

## Sustainability assessment in the CO<sub>2</sub> capture process: Multi-objective optimization

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### ABSTRACT

Electricity production from the burning of fossil fuels, is one of the main sources of Carbon Dioxide (CO<sub>2</sub>) emissions. Therefore, it is necessary to find alternatives to mitigate CO<sub>2</sub> emissions. Having as alternative the implementation of CO<sub>2</sub> Capture and Storage plants (CCS). Highlighting post-combustion technologies with chemical absorption and mono-ethanolamine (MEA) as solvent. Despite its high efficiency to capture CO<sub>2</sub>, MEA is considered toxic, so its implementation entails an environmental impact. Moreover, no studies report a complete design considering environmental impact and the process economies as a sustainable indicator.

This work presents the optimization of the design of a CO<sub>2</sub> capture plant coupled to a power plant considering a stochastic algorithm having as objective function the minimization of the Ecoindicator 99, Condition Number ( $\gamma'$ ) and maximize the return on investment (ROI). To evaluate the environmental implications, control properties and economic of the process, respectively. The analysis considered the most used fuels in the power plant: coal, natural gas, and associated gas. Including the analysis of biogas as a green fuel to produce energy. All the cases were standardized to recover 99% of the CO<sub>2</sub> produced. The results indicate that the design with the best overall performance is when natural gas is burned. Having a lower environmental impact with 22549.43 kEcopoints and a ROI of 73.24%.

### 1. Introduction

Carbon dioxide (CO<sub>2</sub>) is one of the most polluting gases at global level. CO<sub>2</sub> plays a major role in the greenhouse effect contributing to global climate change. This global overheating has drastic consequences for the entire planet. Likewise, CO<sub>2</sub> concentration continues rising because the rate of CO<sub>2</sub> emission in the atmosphere is bigger than the rate of its absorption.

CO<sub>2</sub> emissions are primarily produced by the burning of fossil fuel from industrial activity, transport and electricity production. It is reported that 70% of CO<sub>2</sub> emissions are related to electricity production. According to the International Energy Agency, about 33.4 Gt of CO<sub>2</sub> produced in 2019 came from electricity production from the burning of fossil fuels [1]. Moreover, the COVID-19 pandemic has had a significant impact on how energy is produced, supplied, and consumed worldwide. Due to the pandemic situation, there was an increment of renewable

energy utilization, resulting on the reduction of fossil fuel consumption. Therefore, the global CO<sub>2</sub> emissions related to the electricity sector dropped by almost 5.8% [2,3]. While 2020 marked the biggest decline in global CO<sub>2</sub> emissions in history, in 2022 there is evidence of a rapid rebound in energy demand and therefore the rising of CO<sub>2</sub> emissions. In this sense, almost the 60% of the total electricity production worldwide is generated from the burning of fossil fuels. Having coal, natural gases and oil as the three major fossil sources to obtain energy in power generation plants [4].

Due to the seriousness of the problem, solutions have been sought promoting concrete actions aimed at curbing climate change. According to the sustainability objectives of the United Nations, it is necessary to develop new processes or improve the existing one in order to be sustainable and contribute to the improvement of environmental impact derived from CO<sub>2</sub> emissions. Nowadays, the implementation of CO<sub>2</sub> Carbon Capture and Storage (CCS) technologies has been exhibited as a

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promising option to reduce CO<sub>2</sub> emissions, reduce global warming, and avoid climate change. CCS methods are technologies used to capture carbon dioxide, emitted mainly by burning fossil fuels in power plants, preventing CO<sub>2</sub> from being released into the atmosphere. There are three ways to classify CO<sub>2</sub> capture technologies; Oxy-fuel combustion, Pre-Combustion Capture and Post-Combustion Capture [5]. Within these three categories there are examples of technologies that have been used to capture CO<sub>2</sub>. Post-combustion capture can be divided into three categories: biological methods, physical methods, and chemical methods. One example of biological method is the case of CO<sub>2</sub> fixation through the photosynthesis of plants, algae, and photosynthetic bacteria. This method has low CO<sub>2</sub> absorption capacity to cover the amounts of CO<sub>2</sub> produced worldwide. Some examples of physical methods are the CO<sub>2</sub> capture by physical absorption, cryogenic condensation, and membrane separation methods with an organic solution without chemical reaction occurring during the capture process [6–8]. The physical methods, in comparison with the biological methods, present better efficiency in CO<sub>2</sub> absorption. However, they are more expensive due to the absorbents used. On the other hand, chemical methods absorb CO<sub>2</sub> by reacting with chemical absorbents. Compared to the other methods mentioned, the chemical absorption method turns out to be the best option for the separation of CO<sub>2</sub>, due to its high efficiency and low cost [9,10].

Typical chemical absorption process is used for separating CO<sub>2</sub> from exhaust gases. The process consists of an absorber and a regenerator column where the solvent is regenerated. As a first step in the absorption column, the exhaust gases (CO<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub>) are in contact with a liquid solvent, typically an aqueous amine solution. The amine selectively absorbs the CO<sub>2</sub>, capturing more than 85% of the CO<sub>2</sub>, enabling nitrogen and oxygen to be released into the atmosphere [11]. As a second step, the amine is regenerated, and the CO<sub>2</sub> stripped out of the liquid. The CO<sub>2</sub> is obtained as pure gas at the column top, while the lean amine is recycled to the absorption column.

The most widely used solvent for CO<sub>2</sub> absorption is aqueous monoethanolamine (MEA) solution at 30% by weight [12]. Monoethanolamine (MEA) is the most widely used and studied solvent due to its great CO<sub>2</sub> capture capacity. Since its thermophysical properties are well studied, it is possible to simulate the process with high precision, which has made MEA a comparison basis to evaluate the performance of other more sophisticated solvents. Despite its high efficiency, MEA is considered highly toxic, so its implementation entails a high environmental impact, plus the considerable energy required for its regeneration. Those drawbacks open the opportunity to study new green solvents, which can be capable of replacing the MEA in the CO<sub>2</sub> capture process.

Due to the necessity of developing green processes, new research points to different solvents as potential alternatives that can be used for CO<sub>2</sub> capture. Allowing the study of other solvents, such as Deep Eutectic Solvents (DES), considered green solvents due to the nature of its components [13]. Likewise, using potassium taurate as a solvent presents the advantage of lower corrosion and good stability compared to MEA [14]. Another example is the potential use of piperazine as a solvent, through a thermodynamic analysis it has been proved the CO<sub>2</sub> absorption efficiency [15,16]. Despite the apparent advantages that these solvents have compared to MEA, as long as they are not economically competitive or there are no models at the industrial level, amine-based chemical absorption will still consider the most industrially developed technology for this kind of process.

To improve and convert the traditional CO<sub>2</sub> capture process with MEA into a sustainable process, it is necessary to evaluate the process according to sustainability metrics. Jiménez-González and Constable propose that a good measure to evaluate the sustainability of a process is to analyze the economic, environmental and controllability indicators, which is directly proportional to the safety of the process, as sustainability metrics [17].

In order to minimize and environmental impact due to MEA used as

solvent during CO<sub>2</sub> capture, this work aims to present a novel proposal for the simulation of a CO<sub>2</sub> capture plant coupled to a power plant, where the optimal design and operation conditions are presented, from a sustainable point of view, turning the traditional capture process with MEA, into a sustainable process following the green chemistry principles.

Unlike other works reported in the literature where a mono-objective optimization of the energy requirements where is presented as a preliminary analysis of the CO<sub>2</sub> capture plant [18]. In this work it is presented a multi-objective optimization considering the stochastic algorithm having as objective function the minimization of the environmental implications of capture plants using MEA as solvent (Ecoindicator 99), the minimization of Condition Number (CN) as an indicator of the control properties of the system, as well maximize the return on investment (ROI) as an economic indicator. Another contribution of this work is to consider the power plant and the capture plant within the optimization. Even when the power plant is presented as a simplified model, it is important to remark the complexity of the thermodynamics involved in the model. And therefore, the high non-linearity for the optimization problem. The analysis considered the most used fuels in the power plant: coal, natural gas, and associated gas. As well it is included an analysis of biogas as green fuel to produce energy. All the cases were standardized to recover 99% of the CO<sub>2</sub> produced during the combustion. This works presents

## 2. Sustainability indicators

The indices proposed for developing green chemistry in this work are mainly related to the economy with the Return on Investment (ROI), the environmental impact measured through the Eco-Indicator 99 (EI99), and the process controllability with the Condition Number ( $\gamma^*$ ).

