Optimal Design and Operating Conditions of an Integrated Plant Using a Natural Gas Combined Cycle and Postcombustion CO₂ Capture

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ABSTRACT: This paper deals with the simultaneous optimization of the operating conditions and sizes of each one of the process units of a natural gas combined cycle coupled to a postcombustion CO₂ capture system. Precisely, from the mathematical models previously developed by the authors for each stand-alone process, a new optimization nonlinear programming (NLP) model is proposed in order to optimize the whole process but with the main characteristic that several feasible alternatives to integrate both processes are simultaneously embedded. Therefore, as a result of the model, the best integration schema, optimal operating conditions, and size of each process unit are obtained at the same time. No integer variables are needed to model discrete decisions in both processes. The maximization of the overall thermal efficiency is considered as an objective function. However, the proposed NLP model can be easily extended into a mixed-integer nonlinear programming (MINLP) model if it is necessary for cost minimization. The optimization results are discussed in detail, and they are compared with suboptimal configurations including reference cases.

1. INTRODUCTION

Fossil fuels (coal and natural gas) will still be the primary source for power and electricity generation. However, the combustion of these fuels for electricity generation, industry, and transportation is the largest source of CO₂ emissions which is considered to be one of the main contributors to the greenhouse effect. For this reason, the reduction of CO₂ emissions is a global challenge and requires collective actions and close cooperation between industries and researchers. CO₂ capture and storage (CCS) has a high potential for large reductions in CO₂ emissions. Currently, there are three feasible capture technologies: (1) precombustion, (2) postcombustion, and (3) oxi-fuel combustion.

The postcombustion process includes various techniques: (a) scrubbing with aqueous amine solutions [monoethanolamine (MEA), methyldiethanolamine (MDEA), diethanolamine (DEA)]; (b) combined amine-membrane techniques; (c) molecular sieves; and (d) pressure and temperature swing adsorption (PSA/TSA) using zeolites. These techniques separate the CO₂ from a flue gas environment containing other components (NOx and SO₂). Chemical composition of flue gas depends on the type of fossil fuel used. Certainly, coal emits more NOx and CO₂ per unit of useful energy produced than natural gas.

In particular, the chemical absorption with MEA, which will be addressed in this paper, is considered to be the most mature technology to be implemented in midterm not only for already existing power plants but also for new ones. However, it is considered to be an intensive energy process because of the high heating utility required for the amine regeneration which is the major drawback of this alternative. In this process, there are several trade-offs that must not be ignored (investments and operating costs and energy penalties).

During the last several years, significant research efforts have been directed toward achieving significant savings of the CO₂ costs. Current research activities for postcombustion CO₂ capture technologies have been done in different lines of research from experimental studies at laboratory scale and pilot plants to the development and implementation of mathematical models in computers. Regarding the latter line of research, the application of mathematical modeling to address the optimization of integrated plants of NGCC and postcombustion CO₂ capture processes using amine is receiving special attention. Several articles deal with the systematic optimization of stand-alone power plants.1−8

Bruno et al.2 developed a mixed-integer nonlinear programming (MINLP) model to optimize the structural and operating conditions of utility plants to satisfy fixed demands (electricity, mechanical work, and heating utility). The complexity of the mathematical model was reduced by fixing the steam pressures, and the steam turbine efficiency was calculated using linear and quadratic correlations depending on the extraction pressure. The model has been implemented in the computer package STEAM, and it is useful for both synthesis and analysis of different design alternatives.

Jüdes et al.4 presented a nonconvex mixed-integer nonlinear programming (MINLP) mathematical model considering the partial-load operation already in the design phase of a combined heat and power plant (cogeneration plants). The proposed model was solved with LaGO (Lagrangian Global Optimizer), and it
allows one to find a cost optimal plant design that is feasible for the full-load and the considered partial-load cases.

Martelli et al.\textsuperscript{6} proposed a rigorous mathematical programming model, a linear approximation, and a two-stage algorithm in order to optimize not only heat recovery steam generation (HRSG) of simple combined cycles but also any heat recovery steam cycles (HRSCs) with external heat/steam sources/users and with multiple supplementary firing. The authors successfully applied the proposed model and methodology to highly integrated plants (biomass to Fischer–Tropsch liquids plants, integrated gasification combined cycles (IGCCs) with and without CCS, and coal to synthetic natural gas (SNG) facilities).

