy consumption, amine degradation, and environmental footprint. Despite its high efficiency, low cost, and the facility of implementation to existing power plants, MEA is considered highly toxic so that its implementation entails a high environmental impact. To have a positive environmental impact on CO_2 capture processes, it is necessary to highlight the technical challenges involved in the separation method of CO_2 due to the use of aqueous amine solutions. To achieve high efficiency and low environmental impact, it is important to consider two different aspects: i) To improve the power plant efficiency, which depends on the type of fuel and determines the CO_2 concentration in the flue gases, ii) to optimize the process design and operating conditions for the CO_2 capture. As discussed in Nagy and Mizsey (2015), changing flue gases conditions significantly influence the optimal operation of the capture process, particularly the solvent and energy requirements.

As stated above, carbon capture processes have been considered an alternative to reduce CO_2 emissions, particularly those associated with electricity production. However, to guarantee that implementing these processes present real environmental advantages, it is necessary to evaluate their environmental impact through a systematic methodology. Life Cycle Analysis (LCA) allows the identification, measurement, and evaluation of the potential impacts associated with a product or service throughout its entire life cycle, from obtaining raw materials to final disposal. The results of an LCA are interpreted in terms by Ecoindicators, quantifying the environmental impact by the normalization and weighting of the obtained results for each category indicator. Such Ecoindicators considerer three types of environmental damages: human health, ecosystem quality, and resources depletion, wherein each one may include various subcategories of impacts, such as global warming, human toxicity, ozone depletion, terrestrial eutrophication, among others (Goedkoop and Spriensma, 2001).

Different studies have been reported in the literature in which CO_2 capture is implemented. A few expamples of them aim to carry out an environmental analysis of the implementation of CO_2 capture plants to power plants. Either for a specific fuel (Petrakopoulou and Tsatsaronis, 2014), in different geographical regions (Schreiber et al., 2012), or a comparative LCA for different carbon capture technologies (Garcia-Garcia et al., 2021). The analysis of the literature information, suggests that carbon capture and utilization provide a notable reduction in global warming and climate change indicators, compared to conventional processes. However, there is no work in literature in which there are reported the optimum conditions during the CO_2 capture process implementation, by reducing energy requirements in a rigorous optimization considering the full model and then perform an environmental impacts analysis as an index of sustainability.

On the other hand, due to the large number of degrees of freedom, as well as process variables, process optimization has proven to be a very important tool in the design of CO_2 capture processes. The optimization applied directly to the capture processes can provide an appropriate solution in the search to maximize CO_2 capture, and minimize energy use for that process. In the CO_2 capture process, there are great challenges to overcome due to the inherent complexity that these processes represent. When it comes to modeling these types of processes, a complete model should consider all the interactions resulting from the matter balance, energy balance, thermodynamic model, as well as the existing reactions in the system. CO_2 capture has been addressed on several occasions with the intention of obtaining optimized schemes. Lee and Han (2015) performed the parametric optimization process of the CO_2 capture plant through trial and error. Having as objective function maximize the exergy efficiency, and the total heat transfer capability and minimize the turbine size parameters under the waste heat conditions. The study was carried out for natural gas and the results proposed that the optimization of the design variables will improve the exergy efficiency of the process. Similary, Bravo et al. (2021) presented a parametric optimization of a coal power process with CO_2 capture having as objective function the reduction of energy requirements. As results they present the optimal parameters for the capture plant to reduce energy requirements. Zaman and Lee (2015) performed the optimization of a post-combustion CO_2 capture plant, considering flexible operation with coal as fuel. The modeling was performed using the gproms software.Similarly, Yancy-Caballero et al. (2020) performed a capture process in a Pressure Swing Adsorption process using a discretized model in sections. On the other hand, Mores et al. (2014), developed a rigorous optimization model to address the design and operation of power plants coupled to capture systems. The modeling of the process was limited to mass, and energy balances, design equations for gases, turbines, pumps, condensers and steam generators. Having as objective function the mitigation cost. The optimization process of this surrogate model was performed in gams. Moreover, (Yulia et al., 2021) presented the deterministic optimization of a CO_2 absorption system by maximizing exergy and minimizing exergoenvironmental. The analysis is presented for a coal fired power plant. However, all these optimization studies were carried out without rig-

Table 1 – Industrial utilization of chemical absorption using MEA.

Company	Industry Sector	Location	Reference
KBR	Engineering, procurement, construction and service companies	Texas, USA	(Luis, 2016)
Alstom	Power generation	Saint-Ouen, France	(Luis, 2016)
SaskPower's Boundary Dam Power Station	Power generation	Canada	(IEAGHG, 2015; Wilson et al., 2004)
Ruukki Metals	Steel	Raahe, Finland	(Arasto et al., 2014)
SINTEF Energi	Cement plant	Norway	(Anantharaman et al., 2016)
Norcem AS	Cement Plant	Norway	(Jakobsen et al., 2017)

orously considering the model associated with the combustion and capture process. That is, the original model associated with the process was not considered. In this work, using a black box methodology, it was possible to optimize the CO_2 capture process using the complete process model using a stochastic optimization algorithm. Additionally, this paper proposes optimization for four different fuels. Evaluating the system in a sustainability framework. In other words, rigorous modeling, as well as optimization considering the complete model and the complexity it entails, is important to determine the feasibility of this type of processes, to assume their complexity and to find the adequate combination of variables that allows an optimized operation that guarantees the minimum energy consumption in the CO_2 capture process.