There are works in the literature where it has been shown how the integration of different metrics, such as the indices proposed in this work, can improve the sustainability of the process due to the inherent interconnection between different aspects such as: environmental impact, safety, profitability, energy efficiency problems, among others [19]. According to Jiménez-González and Constable [17], these axes are needed to evaluate green chemistry of a process.

In this way, considering different metrics such as environmental impact, controllability and economic issues provides a broad perspective that can help in the decision-making process where multiple decision variables are commonly evaluated simultaneously that affect the operability of the process, the useful life of the project and the economics of the process [19]. Finally, the indices considered in this work are described below.

### 2.1. Economy of the process: return on investment (ROI)

The Return On Investment (ROI) is a financial indicator that measures the investment profitability; that is, the relationship between the profits or profits obtained or expected to be obtained, and the investment. The ROI calculation is based on the annual revenue, the annual production costs and the total capital investment, as well it is stated as a percentage per year (see Eq. (1)) [20–22].

$$ROI = \frac{P}{I} \quad (1)$$

A process is considered profitable when the ROI is bigger than the bank's annual rate for an investment of an annual term. To establish an economic activity, an investment (I) is needed, in exchange for this investment income is obtained in the form of sales, which must offer a surplus over the operating costs of the process to have commercialization potential. To calculate the total investment of the process (I), the investment must be broken down into fixed investment ( $I_f$ ) and a working capital ( $I_w$ ), as shown in Eq. (2):

$$I = I_f + I_w \quad (2)$$

According to Gutiérrez [20] the  $I_f$  represents 80% of the total investment and represents the expenses per equipment. Likewise, the  $I_w$  represents the cost per raw material, acquiring a value of 20% of the total investment. For the calculation of  $I_f$ , 75% is assumed at the cost of principal equipments ( $I_E$ ) and 25% at the cost of auxiliary equipment ( $I_A$ ) according to Eq. (3).

$$I_f = I_E + I_A \quad (3)$$

To calculate the cost of principal equipment, the Guthrie Method was used [23]. As the purpose of the work is to implement capture systems in existing power plants, for the calculation of investment costs the absorber, desorber and auxiliary equipment are included in the Capital Cost. Here, carbon steel is considered a construction material. All the parameters for the equipment and the utility costs were taken from Turton et al. [24].

To calculate the net profit (P), it is necessary to address some previous concepts. One of them is the cost of operation (C), this concept associates the costs related to investment, variable costs and labor costs. They can be evaluated per unit of time (\$/year) or per unit of production (\$/kg) and are calculated as shown in Eq. (4) [20]:

$$C = aI + \sum bMP + \sum cE + dMO - \sum pSP \quad (4)$$

where C represents the operating cost of the process,  $aI$  is a factor that considers annual expenses such as royalties, maintenance, etc.  $bMP$  represents the unit cost of each raw material MP,  $cE$  represents the cost of each service E,  $dMO$  represents labor costs and  $pSP$  represents the unit cost of each by-product SP. It is important to point out that  $aI + dMO$  represent approximately 5% of the Investment (I). As well, another important concept is gross profit (R), which is defined as the difference between annual sales (S) and the annual operating cost [20] (see Eq. (5)).

$$R = S - C \quad (5)$$

The net profit (P) is calculated by subtracting the equipment depreciation the payment of taxes from the gross profit as shown in Eq. (6) [20]:

$$P = R - eI - t(R - dI) \quad (6)$$

where  $eI$  represents a constant depreciation factor,  $t$  represents a tax rate, and  $dI$  represents a tax depreciation.

## 2.2. Environmental impact measured: eco-indicator 99 (EI99)

The Eco-Indicator 99 (EI99) is a methodology proposed by Goedkoop and Spriensma [25] as a quantitative life cycle analysis. This methodology accounts for the origin of raw material in processing and degradation. It is based on standard ecological indicators, which are numbers that express the total environmental burden of a product or a process. The higher the value of the indicator, the greater the environmental impact. This method is based on the evaluation of three categories:

The first category is human health; this set represents the span of an illness and years lost due to premature death because of environmental causes. The evaluated points in this category are: carcinogenic effects, climate change, destruction of the ozone layer, radiation and respiratory effects. The second category is the quality of the ecosystem, which shows the effects on different species. The effects it evaluates are: ecotoxicity, acidification, and eutrophication due to land use. The third category is the depletion of resources, which refers to the surplus energy needed to extract mineral resources and fossil fuels. This part assesses fossil fuels and mineral extraction. Mathematically, EI99 can be expressed as shown in Eq. (7):

$$EI99 = \sum_i \omega \cdot C_i \cdot \alpha \quad (7)$$

where  $\omega$  represents the weight factor for the damage,  $C_i$  represents the impact value for category  $i$ , and  $\alpha$  represents the amount of what is being evaluated. The unit used for EI99 is the eco-point, where 1 eco-point is representative of one thousandth of the annual environmental burden of an average European inhabitant.

## 2.3. Process controllability: condition number ( $\gamma^*$ )

The singular value decomposition (SVD) is a mathematical method used to compute the pseudoinverse, matrix approximation, and determining the rank, range, and null space of a matrix. The SVD is also extremely useful in all areas of science, engineering, and statistics, such as signal processing, least squares fitting of data, and process control [26].

For example:

- in signal processing, SVD and pseudoinverse have been efficiently applicable in analyzing modifying, and synthesizing signals and sounds.
- in image processing, SVD is used to process images with algorithms.
- SVD it is quite helpful in face recognition, widely known as model analysis, where non-scaled mode shapes can be determined with non-scaled mode shapes.
- SVD is used in numerical weather prediction. Is helpful where mathematical modes of the atmosphere are used weather prediction based on present weather condition.

As SVD helps in the perfect representation of any matrix and it is quite easy to eliminate data that is not that important in a matrix to produce low-dimensional approximation. About process control, SVD is used in the multivariable control theory to measure control properties of a dynamic system as a tool to quantify multivariable directionality as a function of frequency. The magnitude of singular values is associated with the system gains as the direction of the inputs are varied. This might relate to the "force" the inputs require to move the system in a certain direction. On the one hand, the minimum singular value ( $\sigma_*$ ) is associated with the direction where the system has more difficulties moving to. On the other hand, the magnitude of the maximum singular value ( $\sigma^*$ ) indicates the easiest direction the system will move to [27].

The degree to which ill-conditioning prevents a matrix from being inverted accurately depends on the ratio of its largest to smallest singular value, a quantity known as the Condition Number ( $\gamma^*$ ). The S matrix obtained from SVD is shown in Eq. (8).

$$S = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix} \quad (8)$$

From both aforementioned values, the  $\gamma^*$  can be obtained, and it is defined as the quotient between the maximum singular value and the minimum singular value as shown in Eq. (9).

$$\gamma^* = \frac{\sigma^*}{\sigma_*} \quad (9)$$

The Condition Number quantifies the sensitivity of the system to inaccuracies in process parameters and mode errors. Systems with small Condition Number present better control properties. Therefore, it is necessary to identify systems with high values of minimum singular value ( $\sigma_*$ ) and low values of the Condition Number ( $\gamma^*$ ). It is expected that these systems will have the best dynamic behavior. It is necessary to reiterate that the association of high Condition Number is due to ill-conditioning with poor control properties.

Although the Condition Number is reported numerically, its interpretation is qualitative. It is not possible to know how good the control properties of a design are by the simple numerical value obtained. Its representation makes sense when compared with other designs. The design with the lowest value of condition number, compared to all comparative designs, is the one that presents the best control properties. Because of its qualitative representation, it is not possible to define a value from which a design has good control properties, therefore in an optimization problem should be considered as an index and not as a constraint.