Similarly, several articles dealing with the mathematical modeling and simulation of stand-alone CO\(_2\) capture processes using amine have been published. Many of the authors employed process simulators such as Aspen Plus,\textsuperscript{9–15} HYSYS,\textsuperscript{14,15} Aspen HYSYS,\textsuperscript{16} and gPROMS.\textsuperscript{17,18} Other authors developed in-house simulation algorithms.\textsuperscript{19–21} Freguia and Rochelle\textsuperscript{19} integrated a Fortran subroutine into Aspen Plus to perform a rate-based calculation of CO\(_2\) absorption into MEA. In all of the articles, significant insights have been gained for both absorber and regenerator units considering coupled and stand-alone operating modes. Many of the authors analyzed the effect of the pressure and temperature of absorber and different type of amines (primary, secondary, and tertiary amines) on the overall CO\(_2\) absorption efficiency and on the heat duty in the regenerator unit because of its significant influence on the total operating cost.\textsuperscript{22,23} On the other hand, techno-economic evaluations of postcombustion processes have also been the focus.\textsuperscript{24–33}

To the knowledge of the authors, only a few articles dealing with the simultaneous optimization of the dimensions and operating conditions of the entire postcombustion CO\(_2\) capture process (absorption, amine regeneration, compression stages) involving detailed cost equations and rigorous mathematical modeling of the process equipment have been discussed specifically in the literature.\textsuperscript{18,34–37} Finally, it should also be mentioned that there are several articles dealing with the study of the power plants coupled to CO\(_2\) capture processes. Some of the authors focused on the integration of coal power plants with CO\(_2\) capture plants.\textsuperscript{24,26,38,39} Other authors carried out techno-economic analysis of natural gas combined cycles with postcombustion CO\(_2\) capture employing parametric analysis and mathematical models with different levels of details.\textsuperscript{21,25,40–43}

Romeo et al.\textsuperscript{26} compared different possibilities to overcome the energy requirements when integrating amine scrubbing to a commercial pulverized coal power plant. They found that using a gas turbine to supply compression electrical energy and extracting steam from the steam cycle is the optimum option regarding the efficiency penalty on the power plant performance.

Sipočz and Tobiesen\textsuperscript{44} presented thermodynamic and economic analyses of a 440 MWe NGCC plant with an integrated CO\(_2\) removal plant, using an aqueous solution of monoethanolamine (MEA). The absorber intercooling and the lean vapor recompression were included in the flow sheet of the CO\(_2\) capture plant, and exhaust gas recirculation (EGR) was considered in the gas turbine in the NGCC plant which led to

Figure 1. Schematic diagram of the entire process to be optimized.
an increase the CO₂ content in the exhaust gases compared to conventional operating gas turbines. It is shown that EGR in combination with a reduced specific reboiler duty adds significant benefits to both the operational and capital expenditures. Also, the authors concluded that special attention should be put in the calculation of the fuel costs and currency rates because they play important roles in providing reliable cost estimations.

Möller et al. proposed an integrated genetic algorithm solver for optimizing the pressure levels in a natural gas-fired combined cycle with and without CO₂ separation from the flue gas. The authors used two objective functions: efficiency and specific cost. For the analyzed cases, one of the conclusions reveals that a third steam pressure level does not significantly increase the efficiency due to very low mass flow at the intermediate steam pressure level.

Möller et al. addressed the integration of steam production for amine regeneration at a natural gas combined cycle. The steam is extracted from the LP section of the steam turbine and returned to the high pressure feedwater circuit. The combined cycle involved a triple-pressure reheat steam cycle with fixed steam pressure levels. For the CO₂ capture plant, the authors used a simplified model (constant geometry in the absorber and desorber and the regeneration temperature and MEA heat demand were proportional to the mole-flow of captured CO₂). Different ambient conditions and three different operational part-load strategies and their influences on the cycle performance were examined.

The main goal of this paper is to investigate how the NGCC and CO₂ capture plants should be integrated in order to improve the overall thermal efficiency. The major challenge is to develop a robust and detailed nonlinear programming (NLP) mathematical model which allows one to determine not only the optimal operating conditions but also the size of each one of the pieces of equipment. As will be described later, the proposed model embeds three alternative integration diagrams. The proposed model is an extension of previous ones which are used here to describe the NGCC and postcombustion CO₂ capture. Precisely, the mathematical model for the HRSG derived from Manassaldi et al. and the detailed model of the entire CO₂ capture process presented in Mores et al. are used as a basis to derive the new NLP mathematical model.