In the present work aims to present a novel analysis, considering the optimal conditions during CO_2 capture considering as objective function the minimization of the energy requirements. Therefore, a LCA is presented as a metric to evaluate the environmental impact of different scenarios of thermoelectric plants coupled to CO_2 capture processes using monoethanolamine (MEA) as solvent. The case studies for this analysis include the effect of the processes with constant fuel flow and constant energy demand; in that sense, the impact of the type of solvent will not be taken into account as a degree of freedom in this analysis. Both scenarios to be evaluated include the use of the three most used fuels in power plants according to the International Energy Agency (2020): coal, natural non associated gas, and associated gas; as well it is also presented a scenario using biogas as a sustainable alternative. This work is novel since, although the implementation of CO_2 capture plants reduces the environmental footprint caused by CO_2 emissions, it is important to carry out a general study of the environmental implications of implementing such technology. As discussed earlier, there are different works in the literature where the LCA for capture plants is reported. Some of them evaluate the impact of the MEA as a solvent by categories (Asselin et al., 2020). Likewise, the LCA is reported for coal-fired power plants using MEA, DME, or ammonia-ethanol (Strube et al., 2011). However, there are no works where the optimization of the capture process is reported accompanied with the LCA where the performance of 4 fuels is evaluated in a comparative analysis using MEA.

2. Methodology

In order to analyze the environmental impact in different scenarios of electric power generation plants with the coupling of a CO_2 capture process in post-combustion, two cases were studied: constant fuel flow and constant energy demand. For each of these cases, four different fuels were used: biogas, coal, non-associated gas, and associated gas. The simulation of the power plant and the CO_2 capture process was carried out in the Aspen Plus V8.8® process simulator. The study of these two cases using the four most commonly used fuels in thermoelectric plants is important as a preliminary study for industrial applications. It is important to highlight the importance of CO_2 capture in an existing energy production scenario as an overview of the case study. According to the information reported by Hasan et al. (2012), the design of the power generation plant was carried out using the Peng-Robinson method to estimate the thermodynamic properties. The simulation of the combustion chamber was carried out using the RGibbs reactor module (equilibrium modeling in Aspen Plus, which is based on the minimization of the Gibbs free energy of the system in terms of the mole numbers of the species present in all phases) considering a molar ratio of air to fuel of 30:1. With excess air, in order to achieve complete combustion for the four fuels. And a fuel flow of 1000 kmol/h for all the analyzed cases. The compositions in the mass percentage of the fuels used are shown in Table 2. Note, associated gas refers to the natural gas found in association with oil within the reservoir. Some reservoirs contain only natural gas and no oil, this gas is termed non-associated gas.

Table 2 – Fuel composition in mass percent (Hasan et al., 2012; Luyben, 2013).

	Natural Gas	Associated Gas	Biogas	Coal
CH_4	96.00	87.20	60.00	–
C_2H_6	1.80	4.50	–	–
C_3H_8	0.40	4.40	–	–
$i\text{-}C_4H_{10}$	0.15	1.20	–	–
N_2	0.7	2.70	2.00	–
CO_2	0.95	–	38.00	–
C	–	–	–	78.20
H	–	–	–	5.20
O	–	–	–	13.60
N	–	–	–	1.30
S	–	–	–	1.70

Fig. 1 shows the global CO_2 capture process coupled to a thermoelectric plant. The CO_2 capture problem is commonly oriented to the downstream process. However, in this study, we wanted to address the capture problem by considering a slightly more extensive version of the overall process. Although this proposal only presents a proposal of two stages before the capture process, it has been demonstrated that this simplified plant has the necessary characteristics to adequately represent the process as well as its operating parameters, compressor system, compression ratio, etc. Luyben (2013). The CO_2 capture process was designed by chemical absorption using an aqueous monoethanolamine (MEA) solution at 30% weight as the solvent. The 30 wt% aqueous mixture has practical importance: MEA in high concentration is strongly corrosive, and its viscosity increases, making it difficult to handle efficiently at lower temperatures (Kohl, 1985). RadFrac balance stage block (the main separation block in Aspen Plus. The block can perform simulation, sizing, and rating of the tray and packed columns) was used to simulate the absorber and the regenerator (see Fig. 1). An equilibrium stage model of a tower packed with Sulzer Mella-

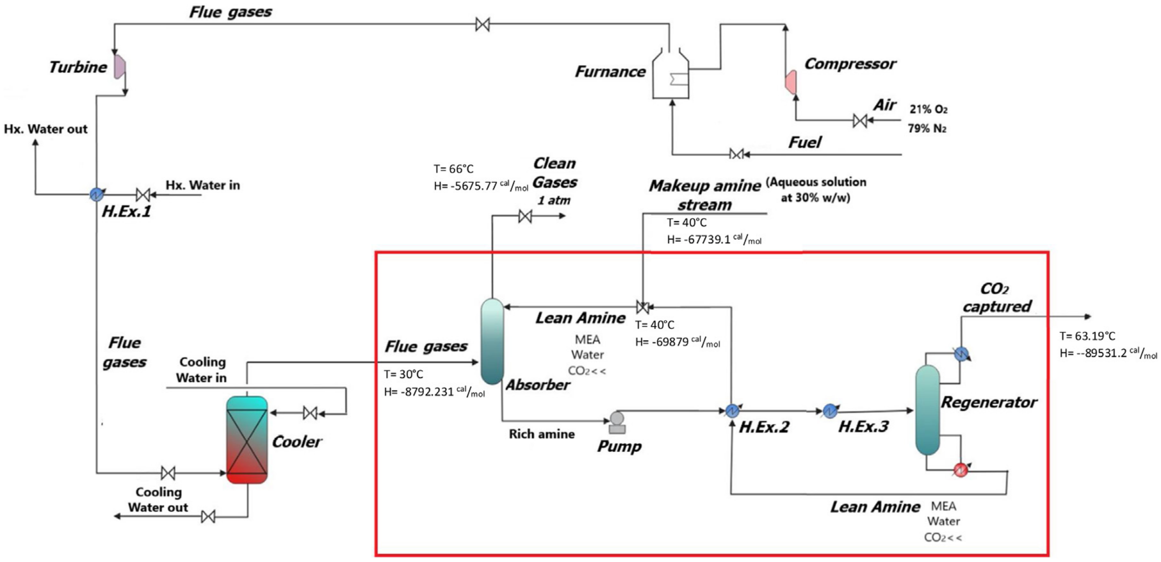

Fig. 1 – Flow diagram of a thermoelectric power plant with CO_2 capture system in post-combustion using chemical absorption with monoethanolamine. Considering energy balance for case 2.