For the control analysis in the case of CO<sub>2</sub> capture, each purification alternative provides a relative gain matrix in its nominal state. To obtain this matrix, the schemes are subjected to a disturbance in a manipulable variable (reflux ratio, reboiler duty, etc.) The magnitude of the disturbance is small enough (0.5%) that a first-order behavior can be assumed according to many previous works [28,29]. To avoid the SVD dependence of the system unit used (variables limited between 0 and 1, and high values for reflux ratio and reboiler heat duties) the approach of the proposal used in here is to limit the variables described. Since the maximum opening of the control valves can be twice the nominal value, the valves are theoretically open by 50%. In this way, to generate the relative gain matrix, a step change must be applied in the manipulated variable, and subsequently, this change must be divided by two. With this consideration, you get the same range of variation when opening and closing the control valves. The consequence of this consideration is to relate both, the amount and magnitude of change in a range of 0–100%. Moreover, with this form of scaling, and with the term 1/2P in Eq. (10), the manipulated variables are simultaneously dimensionless standardized. For example, a relative gain matrix for the purification of three components could be stated as:

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} = \begin{bmatrix} \frac{x_{C1}^{V1} - x_{C1}^{SP}}{\frac{1}{2}P} & \frac{x_{C1}^{V2} - x_{C1}^{SP}}{\frac{1}{2}P} & \frac{x_{C1}^{V3} - x_{C1}^{SP}}{\frac{1}{2}P} \\ \frac{x_{C2}^{V1} - x_{C2}^{SP}}{\frac{1}{2}P} & \frac{x_{C2}^{V2} - x_{C2}^{SP}}{\frac{1}{2}P} & \frac{x_{C2}^{V3} - x_{C2}^{SP}}{\frac{1}{2}P} \\ \frac{x_{C3}^{V1} - x_{C3}^{SP}}{\frac{1}{2}P} & \frac{x_{C3}^{V2} - x_{C3}^{SP}}{\frac{1}{2}P} & \frac{x_{C3}^{V3} - x_{C3}^{SP}}{\frac{1}{2}P} \end{bmatrix} \quad (10)$$

where all elements  $K_{ij}$ , are the relative gain matrix. The elements of the first row on the right side correspond to the differences among the mass purity of component A in the nominal state  $x_A^{SP}$ , and the mass purities after disturbance  $p.x_A^{V1}$  is the mass purity of a chemical compound after a disturbance in manipulated variable 1,  $x_A^{V2}$  is the mass purity of a chemical compound after a disturbance in manipulated variable 2,  $x_A^{V3}$  is the mass purity of a chemical compound after a disturbance in manipulated variable 3. In this work, the relative gain matrix was built as N x N, according to the N output streams of the separation scheme.

The SVD technique requires transfer function matrices, which are generated by implementing step changes in the manipulated variables of the design of the configuration and registering the responses of products. For process presented in this work, controlled variables were considered the purity of the products. Similarly, manipulated variables were defined, for each equipment. After the designs were generated, open-loop simulations were obtained in Aspen plus in order to obtain the transfer function matrix according to the methodology presented by Vazquez-Castillo et al. [30]. The calculation of the condition number has been carried out through the singular value decomposition of the relative gain matrix. Lower values of the condition number of a design are preferable over upper values so that the process may assimilate the perturbations without system destabilization [31].

### 3. Study case

The study case presented in this work evaluates the scenario of a power plant coupled to a post-combustion CO<sub>2</sub> capture process. For all cases, it is considered a fuel feed flow of 1000 kmol/h, considering the 3 most used fuels for electricity production: coal, natural gas and associated gas. As well, it is considered biogas as a green option biofuel. It is important to highlight, that the associated gas refers to the natural gas found in association with oil within the reservoir. In Table 1 it is shown the composition of each fuel in mass fraction.

The process can be explained in two step process, first the power plant and second the CO<sub>2</sub> capture process, both were simulated in the Aspen Plus V8.8® process simulator as is shown in Fig. 1. For the power plant, the design of the chemical process system for operating a combustion turbine is not trivial. The mechanical design of combustion turbines is a very complex fluid mechanics problem that includes issues of heat transfer, ignition, flame speed, flame stability, stress analysis, and materials of construction. As well, the design of the chemical process system for operating a combustion turbine is also not a trivial exercise. The chemical engineering design issues in air-fired systems involve finding the amount of air to be fed and the optimum combustor pressure because of the trade-off between compressor work and turbine power. Some literature details the complex issues associated with gas turbine and energy systems simulation [35–37]. If the goal of this work were to represent just the power generation plant, then a combined cycle for the power generation plant would be adopted to represent a realistic situation for the case of gases fuels. Moreover, in the case of coal as fuel, several technologies, such as integrated gasification combined cycle, pressurized fluidized bed combustor and pulverized coal injection, have been proved for the clean utilizations of coal due to the use of combined cycles [38,39].

The representation of this kind of models for the power generation plant, would considerably increase the complexity and robustness of the optimization problem. Therefore, to represent the power generation coupled to the capture process, considering the thermodynamic behavior included during the combustion as well as in the capture, it is necessary to use a simplified model that represents the combustion behavior, avoiding mathematical robustness from a more complex model. Therefore, Luyben [32] proposes that it is possible to represent the combustion process with a simplify power plant model. Which consists of a conventional combustion turbine system and a single-stage air compressor, was considered for energy production from burning fuels [32]. In this type of system, a fuel and an oxygen source (air) are combined to produce a gas stream of high volume, high temperature and pressure.

For the case of gaseous fuels, the scheme of Fig. 1 was used. In the case of coal, because it is a solid fuel, the combustion process should be represented as a Rankine-cycle. So, in order to use the proposed scheme, the flue gases at the exit of the combustion chamber were considered as the beginning of the process.

There is an important stoichiometric relationship in the proportions of fuel and air supplied to the process, which can be analyzed on a molar basis according to the combustion reaction with methane, which is the simplest of hydrocarbons and constitutes 70–90% of natural gases [40]. Methane reacts with oxygen in the air according to Eq. (11).

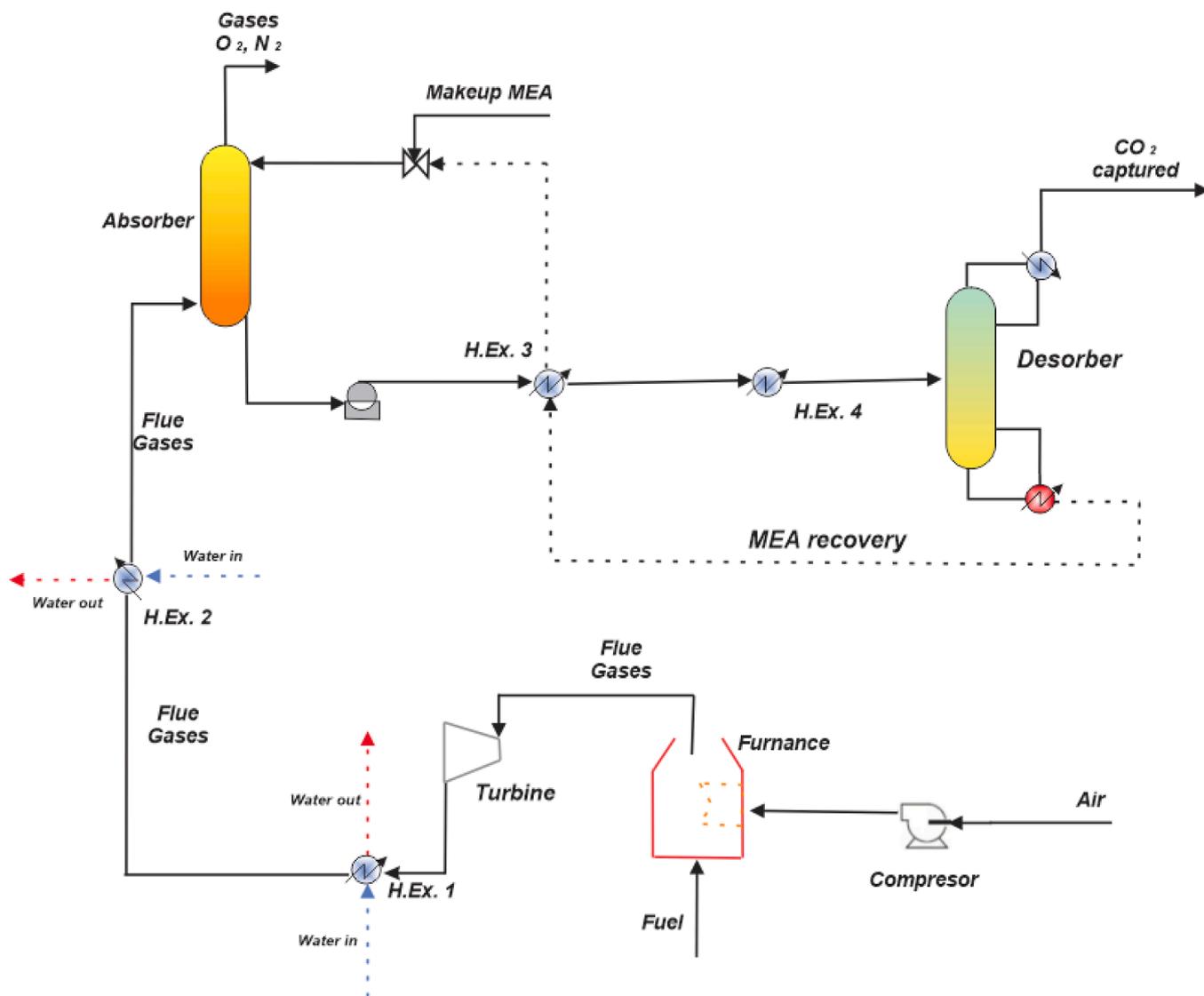


For every mole of methane, 2 moles of oxygen are required. Now, the composition of oxygen in air is 21 mol%, so there are 3.762 moles of nitrogen for every mole of oxygen. If only the amount of oxygen required stoichiometrically were fed into the process, a fuel feed of 1000 kmol/h would require 2000 kmol/h, representing an airflow of 9523 kmol/h. As reported in Luyben [32], an excess of air of at least 5 mol% of oxygen, and a maximum of 30:1 air to fuel ratio is required to ensure complete combustion.

Once the fuel and process feed air ratios are established, they are

**Table 1**  
Fuel composition in mass and mole fraction [32,33].

		CH <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>8</sub>	i-C <sub>4</sub> H <sub>10</sub>	N <sub>2</sub>	CO <sub>2</sub>
Natural Gas	Mass	0.96	0.018	0.004	0.001	0.007	0.0095
	Mole	0.98	0.009	0.001	0.0004	0.004	0.003
Associated Gas	Mass	0.872	0.045	0.044	0.012	0.027	-
	Mole	0.93	0.026	0.017	0.01	0.017	-
Biogas	Mass	0.6	-	-	-	0.02	0.38
	Mole	0.8	-	-	-	0.015	0.185
Coal		C	H	O	N	S	
	Mass	0.782	0.052	0.136	0.013	0.017	
	Mole	0.51	0.41	0.066	0.007	0.004	



**Fig. 1.** Scheme of a power plant coupled to a post-combustion CO<sub>2</sub> capture process using MEA 30wt% as solvent.

combined in a combustion reactor. For reactor modeling, a combustion chamber is considered an RGibbs type reactor operating adiabatically, likewise to model the thermodynamic properties involved in the combustion processes, the Peng-Robinson thermodynamic model is used. Peng-Robinson equation of state has been successfully applied for predicting dew points, liquid dropouts and thermodynamic properties of natural gases and other hydrocarbons [41]. The combustion was modeled based on the minimization of the Gibbs free energy using a RGibbs reactor module from Aspen Plus. The generated combustion reaction can reach pressures between 4.5 and 9 atmospheres [42] and

temperatures from 800°C till 1400°C depending on the burning fuel [42–44]. The flue gases, obtained at high pressure and high temperature, are fed to the turbine. Turbine power is generated as gases flow from the high-pressure inlet to the low-pressure outlet, and this power is used to drive electrical generators. Therefore, the bigger this pressure difference, the greater the power generated in the turbine. The inlet pressure is the limiting design parameter of the combustion turbine, that is, the conditions of the combustion reactor govern the limitations of the inlet pressure to the turbine. The air-fuel ratio is very important to complete combustion during the combustion process. For this stage, the

main design aspects are related to finding the amount of air to be fed and the optimum combustor pressure because of the trade-off between compressor work and turbine power [32]. This factor directly influences the capture, as it is stated that the capture efficiency depends on the composition of flue gases. To ensure high capture efficiency, flue gases must be high in CO<sub>2</sub>.

To model the CO<sub>2</sub> capture plant, the process consists of two columns, the absorption and desorption units. The flue gases enter at the bottom of the absorber column and the MEA at the top. Therefore, both streams interact, driving the CO<sub>2</sub> to the liquid stream in the column bottom. In the desorber column, it is important to regenerate the solvent and make the desorption of the CO<sub>2</sub>, which strongly depends on the reboiler duty. The capture process is complex because the chemical absorption includes several dissociation reactions as is shown from (Eqs. (12)–(16)). In Tables 2 and 3 it is shown the kinetic data for (Eqs. (12) and (13)), considering an Arrhenius form [12,45,46].

Additionally, Table 3 shows the kinetic and equilibrium constants corresponding to (Eqs. (14)–(16)).

For simulation purposes, design specification related to the CO<sub>2</sub> recovery is specified for the gas outlet, to avoid convergence problems related to dissociation reactions in liquid phase. For the regeneration column, the distillate flow and the reflux ratio are operating variables that must be manipulated to recover the greatest amount of CO<sub>2</sub> from the combustion gas stream and thus store it. In this way, CO<sub>2</sub> emissions into the atmosphere and the associated environmental impact are reduced. Another factor to consider during the capture is the type and amount of solvent required during the capture. The CO<sub>2</sub> capture plant is based on chemical absorption with an aqueous solution of Monoethanolamine (MEA) at 30% by weight as solvent was considered [12]. The Water/MEA ratio directly impacts the reaction environment. Water accelerates reactions by participating in the deprotonation of MEA-zwitterion and changing the solvation environment [47]. Moreover, by having bigger amount of MEA the viscosity would increase, affecting the capture efficiency as well [48].

In order to model the electrolyte behavior during the chemical absorption, it is important to consider all the kinetics and the binary interaction parameters. Likewise, the reactions involved in the CO<sub>2</sub> absorption/desorption process, include the formation of various ionic species involved in using MEA as a solvent. Therefore, using of the Electrolyte Non-Random Two Liquid (e-NRTL) thermodynamic model allows modeling of the thermodynamic parameters involved and provides satisfactory results for post-combustion capture processes [49]. For the capture process, some design aspects related to the process configuration and operational conditions should be considered to reduce the energy consumption and use of MEA. For the desorber column, in order to capture the maximum amount of CO<sub>2</sub> from the flue gas obtained from the power plant, it is necessary to manipulate the distillate flow and the reflux ratio. All the cases were standardized to a purity of 99 mol % CO<sub>2</sub> and at 99% recovery of the CO<sub>2</sub> produced during the combustion. This design specification directly affects the energy requirements of the process and, therefore directly influences environmental and cost indicators.

#### 4. Optimization

As stated above, it can be noted that the process for CO<sub>2</sub> capture and storage is an appropriate case to be optimized, considering as objective

**Table 2**  
Kinetics of reactions [34].

Reactions	Kinetic constant, k	Activation energy, E (kJ/mol)	Eq.
$OH^- + CO_2 \xrightleftharpoons[k_2/k_1]{} HCO_3^-$	k1	$1.33 \times 10^{17}$	55.38 (12)
	k2	$6.63 \times 10^{16}$	107.24
	k3	$3.02 \times 10^{14}$	41.2 (13)
$HO - C_2H_4 - NH_2 + CO_2 + H_2O \xrightleftharpoons[k_4]{k_3} HO - C_2H_4 - NH - COO^- + H_3O^+$	k4	$5.52 \times 10^{23}$	69.5

function the analysis of economic, environmental, and process control properties. This can be explained as the design parameters involved in the process directly impact the economic and environmental indexes, as well it is also necessary to consider the control properties of the system. It is important to highlight that to have a positive environmental impact in CO<sub>2</sub> capture processes, it is necessary to overcome the technical challenges involved in the CO<sub>2</sub> capture due to the use of aqueous amine solutions. In order to obtain a design with high CO<sub>2</sub> recovery, low environmental impact, good control properties and low operating cost, it is necessary to have a high concentration of CO<sub>2</sub> in the flue gases, which strongly depends on the type of fuel used in the power plant. As well, the election of the solvent used plays an important role in the CO<sub>2</sub> capture process.