Table 3 – Kinetics of reactions (Zhang et al., 2018).

Kinetic constant, k		Activation energy, E (kJ/mol)
1	1.33×10^{17}	55.38
2	6.63×10^{16}	107.24
3	3.02×10^{14}	41.2
4	5.52×10^{23}	69.5

Table 4 – Equilibrium constant values (Nagy and Mizsey, 2015).

$\ln keq = A + B/T + C \ln(T) + D(T)$
A[=] dimensionless
B[=] K
C[=] 1/K
D [=] 1/K
T [=] K

	A	B	C	D
Equation 3	−3.038325	−7008.357	0	−0.00313489
Equation 4	132.89888	−13445.9	−22.4773	0
Equation 5	216.050446	−12431.7	−35.4819	0

pak 250 Y™ type packaging was used in the absorber and the regenerator a non-equilibrium stage model of a tower packed with Sulzer Mellapak 150 Y ™ packaging (Bui et al., 2018).

The chemical reactions involved in the reactive absorption/desorption process are presented in Eqs. 1–7. Table 3 shows kinetic data for Eqs. 1–4, considering an Arrhenius form. Additionally, Table 4 shows the kinetic and equilibrium constants.

Reactions with kinetics

$$OH^- + CO_2 \leftrightarrow k_1/k_2\, HCO_3{}^- \tag{1}$$

$$HMEA + CO_2 + H_2O \leftrightarrow k_3/k_4\, MEACOO^- + H_3O^+ \tag{2}$$

Equilibrium reactions

$$MEA^+ + H_2O \rightarrow MEA + H_3O^+ \tag{3}$$

$$2H_2O \rightarrow OH^- + H_3O^+ \tag{4}$$

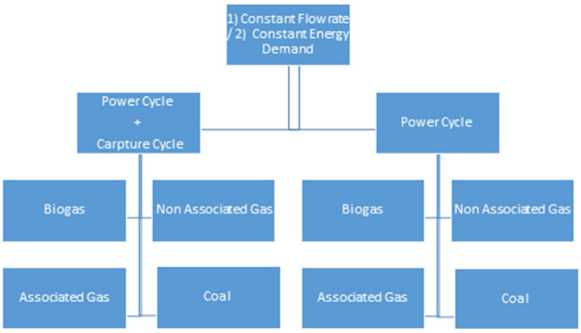

Fig. 2 – Carbon Capture scenarios: analyzed at 1) Constant fuel flow and at 2) Constant energy demand.

$$HCO_3^- + H_2O \rightarrow CO_3^{2-} + H_3O^+ \tag{5}$$

The power plant and capture process were simulated separately considering the combustion gases of the first process as a feed of the absorption tower. In order to carry out the life cycle analysis of the different scenarios, it was necessary to standardize the processes so that they could be comparable to each other. In this case, the variables were manipulated to guarantee a 95% molar recovery in the CO_2 stream in the absorber. Because the components present in the absorption process dissociate, it is necessary to achieve a recovery of CO_2 in the gas output stream of the same equipment. In the case of the regenerator, the distillate flow and the reflux ratio were manipulated to capture the greatest amount of CO_2 from the combustion gas stream coming from the thermoelectric power plant and thus reduce the CO_2 emissions to the atmosphere and the environmental impact that they generate. For this reason, in all the analyzed cases, they were standardized to a purity of 99 mol% of CO_2. Scenarios evaluated for CCS at constant fuel flow and constant energy demand are presented in Fig. 2.

To carry out the LCA it is necessary to define the system boundaries and the functional unit. This work considers a cradle to gate analysis, wherein it is quantified the environmental impact from obtaining raw materials until the output of processing plants; the power generation process and/or CO_2 capture plant. The associated inputs are raw materials (fuel, air, water, solvent) and energy requirements during solvent regeneration. Additionally, the definition of the functional unit is fundamental to developing the LCA. The functional unit refers to the calculation base for the analysis, which should be selected to reflect the function that is going to be compared. In the case of power plants, the functional unit is 1 MW h produced, while the functional unit is 1 kg of CO_2 captured for the capture process. Impact Assessment was performed with SimaPro 8® software using ReciPe EndPoint (H) method. ReCiPe method evaluates the environmental impact in three damages categories: human health, ecosystem, and resources, obtaining a single score derived by aggregating the weighting results of the different impact categories (Goedkoop and Spriensma, 2001).