Similarly, optimization in terms of control will result in a sustainable and green process by increasing CO<sub>2</sub> recovery providing economic competitiveness by maximizing process efficiency. Reliable indices are needed in process optimization to assess green chemistry. It is expected that the analysis framework developed in this paper can contribute to the use of indices that can assess more than one aspect of green chemistry, to be easily integrated into green process-based optimization.

##### 4.1. Multi-objective optimization method

For optimizing the electricity production process with post-combustion CO<sub>2</sub> capture, the hybrid stochastic algorithm known as Differential Evolution with Tabu List (DETL) is selected. 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 Rangaia [50], it has been shown to have several advantages compared to other optimization methods. For example, DETL has faster convergence, smaller computational efforts, less computational time to solve non-linear and non-convex problems than other methods like genetic algorithms or simulated annealing. Another advantage of DETL is its ability to memorize previously tested solutions, thus avoiding the evaluation of previously tested solutions. This ability reduces the computational time needed to obtain the optimal solution [50,51].

The DETL method consists of four basic steps based on the biological evolution theory, these steps are: initialization, mutation, crossover and selection.

- 1 Initialization step: In this step, a random vector of possible solutions ( $x_i$ ) is generated. The values of this random vector are constrained to upper (max) and lower (min) bounds of each decision variable ( $i$ ). These decision variables are arranged into two D-dimensional vectors. Finally, vector of variables ( $x_i$ ) generated as is shown in Eq. (17):

$$x_i^n = \text{rand}_i(0,1) \cdot (b_{i,\max} - b_{i,\min}) + b_{i,\min} \quad (17)$$

where the rand (0,1) is a random generator constrained in the interval 0,1,  $n$  is the number of generations considered to solve the optimization problem.

**Table 3**  
Equilibrium constant values [34].

$eq = A + B/T + C \ln(T) + D(T)$	A [dimensionless]	B [K]	C [1/K]	D [1/K]	Eq.
$MEA^+ + H_2O \rightarrow MEA + H_3O^+$	-3.038325	-7008.357	0	-0.00313489	(14)
$2H_2O \rightarrow OH^- + H_3O^+$	132.89888	-13445.9	-22.4773	0	(15)
$HCO_3^- + H_2O \rightarrow CO_3^{2-} + H_3O^+$	216.050446	-12431.7	-35.4819	0	(16)

1 Mutation step: This step consists in the generation of new vector sets also known as donor vectors ( $v_i^{n+1}$ ). The donor vectors ( $v_i^{n+1}$ ) are created from three different vectors  $x_a, x_b, x_c$  randomly chosen for each generation  $n$ . The mutation step can be summarized with the next Eq. (18):

$$v_i^{n+1} = x_c^n + F(x_a^n - x_b^n) \quad (18)$$

where  $F$  is called differential weight and it takes values in the continuous interval of 0–2. Differential weight provides stability and avoids the standstill of methods in similar solutions [52].

1 Crossover step: In the crossover step the donor vectors ( $v_i^{n+1}$ ) are combined with the vector of variables ( $x_i$ ) generated during the initialization step. The objective of this step is to generate a trial vector ( $u_i^{n+1}$ ). The crossover is carried out through a binomial scheme where the method randomly decides how each variable is exchanged with the donor vector. The Mathematical formulation of the crossover step is shown in Eq. (19).

$$u_{j,i}^{n+1} = \begin{cases} v_i & \text{if } (rand_{ij}[0, 1]) \leq Cr \\ x_i & \text{otherwise} \end{cases} \quad (19)$$

2 Selection: Lastly, in the selection step, sets of vectors with the best fitness function values are chosen to be part of the next generation. This selection is executed as is shown in Eq. (20).

$$x_{j,i,G+1} = \begin{cases} u_i^{n+1} & \text{if } fit(u_i^{n+1}) > fit(x_i^n) \\ x_i^n & \text{otherwise} \end{cases} \quad (20)$$

This process is repeated until the best value of the objective function is found (global solution) or until the maximum number of generations is reached.

The DETL optimization method has been tested using different benchmark functions to check its convergence in the neighborhood of the optimum for single and multi-objective systems [50,51,53,54]. Generational Distance (GD) and Spread (SP) Eqs. (21) and (22) are used as performance metrics to quantify the performance of DETL algorithm on test problems. GD is calculated between the obtained Pareto-optimal front (after global search or normalized normal constraints) and the true Pareto-optimal front (analytical solution). SP is calculated for the obtained Pareto-front.

$$GD = \frac{\sqrt{\sum_{i=1}^n d_i^2}}{n} \quad (21)$$

$$SP = \sqrt{\frac{1}{n} \sum_{j=1}^n (d_j - \bar{d})^2} \quad (22)$$

Here,  $n$  is the number of non-dominated solutions in the Pareto-optimal front,  $d_i$  is the distance of each solution in the obtained Pareto-optimal front to its nearest point in the true Pareto-optimal front,  $d_j$  is the distance of each solution point in the obtained Pareto-front to its

nearest points in the same Pareto-optimal front, and  $\bar{d}$  is the average of  $d_j$  for all solution points in the obtained Pareto-optimal front.

As a result of the optimization process, a Pareto front that presents the non-dominated solutions in the search space is obtained. Due to the stochastic nature and being a method based on evolutionary theories, it is possible to obtain several points that can be optimal in the trade-off of the various objective functions. Then, it is possible to generate a catalog of several feasible optimal solutions that are in the zone where the objective functions converge in their minimum/maximum value. In that sense, according to the needs of the final design, it is possible to choose a process with characteristics associated to one or several particular objectives.

The optimization parameters can be pre-tuned to improve the performance during the optimization process. However, the search space formed by the model representing the capture process, the objective functions and the constraints considered does not depend at all on the optimization parameters used.

#### 4.2. Multi-objective optimization problem statement

The optimization problem was solved through Normalized normal constraints (NNC) that formulates the multi-objective optimization problem as a solve single objective optimization (SOO) based on linear mapping of objectives. NNC does not assign any weight to different objectives but incorporates extra constraints in the problem formulation. The newly formulated constrained SOO problem can be solved using an efficient SOO method. NNC method is unlikely to find the global Pareto-optimal solutions for non-convex search space. Hence, a stochastic global search before NNC method is used to escape from local Pareto-optimal solutions [51].

In an optimization problem, an objective function is an important mathematical formulation from a set of design responses that are constrained by a specific condition. During the optimization, the objective function tries to minimize or maximize the design response from that set of variables. During each design cycle the optimization module determines which of the set of weighted design responses has the minimum value of that design response. The Optimization module can arrive at a solution that optimizes the objective function; however, if the constraints are not satisfied, the result of the optimization is not a feasible design.

In this work the objective function involves three important axes to analyze: Return on Investment (ROI) as an indicator of the economy of the process by calculating return on investment due to the coupling of a capture plant to an existing power plant. Condition Number ( $\gamma^*$ ) as an indicator of the dynamic behavior of the process considering low condition number for systems with good controllability and eco-indicator 99 (EI99) to quantify the environmental impact derived from the coupling of the capture process, use of MEA as a solvent. It is expected that the analysis framework developed in this paper can contribute to the use of indices that can assess more than one aspect of green chemistry to be easily integrated into a green process-based optimization. Similar works have been reported by Sánchez-Ramírez et. al. [55] and Contreras-Zarazúa et al. [56] applying these indexes for distillation columns. Based in the previous information about the indices, a general mathematical expression for the objective function and its respective decision variables involved in the optimization procedure are shown in Eq. (21n).

$$\text{Min} [-ROI, \gamma^*, EI99] = f(\text{Air}, PR_{\text{com1}(\text{out/in})}, CP_{\text{reactor}}, DP_{\text{turbine}}, N_{ij}, NF_{ij}, D_{ij}, MEA, RR, Q) \quad (21)$$

$$\text{Subject to: } \begin{cases} y_{i,f} \geq x_{i,f} \\ w_{i,f} \geq u_{i,f} \end{cases}$$

where the Air is the air feed flow that enters to the power plant.  $P_{\text{com1}}$ ,  $P_{\text{reactor}}$  and  $P_{\text{turbine}}$  represents the pressure in the compressor, reactor, and turbine, respectively operating in the power plant. For the variables related to the capture process  $N_{ij}$  represents the number of stages,  $NF_{ij}$  represents the feed stage,  $D_{ij}$  represents the diameter where the  $i$  is specified for the absorber and  $j$  corresponds to the desorber. MEA represents the solvent feed flow in the absorber, RR represents re reflux ratio and Q the reboiler duty, both in the desorber column. The objective function is restricted to satisfy the recuperation of 99% of the  $\text{CO}_2$  produced during the combustion and also to achieve a purity of 99% mol of  $\text{CO}_2$ . Where  $y_{i,f}$  represents the  $\text{CO}_2$  recovered in the desorber column and  $x_{i,f}$  represents the 99% of the  $\text{CO}_2$  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 99% mol of  $\text{CO}_2$ .