Regarding the optimization process, due to the preponderant role of energy consumption in the overall CO_2 generation, the objective function will focus on minimizing the energy consumption according to the following equation. A hybrid stochastic optimization algorithm, Differential Evolution with Tabu List (DETL), was used to solve the objective function and the model associated with the equipment. Note that the solution of this type of model involves solving the MESH equations (matter and energy balance, summation constraints, thermodynamic equilibrium) as a whole, not to mention the solution of the chemical reaction. For example, for a column of N stages and C components, the model for that column is represented by N(2C + 3) equations in [N(3C + 10) + 1] variables, which represents a set of nonlinear algebraic equations. Fortunately, using this solution strategy allows us to solve this complex model completely and unchanged in a “black box” fashion. This methodology selection is due to the nature of the model to be solved, that is, the model is highly non-linear and potentially non-convex, understanding a convex model as any problem where the objective or any of the constraints are non-convex. Such a problem may have multiple feasible regions and multiple locally optimal points within each region. It can take time exponential in the number of variables and constraints to determine that a non-convex problem is infeasible, that the objective function is unbounded, or that an optimal solution is the “global optimum” across all feasible regions. Additionally, these types of strategies have shown to be capable of solving these types of relatively complex problems (Contreras-Zarazua et al., 2019). The following is the objective function to be considered in the optimization problem.

$$\mathrm{Min}\,(Q) = f(N_{tn}, N_{fn}, R_{rn}, F_{rn}, F_{ln}, A_{vn},)$$

where *Ntn* is the total number of column stages, *Nfn* is the feed stage in a column, Rrn is the reflux ratio, Frn is the distillate/bottoms flux, *Avn* is the amount of solvent. While several target functions can be associated with the performance of a distillation column, energy consumption is key to evaluating the performance of a separation operation of this nature. According to the U.S. Department of Energy, separation columns in operation in the U.S. consume about 40% of the total energy used to operate chemical plants (White, 2012). On the other hand, the thermal load can represent up to 80% of the total annual cost (Segovia-Hernández et al., 2015). In this sense, the impact of energy consumption on the conceptual design of a separation column is clear. Additionally, by reducing the total energy consumption of the process, a minimization of the generation of greenhouse gases is achieved, according to Gadalla et al. (2005). Under these conditions, the design of a CO_2 capture process is achieved with a low environmental impact: to generate low CO_2 emissions by minimizing the use of energy in the reboiler and at the same time generate the capture of CO_2 from the external fuel burning. To solve the objective function, as well as the model associated with the equipment, a hybrid stochastic optimization algorithm, Differential Evolution with Tabu List (DETL), was used. The use of this type of methodology is due to the nature of the model to be solved, that is, the model is highly non-linear and potentially non-convex. Additionally, these types of strategies have shown to be capable of solving these types of relatively complex problems (Contreras-Zarazua et al., 2019; Srinivas and Rangaiah, 2007). The constraints were defined as a CO_2 and amine recovery of 95%, and purity of amine and CO_2 bigger than 99% wt, whereas the mass flow for the feed stream was set as 1000 kmol/h, at 148.85 °C. Table 5 shows detailed information about the decision variables considered and the ranges for the designs variables

Table 5 – Decision variables of the process.

Type of variable		Search range
Number of Stages	Discrete	5–100
Feed Stages	Discrete	4–99
Reflux Ratio	Continuous	0.1–75
Distillate Rate	Continuous	10–248 (kmol h^{-1})
Diameter	Continuous	0.9–5 (meters)
Solvent	Continuous	25,000–27,000 (kmol h^{-1})

3. Results

For the results analysis, it is important to remember that the characteristics of the flue gases depend on the type of combustion and fuel used within the power plant, particularly the volumetric flowrate and CO_2 content, which may affect the capture effectiveness during the CO_2 sequestration. In this work, the analysis of two different scenarios, plant simulation with or without CO_2 capture system by chemical absorption, was conducted. The type and flowrate of flue gas have a significant effect on the capture effectiveness, because of the high variation in CO_2 content. Energy production in power plants may vary depending on peaks of power demands and/or variations in electricity prices, or even due to changes in the fuel characteristics. Therefore, capture plants should be able to capture different CO_2 loads, depending on those changes. Two different operating policies for the power plant were considered, the first one for a specified flowrate of fuel to be burned and the second one for specified energy production in the turbine of the power plant. This allows us to evaluate variations in the type of fuel and energy production. Four different types of fuels were selected. To evaluate the effect of the type of fuel and the capture plant implementation on the environmental impact of the process, an LCA was developed through the commercial software SimaPro.

3.1. *Case study 1: Carbon capture scenarios, at constant fuel flow*

It has been stated that the type of fuel has not only an important role in the energy production of the power plant but in the composition of the flue gases. As reported by Nagy and Mizsey (2015), the composition of combustion gases varies depending on the fuel (Table 6). The flue gas obtained when mineral coal is burned presented the lower CO_2 content, while the larger concentrations of CO_2 were observed for flue gases coming

Table 6 – Flue gas composition, reported in molar fraction, from the combustion of the different fuels, Case 1.

	N_2	O_2	CO_2	H_2O
Biogas	0.767	0.168	0.029	0.035
Coal	0.786	0.189	0.024	0.002
Non associated gas	0.767	0.144	0.030	0.059
Associated gas	0.766	0.139	0.034	0.062

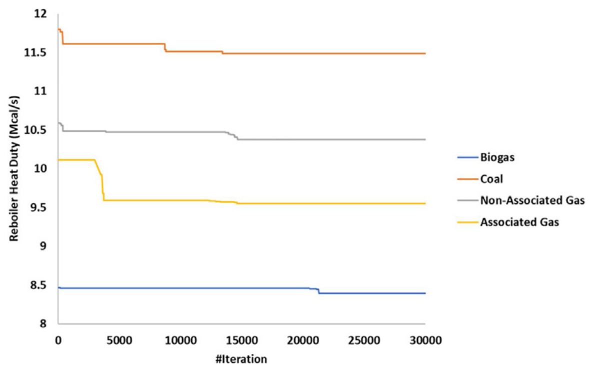

Fig. 3 – Optimization results for case study 1.

from burning natural gases. For all studied cases, the flowrate of combustion air was specified in the same value so that there is a larger excess for the coal system (this can be observed in the larger composition of N_2 and O_2 in the flue gas). Furthermore, CO_2 concentration also depends on water generation during combustion, which is larger during burning gases.