According to other optimization works, it has been shown that the selected design variables have a direct impact on the sustainability indicators that are evaluated [22,55–57]. One way to verify this is by analyzing the formulation of the evaluated indices. To calculate the economic indicator, it is necessary to obtain the operating cost, which depends on the reboiler duty, feed flows, operating pressures, etc. It also depends on the cost of capital, which depends on the sizing of the equipment. On the other hand, for the calculation of the environmental indicator, it is important to consider quantities of what is being evaluated. In this case, it is necessary to consider the sizing of the equipment, the solvent flows, and heating services.

The proposed model has a significant number of variables to be optimized to have an optimal design and operation conditions, by aiming a maximum capture of  $\text{CO}_2$ , the best control criteria, maximum return on investment and lowest environmental impact. In this context, due to the electrolytic behaviour present in the liquid phase, the  $\text{CO}_2$

**Table 4**  
Design variables considered for the multi-objective constrained optimization.

Variables	Type of Variable	Symbol	Range	Units
<b>COMBUSTION</b>				
Air Flow	Continue	Air	9 000–35 000	kmol/h
Compressor Pressure Ratio (pressure out/ pressure in)	Continue	$PR_{\text{com1}(\text{out/in})}$	1–8	—
Combustion Reactor Pressure	Continue	$CP_{\text{reactor}}$	4.5–9	Atm
Turbine Discharge Pressure	Continue	$DP_{\text{turbine}}$	1–8	Atm
<b>ABSORPTION</b>				
Number of stages	Discrete	$N_i$	4–99	—
Fed Stage	Discrete	$NF_i$	4–99	—
Diameter	Continue	$D_i$	0.5–3.5	m
Solvent Flow	Continue	MEA	43000–44 000	kmol/h
<b>DESORPTION</b>				
Number of stages	Discrete	$N_j$	4–99	—
Fed Stage	Discrete	$NF_j$	4–99	—
Diameter	Continue	$D_j$	0.5–3.5	m
Reflux Ratio	Continue	RR	0.1–75	—
Reboiler Duty	Continue	Q	0.03–151.38	GJ/h

capture process represents a highly non-linear model. With a certain number of discrete and continuous variables, the  $\text{CO}_2$  capture model is suitable for optimizing. The bounds of the decision variables considered in this work are presented in Table 4. The bounds were determined based on the description mentioned in previous section.

The implementation of the global optimization approach involved a hybrid platform which linked Aspen Plus, Microsoft Excel, and Matlab through the implementation of a COM technology (see Fig. 2). To start the optimization process, design variables are specified in Microsoft Excel. Using the DETL algorithm programmed in Excel through a Visual Basic macro, initial values are randomly selected according to the methodology provided in the last Section 3.4.

During the optimization process, a decision vector of design variables is sent from Excel to Aspen Plus. In this process simulator, rigorous calculations for the data that identify a particular design of the distillation systems are obtained (e.g., temperature profile, molar composition profile, molar flow profile, etc.) via resolution of phase equilibria along with the complete set of modeling equations. If the decision vector from Excel provides an infeasible combination of variables, ASPEN PLUS will detect the model as not feasible and then the optimization algorithm will provide a new combination of variables. Then, if the combination of variables performs a feasible design, the result data is returned from Aspen Plus and stored in Excel. Then perturbations are applied to the manipulated variables, and new simulations are executed in Aspen Plus. After these simulations are completed, the differences among the components' molar purities in the nominal state and the components' molar purities after the perturbations are estimated. These data along with the necessary data to estimate the condition number are sent from Excel to Matlab. In this software, the calculation of this objective function is carried out. The value obtained for the condition number is returned to Excel. Then the ROI and Ecoindicator 99 are calculated. The method DETL evaluates the objective function, and after that, a new vectors of design variables are generated according to the stochastic procedure of this method. Once the DETL parameters are complete, the method stops the optimization.

The parameters used for DETL were taken from previous works of Rangaiah [51]. Considering population size: 120 individuals, Generation number: 1000, Tabu list size: 60, Tabu radius: 0.0001, Crossover fractions: 0.9, Mutation fractions: 0.3. These parameters have proven to work exceptionally well with nonlinear problems providing great results.

## 5. Results and discussion

This section presents the results obtained from the multi-objective optimization for a  $\text{CO}_2$  capture plant coupled to a power generation plant. To analyze the operating conditions for each design, it is important to highlight the  $\text{CO}_2$  composition of the flue gases obtained for each fuel used for the simulation. So, the  $\text{CO}_2$  composition in molar fraction for Biogas, Coal, Natural Gas and Associated Gas is: 0.054, 0.124, 0.050 and 0.042, respectively. It is possible to observe that the flue gases with the highest concentration of  $\text{CO}_2$ , is the one that is obtained from burning Coal, followed by those obtained from Biogas and Natural Gas. This concentration directly affects the parameters related to operational conditions, such as solvent requirement and reboiler duty, which impact on economic and environmental indexes. In Fig. 3, a 3D representation of the Pareto Front shows each indexes trend during the optimization process for each fuel. According to the analysis of the 3D Pareto Fronts, it can be observed globally that the objectives are in competition. Having a

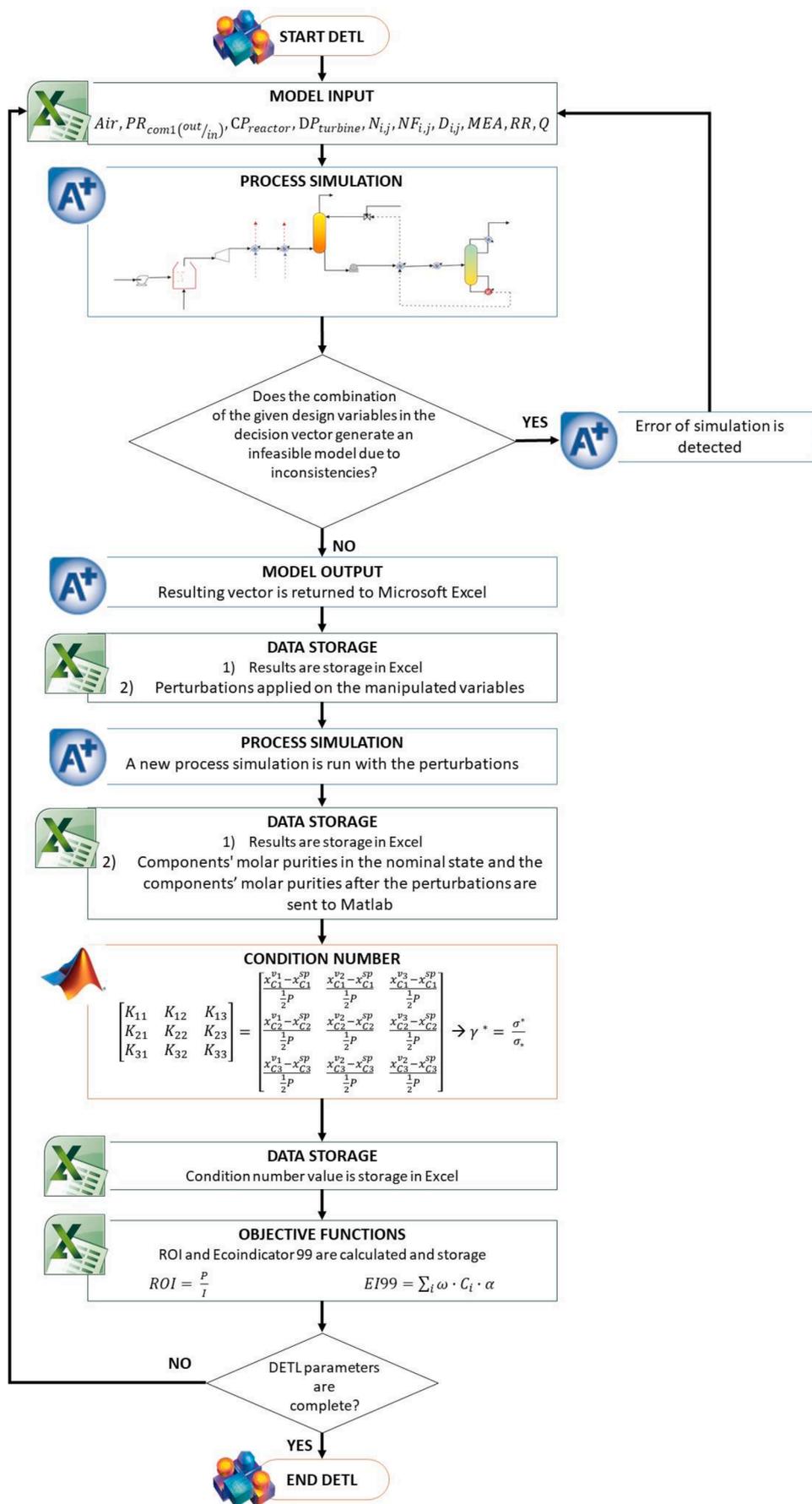


Fig. 2. Software interaction used for hybrid optimization platform.

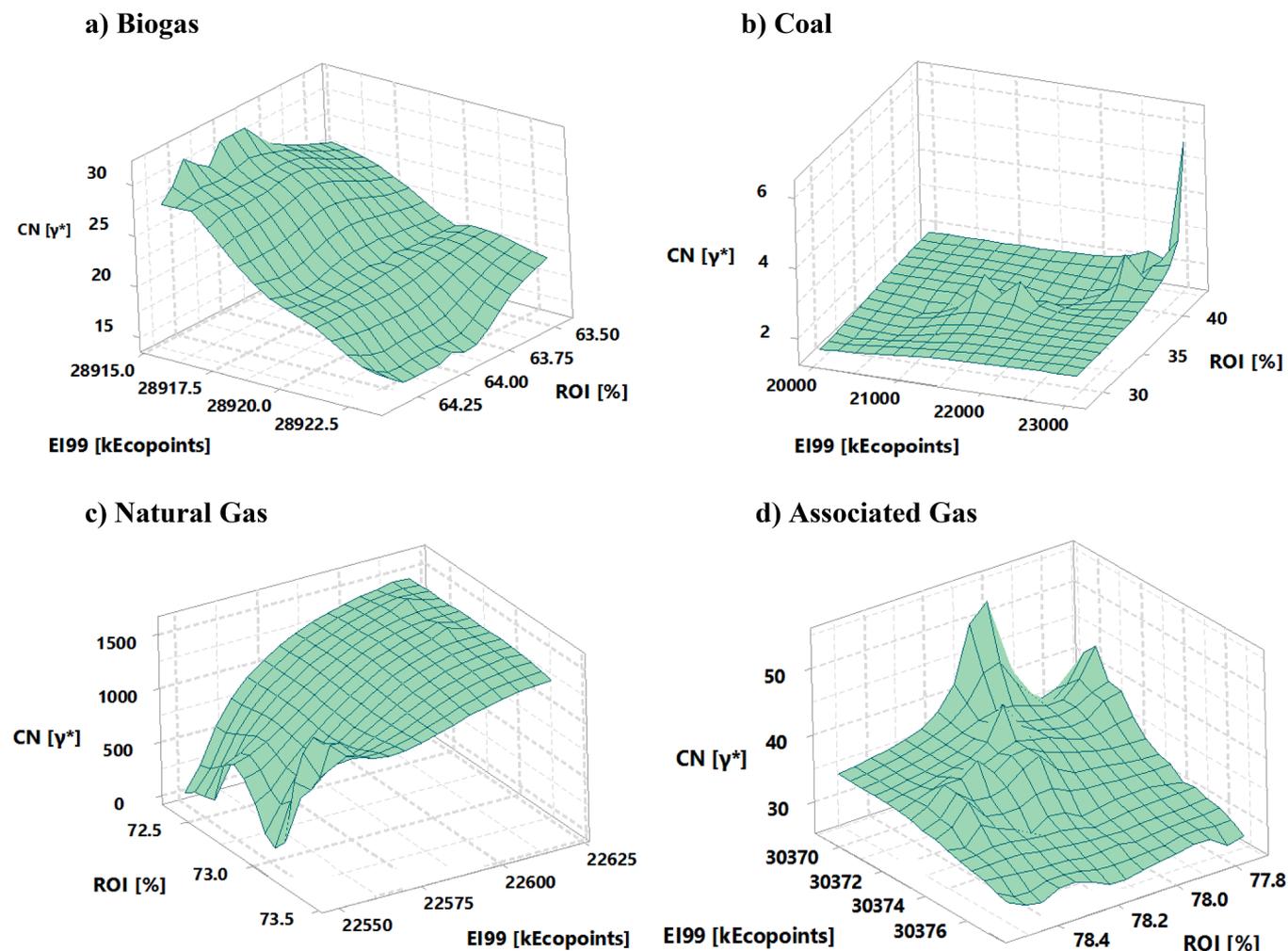


Fig. 3. Pareto fronts between the Condition Number (CN), Return on Investment (ROI) and Ecoindicator 99 for (a) Biogas, (b) Coal, (c) Natural Gas and (d) Associated Gas.

design with lower environmental impact and good control properties implies sacrificing economic recovery. Conversely, having a design with favorable economic recovery represents having a bigger environmental impact. Therefore, the design with the objectives in balance was chosen as the optimal design.

For the Biogas, Fig. 3a, when the value of the eco-indicator 99 is low, then the value of the ROI is high, under this scenario it could be said that the two objectives trade off. However, there still missing the control index. For the condition number it is found that when the other two objectives trade off, the control objective is opposed, the system would not present a good controllability when high values of condition number are presented. One way to explain this behavior is through the design variables. For low values of eco-indicator and a high value of ROI, the topology of the process is smaller and there is an increase in  $\text{CO}_2$  recovery due to the increase of air flow, solvent flow, thermal flow, reboiler duty and reflux ratio. In that sense, by having a smaller equipment size there will be a direct impact on process costs. On the other hand, despite increasing reboiler duty and reflux ratio, the impact of these variables on the economic indicator is leveled off due to the high  $\text{CO}_2$  recovery. On the other hand, by having an increase in the process flows and in the reboiler duty, the condition number will increase. So, the obtained designs will not present good control properties compared to those with low condition numbers. By having bigger systems, the disturbances will be bigger and can be directly related to the security indicator, since the bigger the process is, the bigger the risk.

For the Coal, Fig. 3b, when the value of the eco-indicator 99 and

condition number is low, then the value of the ROI is also low, under this scenario it could be said that when the process has good environmental impact and good control properties, there will be the case in which the process is not economically profitable.

For the Natural Gas, Fig. 3c, when the value of the eco-indicator 99 is low then the value of ROI is low and the value of condition number is high, under this scenario it is possible to observe that none of the objectives trade off. Otherwise, when the eco-indicator's values are high, then the value of ROI will be high and the condition number will be low. For the Associated Gas, Fig. 3d, when the value of the eco-indicator 99 is low then the value of ROI is low and the value of condition number is high, under this scenario it is possible to observe that none of the objectives trade off. Otherwise, when the eco-indicator's values are high, then the value of ROI will be high and the condition number will be low. For this scenario could be said that when the process is economically profitable and presents good control properties, it will have a high environmental impact. It is important to highlight that spikes are observed in the results obtained for the condition number in the optimization curves. It is well reported in the literature that this behavior is observed due to the nonlinearity of the open-loop response, in the system under study, when find design specifications are far from optimal values [58,59].