As expected, these variations on CO_2 concentration influence the capture plant effectiveness, energy, solvent requirements, and CO_2 recovery. Table 7 summarizes the energy production-consumption among each stage of the power plant and the energy consumption due to the implementation of the capture process. As expected, when implementing the capture plant, there is a significant reduction in the efficiency of energy production, due to the energy consumption in the column for the amine regeneration. Such reductions range from 19.47% to 65.27%, wherein the larger efficiency reductions are observed for working with mineral coal. This result can be explained in terms of lower energy production during electricity generation, in this case, 30% lower than that obtained by burning gases. Additionally, energy demand in the desorber column is also larger during the CO_2 capture; there is a direct relationship between CO_2 content and capture process efficiency.

Fig. 3 shows the results obtained once the optimization process was completed. As shown in the reboiler duties obtained as an endpoint, the design in charge of capturing CO_2 using biogas as fuel was the most promising in terms of energy requirements.

The optimization strategy allowed to observe some behaviors in the design variables and the process in general. There is a well-known relationship between the number of equilibrium stages and the reboiler duty. When minimizing the energy requirement, it is necessary to compensate for the separation process by considering larger columns. Considering the above, the established optimization limits take value. On the other hand, although the amount of solvent was considered as a degree of freedom, due to the minimization of the reboiler duty, it was possible to obtain schemes that used the smallest possible amount of amine as solvent. In this way, the tradeoff generated between the design variables and the restrictions of the problem, CO_2 capture, and recovery, was observed. The solution, in appearance, could lead to a trivial solution where it is convenient in the capture section, relatively large columns. However, the fact of modeling reactive stages generates an additional interaction between the energy requirements, the size of the equipment, and the possibility to adequately perform the chemical reaction. As an effect of this behavior, the scheme with the lowest energy consumption was the one with the greatest flexibility in terms of the design variables, beyond the obvious relationship between the variables.

Regarding impact assessment for the power plant working with the different fuels (Fig. 4a), the use of mineral coal and non-associated gas present the major impact in most categories, followed by associated gas and biogas. This could be explained because in these two cases the fuels are directly obtained from nature as raw materials, while the associated gas is obtained as a sub-product from oil wells and biogas is produced from residual biomass, such that all the impacts related to the ecosystems exploitation are reduced. After normalization and weighting to obtain a single score (Fig. 4c), it is observed that the use of coal generates the greatest potential impact. This is due to Climate Change has a high weight within the single score calculation and coal has the biggest impact in this category.

Fig. 4b shows the potential impact when the power plant is coupled to the capture process. It is noticed that in this case, the impact of coal is reduced in several categories, while for the gases the impact is redistributed.The efficiency and solvent flowrate have an important role in these results (Table 7, Case 1). Fig. 4d shows the single score results, where it is observed that implementing the CO_2 capture significantly reduces the environmental impact of the energy production for the biogas and coal systems, while for the natural gases this process does not represent a friendly environmental technology.

As shown in Table 7, when equivalent flows of all fuels are considered, CO_2 obtained during the energy production with biogas and mineral carbon almost duplicates the amount of CO_2 production for burning natural gas, such that the capture process represents a larger benefit for those systems.

It is important to highlight that natural gases present a lower environmental impact during energy production, as these systems generate a lower amount of CO_2 to produce a kW in the power plant than the mineral coal or biogas. For the implementation of the capture process, however, those systems present a similar requirement of solvent and energy to recover a kg of CO_2, compared to the coal system, and therefore seem to be the less effective. Furthermore, for all gases, the impact associated with the resources is increased for the CO_2 capture implementation, due to the solvent requirement and energy demand.

3.2. *Study case 2: Carbon capture scenarios, at specified energy production*

The second scenario here evaluated considers a specified energy production within the turbine of the power plant. In this case, the feed flowrate of each fuel was adjusted such that the energy production goal is reached. As in the first case, the composition of combustion gases varies depending on the fuel. From these results, we can see that flue gases with larger CO_2 content are obtained from biogas and coal combustion (Table 8). Although the CO_2 concentration increases in this second scenario, the CO_2 generation per MW produced in the

Table 7 – Case 1. Simulation of the Power plant (CP) + Capture process (CC), with a feed flowrate of Fuels equal to 1000 kmol/h.

Power plant (CP)

Fuel	Compressor Energy Consumption [MW]	Turbine Energy Production [MW]	Heat Exchanger Energy Recovery [MW]	CP Net Energy [MW]	CP CO_2 Generation [$kgCO_2/MW$]	CP Fuel Flowrate [kg/h]
Biogas	93.55	109.65	89.49	105.60	408.22	26,910
Coal	93.55	100.07	72.68	79.20	433.86	14,759
Non-Associated Gas	93.55	138.58	151.21	196.25	228.12	16,820
Associated Gas	93.55	145.26	165.93	217.65	230.81	18,737

Power plant + Capture process (CP + CC)

Fuel	Net Energy (CP + CC) [MW]	Energy Efficiency Reduction (CP + CC) [%]	Solvent Requirement [kg amine/kg CO_2rec]
Biogas	61.79	41.48	8.3
Coal	27.51	63.27	4.17
Non Associated Gas	151.87	22.61	4.65
Associated Gas	175.26	19.47	4.13