For the Coal, Natural Gas and Associated Gas; the variables regarding the topology of the process do not maintain a trend that allows for a clear explanation of how they affect the economic, control, and environmental indices. However, despite this behavior in the variables, it can be

**Table 5**  
Design parameters for the best scenario of CO<sub>2</sub> capture for each fuel.

Variables	Biogas	Coal	Natural Gas	Associated Gas
<b>COMBUSTION</b>				
Air Flow [kmol/h]	17133.95	20519.78	19602.76	24221.83
Compressor inlet Pressure [atm]	4.3	—	3.72	3.02
Compressor outlet Pressure [atm]	16.05	—	13.55	13.93
Compressor Pressure Ratio (out/in) [-]	3.72	—	3.64	4.60
Combustion Reactor Pressure [atm]	5.13	—	7.46	6.79
Combustion Temperature [°C]	1250.8	—	1351.3	1227.5
Turbine Discharge Pressure [atm]	4.8	2.73	6.89	5.53
<b>ABSORPTION</b>				
Number of stages [-]	39	34	29	33
Fed Stage [-]	3	3	3	3
Diameter [m]	3.2	1.18	2.59	2.76
Solvent flow MEA [kmol/h]	43681	43258.06	43504.63	43509.26
<b>DESORPTION</b>				
Number of stages [-]	33	24	24	22
Fed Stage [-]	3	3	3	3
Diameter [m]	2.36	1.33	2.04	1.45
Reflux ratio (RR) [-]	3.53	2.24	2.32	3.67
Reboiler duty (Q) [GJ/h]	470.08	210.50	364.45	491.86
CO <sub>2</sub> recovered [ton/h]	67.57	32.72	65.84	70.40
Q/CO <sub>2</sub> [GJ/ton]	6.9	6.4	5.5	6.9
L/G [kg/h/kg/h]	2.06	1.68	1.47	1.82
CO <sub>2</sub> Purity [%mol]	0.99	0.99	0.99	0.99
O <sub>2</sub> impurities [ppmv]	0.15	0.89	1.39	0.15
H <sub>2</sub> O impurities [ppmv]	1.9	1.62	6.64	4.79
<b>OBJECTIVE FUNCTION</b>				
ROI [%]	64.25	40.86	73.24	77.83
γ*	20.17	2.39	6.7	34.82
EI99 [kEcopoints]	28920.05	22615.53	22549.43	30369.51

said that the relationship between solvent, reflux ratio and reboiler duty are maintained. That is, if the amount of solvent increases, the reflux ratio increases and, therefore the reboiler duty. So, this behavior could give us an indication of how the sustainability indices are affected.

Table 5 shows a summary of the optimal designs for each fuel, the optimal design for each case is when the objectives functions are in equilibrium between them and competition between targets is balanced. For the case of coal, as the flue gases at the exit of the combustion chamber were considered as the beginning of the process, there is no results about compressor pressures and combustion temperature.

It is possible to observe the impact of some design parameters on the process performance. For the absorption unit, when the CO<sub>2</sub> concentration is low, the efficiency in the capture is affected. In order to capture a bigger amount of CO<sub>2</sub>, the solvent requirement increases. Moreover, the reflux ratio is directly related to the energy requirements. As higher is the reflux ratio the energy requirements for the capture will increase. For the analysis of the sustainability indexes, it can be observed that the better return on investment when implementing a capture process is when associated gas and natural gas are used as fuels, this trend is related to the topology of the process. The process configuration is smaller for these two fuels, directly impacting construction costs. Also, as the flue gasses for those fuels have a bigger concentration in CO<sub>2</sub>, the solvent requirements will be less compared to the other two fuels. It is possible to see that the least environmental impact occurs when natural gas is used as a fuel. Several factors can explain this. First of all, it is the process with the biggest CO<sub>2</sub> recovery, therefore the environmental footprint related to CO<sub>2</sub> emissions tends to decrease.

Likewise, the reduction in environmental impact can be explained because it is the process that has the lowest energy requirements and uses of solvents; these factors have a significant impact on the

environmental weighting. On the other hand, it can be observed that the process where coal is used has an environmental score approximate to that obtained with natural gas. However, this process requires the highest use of solvent, due to the low concentration of CO<sub>2</sub> in its flue gases. As well as the process in which there is a lower recovery of CO<sub>2</sub>. About the control properties, it can be seen that the processes where coal and natural gas are used, are those that present the best control properties by presenting lower condition numbers. However, through the optimization process, it is possible to obtain the best combination of design variables generating the design that meets the lowest environmental impact, highest return on investment and the best control properties for each fuel studied. The results obtained show that the process in which natural gas is used globally presents a balance in the three objectives of costs, environmental, and control properties.

To validate the results obtained in this study, the Liquid/Gas ratio (L/G) and the thermal need [GJ/Ton CO<sub>2</sub>] are presented for all the fuels studied. Thus, for the L/G ratio, the values obtained are between 1 and 3, matching with the state of the art [34]. On the other hand, the reboiler duty of amine regeneration per ton of CO<sub>2</sub> capture is presented, obtaining results between 5 and 7 GJ/Ton CO<sub>2</sub>, likewise these results match with those reported in literature [46,34].

Moreover, to achieve circular economy and green chemistry goals, it is necessary to consider CO<sub>2</sub> recovered as a feed flow for another process. Nevertheless, after capturing CO<sub>2</sub>, the product stream contains several impurities which may negatively impact pipeline transportation, geological storage, and applications. Oxygen (O<sub>2</sub>) and water (H<sub>2</sub>O) are the two major impurities in the CO<sub>2</sub> product stream. It is reported that the levels of impurities present in the CO<sub>2</sub> stream should be less than 50 ppmv for H<sub>2</sub>O and to 10 ppmv for O<sub>2</sub> [60]. From the results obtained, it is possible to see in Table 5 that for all the fuels analyzed, the O<sub>2</sub> and H<sub>2</sub>O contained in the CO<sub>2</sub> product stream are below than the restricted level reported in the literature. In this way, further studies, including the transportation and application of the recovered CO<sub>2</sub> should be considered in the future.

## 6. Conclusion

This work proposes a simultaneous design and optimization of a CO<sub>2</sub> Capture plant coupled to a power plant. The implementation of CO<sub>2</sub> capture plants can be considered a short-term sustainable alternative to reduce CO<sub>2</sub> emissions while waiting for the growth of renewable energies that can cover the world's energy needs. In this study, different aspects of the process such as controllability, environmental impact and economic issues were considered. The evaluation of different metrics provides a wide overview of how different variables can affect the sustainability of the process. Therefore, we have considered different metrics that aid in evaluating and selecting the most sustainable process [61].

As shown, it is important to consider the type of fuel used for electricity production. Due to the CO<sub>2</sub> concentration contained in the flue gasses, there will be variations in the design specifications of the capture process. However, before implementing a CO<sub>2</sub> capture plant, it is necessary to analyze the environmental implications of the implementation, use of solvents, control properties and energy consumption.

The optimal operating conditions of the different systems were found, showing that system operating with the natural gas presents a better balance in all the objectives to analyze. Having the lower impact with 22549.43 kEcopoints and a return on investment of 73.24%. From the results obtained, it can be pointed out that it is possible to find designs that operate under the reported theoretical ranges, having an improvement in CO<sub>2</sub> recovery of 90% to 99% [34]. Although there is an increase in energy requirements compared to studies where mono-objective optimization is performed for the same process, this is necessary to achieve greater CO<sub>2</sub> recovery compared to data reported in the literature [18]. Likewise, multi-objective optimization allows us to visualize a feasible panorama of a sustainable process and gives

indications of which is the best fuel to achieve electricity production in a sustainable process.

To conclude, this work creates the opportunity for future research in the field. Showing that in order to maximize the sustainability of the proposed process there is a huge area of opportunity in the study of new solvents; such as ionic liquids and deep eutectic solvents, to improve the efficiency of CO<sub>2</sub> capture, to replace the use of MEA as the main solvent for CO<sub>2</sub> capture and minimize the environmental impact that entails the use of such a toxic solvent.

### 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.

### Data availability

The data that has been used is confidential.

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