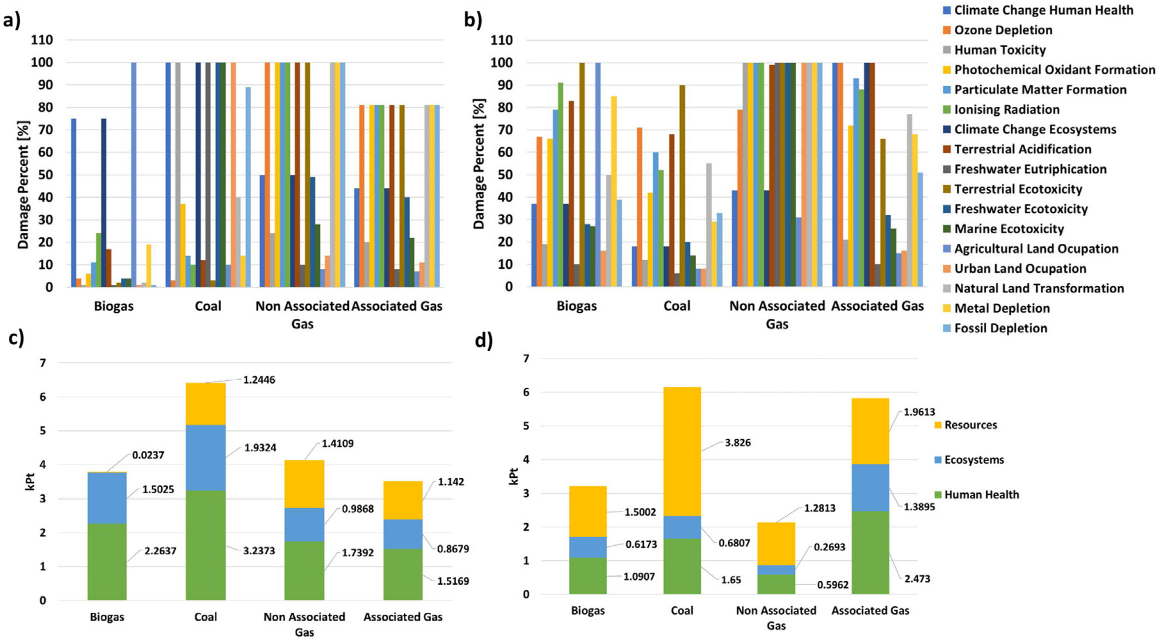

Fig. 4 – Life Cycle Impact Assessment results, Case 1. a) potential impact of power plant (CP) damage percentage by category, b) potential impact of power plant + capture process (CP + CC) damage percentage by category, c) Power plant single score (CP) in kEcopoints [kPt], d) Power plant + Capture process single score (CP + CC) in kEcopoints [kPt].

Table 8 – Flue gas composition, reported in molar fraction, from the combustion of the different fuels, Case 2.

	N_2	O_2	CO_2	H_2O
Biogas	0.749	0.135	0.052	0.064
Coal	0.781	0.162	0.053	0.004
Non associated gas	0.765	0.139	0.033	0.064
Associated gas	0.766	0.139	0.034	0.062

power plant for both fuels is reduced in comparison to the first scenario (case 1), because of an increase in the energy production (Table 9).

Table 9 presents a comparison between the net energy of the power plant and the net energy of the same process when the capture process is coupled. In this scenario, the study cases with the lowest reduction in the energy efficiency were the associated and the non-associated gas, with 19.50% and 19.60%, respectively, and the biogas was the one with the highest reduction since is the system with the larger energy requirement during the capture process.

Regarding the LCA, the fuel with the greatest impact in most of the categories is mineral coal, to mention some categories, a noticeable impact is observed in *Climate Change and Human Health, Human Toxicity, Terrestrial Acidification, Terrestrial Toxicity, and Eutrophication*, among others. After normalization and weighting to obtain a single score, Fig. 5b seems to show a different trend than that observed for case 1. However, it is important to realize that in both cases natural gases present a single score close to 3 (similar to that obtained in case 1). The real difference is in the Eco points obtained for biogas and mineral coal, which are significantly reduced because of the increase in energy production.

In this case, the single score (Figs. 5c and 5d) showed that implementing the capture process to the power plant working with biogas greatly reduces the environmental impact from 1.8494 kPt to 0.5684 kPt. This result can be attributed to the

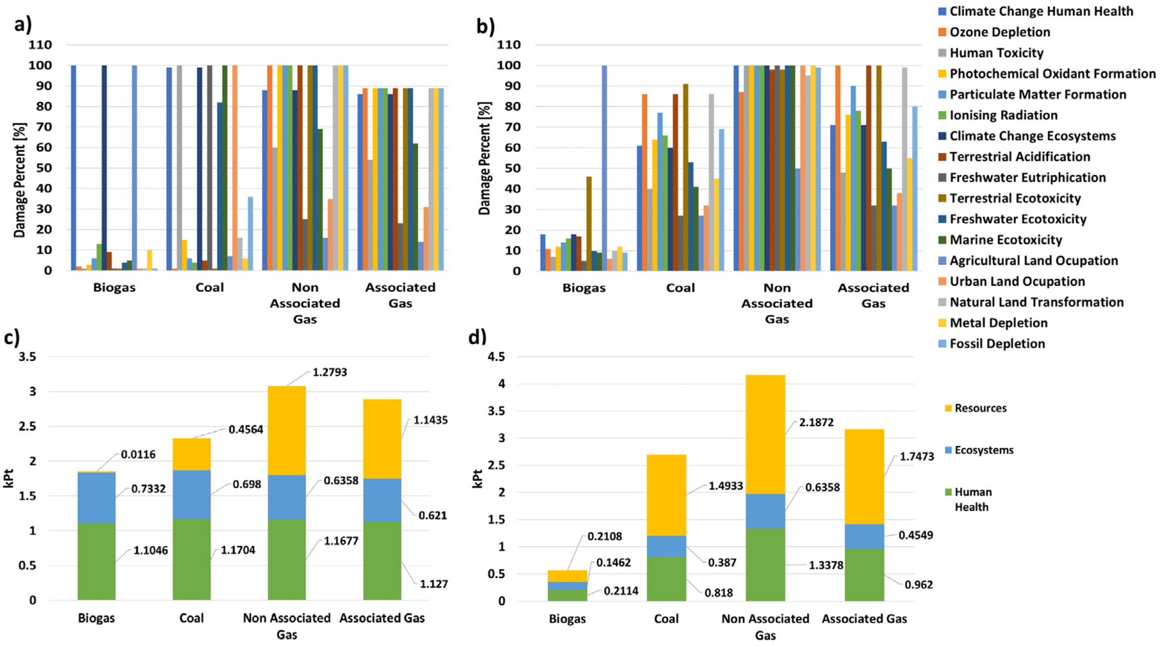

Fig. 5 – Life Cycle Impact Assessment results, Case 2. a) potential impact of power plant (CP) damage percentage by category, b) the potential impact of power plant + capture process (CP + CC) damage percentage by category, c) Power plant single score (CP) in kEcopoints [kPt], d) Power plant + Capture process single score (CP + CC) in kEcopoints [kPt].

Table 9 – Case 2. Simulation of the Power plant (CP) +Capture process (CC), with energy production in turbine equal to 145 MW.

Power plant (CP)

Fuel	Compressor Energy Consumption [MW]	Turbine Energy Production [MW]	Heat Exchanger Energy Recovery [MW]	CP Net Energy [MW]	CP CO_2 Generation [kgCO_2/MW]	CP Fuel Flowrate [kg/h]
Biogas	93.55	145	164.99	216.44	367.26	49,514
Coal	93.55	145	164.52	215.97	366.54	33,502
Non-Associated Gas	93.55	145	164.99	216.44	228.11	18,334
Associated Gas	93.55	145	165.93	217.38	231.09	18,737

Power plant + Capture process (CP + CC)

Fuel	Net Energy (CP + CC) [MW]	Energy Efficiency Reduction (CP + CC) [%]	Solvent Requirement [kg amine/kg CO_2rec]
Biogas	138.29	36.11	3.90
Coal	153.71	28.83	4.05
Non Associated Gas	174.02	19.60	4.15
Associated Gas	175.00	19.50	4.13

following aspects: i) the energy production was increased in the power plant so that the CO_2 generated per kW produced was diminished, iii) The CO_2 concentration in the flue gas was augmented in such a way that solvent requirement is reduced in the capture process.

On the other hand, the global impact of implementing this CO_2 sequestration technique to the process with the other three fuels seems to be only redistributing among the different categories and does not show a significant effect on the environmental impact among them when the single scores are evaluated.

Furthermore, for all fuels in both cases, is observed that even if the CO_2 capture implementation may reduce the environmental impact associated with human health and/or ecosystems, the impact associated with the exploitation of the resources is always increased due to the energy and solvent requirements within the capture process. As noted, there is a clear incentive for developing new capture technologies, or optimizing the operating conditions of this post-combustion alternative to enhance its effectiveness.

On the other hand, Table 10 shows the mass balances for each stream related to the capture process (marked in red square according to Fig. 1) in case study 1 and 2, as well Table 11 shows the basic design parameters for the CO_2 capture zone.

Regarding the process variables that have a preponderant role in the performance of the capture alternatives presented in this work. Throughout the optimization process, it was clear the great impact generated by some design variables. Particularly, the desorber reflux ratio has a direct relationship with the energy requirements of the system. That is, the higher the reflux ratio, the higher the energy expenditure. Similarly, the amount of solvent used directly affects energy consumption. It can be observed that, once the MEA acts to absorb the CO_2, it must be recovered in the second column. This means that the greater the amount of MEA, the greater the amount of material to be heated in the second column, and the

Table 10 – Mass balance for the best design in each case.

Case study 1 with non-associated gas

Stream	Flue gases	Clean Gases	Makeup Amine Solution	Lean Amine	CO_2 Captured
Total Feed Flow [kmol/h]	33995	34166	1267	26079	1096
Water [kmol/h]	2176	3438	1264	22779	2.4
CO_2 [kmol/h]	1122	29	0	28.65	1093
N_2 [kmol/h]	26006	26006	0	0	Trace
O_2 [kmol/h]	4691	4691	0	0	Trace
MEA [kmol/h]	0	2.3	2.3	3272	Trace
Temperature [K]	303.15	319.36	313.15	313.15	305.18
Reboiler Duty [GJ/h]	143.99				
CO_2 Recovery [tonCO_2/h]	46.07				
Thermal needs [GJ/tonCO_2]	3.12				
L/G ratio [kmol h^{-1}/kmol h^{-1}]	0.8				

Case study 2 with biogas

Stream	Flue gases	Clean Gases	Makeup Amine Solution	Lean Amine	CO_2 Captured
Total Feed Flow [kmol/h]	34734.49	34226.45	1473.3	14214.09	1980.354
Water [kmol/h]	2223.007	3301.818	1307.435	5417.491	228.9609
CO_2 [kmol/h]	1806.193	54.80071	0	Trace	1751.363
N_2 [kmol/h]	26016.13	26016.11	0	0	Trace
O_2 [kmol/h]	4689.156	4689.149	0	0	Trace
MEA [kmol/h]	0	164.5688	164.785	8796.60	0
Temperature [K]	303.15	339.22	313.15	313.15	336.34
Reboiler Duty [GJ/h]	280.10				
CO_2 Recovery [tonCO_2/h]	77.06				
Thermal needs [GJ/tonCO_2]	3.6				
L/G ratio [kmol h^{-1}/kmol h^{-1}]	0.83				

Table 11 – Design parameters for the best CO_2 capture alternatives of both study cases.

	Biogas		Non-Associated Gas		Associated Gas		Coal	
	Absorber	Desorber	Absorber	Desorber	Absorber	Desorber	Absorber	Desorber
Number of Theoretical Stages	20	39	20	31	19	17	48	25
Reflux ratio	-----	0.81	-----	0.82	-----	0.79	-----	0.91
Feed stage	20	3	20	4	19	3	48	3
Section packed height (m)	11.19	13.5	12	13.5	8	12	11.55	3.45
Operative pressure (kPa)	88	202.65	88	202.65	88	202.65	88	202.65
Distillate flowrate (kmol h^{-1})	----	936.38	----	1095.81	----	1050.13	----	797.19
Condenser duty (kW)	----	10,668	----	13,103	----	11356.92	----	14424.35
Reboiler duty (kW)	-----	35157.7	-----	41,876	----	39101.72	----	48074.36
Thermal needs [GJ/tonCO_2]	----	3.23	----	3.12	----	3.02	—	2.95

energy requirement increases. According with Lu et al. (2021) and Nagy and Mizsey (2015) the thermal needs are within the reported ranges. In this sense, the optimization work allowed us to obtain the appropriate combination of design variables to generate a design with the lowest possible energy requirement.

4. Conclusions

In this work, a Life Cycle Analysis was conducted to evaluate the environmental impact of different scenarios during the generation of electricity, as well as the energy and environmental implications of coupling a CO_2 capture process. For a specified feed flowrate of fuel to a power plant, the fuel with the lowest environmental impact is the associated gas with a single score of 3.52 kEcopoints. When the CO_2 capture process is coupled to the power plant, the fuel with the lowest overall impact is the non-associated gas with 2.14 kEcopoints. For the scenario of specified energy demand, the fuel with the lowest environmental impact is the biogas, with a single score of 1.85 kEcopoints, and such impact is further reduced up to 0.57 kEcopoints, when the CO_2 capture plant is implemented. According to the results obtained, for the scenario with a constant flow, the best alternative for capture is the one that considered biogas as fuel. On the other hand, for the scenario with constant energy demand, non-associated gas was the most promising alternative. Both alternatives with an energy consumption per ton of CO_2 captured of 3.12 and 3.23 GJ/tCO_2. Further discussions should focus on exploring the benefits and weaknesses of CO_2 capture during real operation, considering combined technologies able to use different fuels, as well as variable energy demands. Moreover, to enhance the energy efficiency of the power plant and CO_2 capture effectiveness, a multiobjective optimization problem needs to be addressed, for each process variable and design parameters in both processes.

Declaration of interests

Data availability

Data will be made available on request.

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Appendix A

The Differential Evolution with Tabu List (DETL) method has its basic foundations in the theory of natural selection. The method was not originally proposed as a hybrid method; Differential evolution (DE) was initially proposed by Storn (1997) to solve single-objective problems, and later it was adapted by Madavan and Field (2002) to solve multi-objective problems. There are five essential steps in differential evolution: initialization, mutation, crossover, evaluation, and selection, all expressed by the equations described below.

In the initialization step, the algorithm search in a D-dimensional space $\Re^D$ starts randomly as:

$$X_{\vec{i},G} = [X_{1,i,G}, X_{2,i,G}, X_{3,i,G}, \ldots, X_{D,i,G}] \tag{A1}$$

The mutation process begins with a parent vector, and by using a trial vector, a donor and target vector can be obtained in a process described as:

$$V_{\vec{i},G} = X_{\vec{r^i_{1,G}}} + F.(X_{\vec{r^i_{2,G}}} - X_{\vec{r^i_{3,G}}}) \tag{A2}$$

In the crossover step, the target vector exchanges its components with the donor vector, in such a way that a trial vector is obtained such as:

$$u_{j,i,G} = v_{j,i,G}\, for\, j = \langle n\rangle_D \quad \langle n+1\rangle_D, \ldots, \langle n+L-1\rangle_D \tag{A3}$$

$$x_{j,i,G}\, for\ all\ other\ j \in [1, D]$$

Finally, in the selection stage, it is determined whether or not the trial vector survives the next generation. This process is described as:

$$\begin{aligned} X_{\vec{i},G+1} &= U_{\vec{i},G} \quad if\ f(U_{\vec{i},G}) \leq f(X_{\vec{i},G}) \\ X_{\vec{i},G+1} &= X_{\vec{i},G} \quad if\ f(U_{\vec{i},G}) > f(X_{\vec{i},G}) \end{aligned} \tag{A4}$$

Where $f(\vec{X})$ is the objective function to be minimized/maximized.

On the other hand, the tabu concepts (tabu list and tabu search) were proposed by Glover (1989). The Tabu list avoids revisiting the search space by keeping a record of visited points. The Tabu list is updated with each new generation of trial vectors. This tabu check is carried out in the generation step to the trial vector, and the new trial individual is generated repeatedly until it is not near to any individual in the Tabu list. Both methods together increase computational efficiency; the first version of this hybrid method was reported by Sharma and Rangaiah (2013).

In the practical implementation, the hybrid method is written in visual basic within Microsoft Excel using DDE (Dynamic Data Exchange) the numerical method exchanges input vectors (column stages, reflux ratio, etc.) and output (flows, reboiler duty, etc.) with the process model (modeled in Aspen Plus). The stochastic method analyzes the values of the objective functions and proposes new values for the input vectors. The parameters used for the optimization process were: obtained from the literature and tuning process via preliminary calculations (Srinivas and Rangaiah, 2007).

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