The paper is outlined as follows. Section 2 introduces the problem formulation. Section 3 summarizes the assumptions and details of the mathematical model. Section 4 presents applications of the developed NLP model and discusses the results. Finally, Section 5 presents the conclusions and future work.

\[ \eta_{\text{gen-cap}} = \frac{\sum_{i=1}^{N_{\text{GT}}} (W_{\text{GT}} - W_{\text{CP}}) + \sum_{j=1}^{N_{\text{ST}}} (W_{\text{ST}}) - \sum_{k=1}^{N_{\text{PP}}} (W_{\text{PP}}) - \sum_{l=1}^{N_{\text{CT}}} (W_{\text{CP}} + W_{\text{CP}} + W_{\text{CP}})}{m^{\text{LHV}}} \]

where the first sum of the right-hand side refers to the total net electricity produced in the gas turbines; the second sum refers to the total electricity produced in the steam turbines; the third sum represents the total electricity consumed by pumps in the NGCC plant; and the last accounts for the total electricity required by pumps, blowers, and compressors in the CO₂ capture plant. The parameters \(N_{\text{GT}}, N_{\text{ST}}, N_{\text{PP}},\) and \(N_{\text{CT}}\) refer to the number of gas turbines (2), the number of steam turbines (1), the number of pumps (depends on the configuration), and the number of CO₂ capture trains (6), respectively. Superscripts PP and CP refer to the power plant and the capture plant. Finally, \(m^{\text{LHV}}\) and LHV are the flow rate and the lower heating value of the fuel (CH₄).

### 2. PROBLEM STATEMENT

The goal of the optimization problem is to determine the best integration arrangement, optimal operating conditions, and equipment dimensions in order to maximize the thermal efficiency and to satisfy minimum levels of electricity demand (700.0 MW) and CO₂ capture (90.0%). As it will be described later, both levels are imposed through lower bounds.

Figure 1 shows the entire process to be optimized. Two (2) NGCC cycles, one (1) steam turbine with three pressure levels, one (1) deaerator, and six (6) CO₂ capture trains operating in parallel mode are considered. It should be noted that only one of the six capture trains is represented in Figure 1. The gas turbine model has been tuned to reproduce, approximately, the performance of a SGT5-4000F gas turbine reported by Siemens. Certainly, data taken from the corresponding turbine catalogue are employed in order to define lower and upper bounds for some optimization variables (pressure ratio, exhaust mass flow rate, and temperature, among others).

As it is shown in Figure 1, the following three integration schemas are embedded: (1) The total steam required in the amine regeneration process of the CO₂ capture system may be extracted from the steam turbine IP/LP ST (red stream). (2) The total steam required in the reboiler of the CO₂ capture process may come from the evaporator of the heat recovery steam generator HRSG. This alternative is marked in green in Figure 1. (3) The steam used in the reboiler of the CO₂ capture process may be partially extracted from both steam turbine IP/ LP ST and HRSG.

The objective function is to maximize the overall thermal efficiency \(\eta_{\text{gen-cap}}\) which is defined in eq 1.

### 3. HYPOTHESIS AND MATHEMATICAL MODEL

As shown in Figure 1, both processes (NGCC and CO₂ capture plant) are coupled through mass and energy balances in the mixers M1 and M2 and deaerator D. As mentioned earlier, the
Table 2. Model Optimization Variables

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure, temperature, and flow rate of the main streams (water and MEA makeup, lean and rich MEA solution)</td>
<td>CO2 capture plant</td>
<td>natural gas combined cycle</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Pressure, temperature, and flow rate of fuel, vapor, water, and exhaust gases in the economizer, evaporator, and superheaters</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Heat transfer area of economizer, evaporator, and superheaters</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Fuel and air consumption</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Electricity produced by the gas and steam turbines</td>
</tr>
</tbody>
</table>

P, x, y, and T profiles in the liquid and vapor phases at the absorber and regenerator units

Heat transfer area of condenser, reboiler, MEA cooler, economizer, and interstage coolers

Packing volume of the absorber and regenerator (both height and diameter are optimization variables)

Reboiler heat duty

Electricity required by pumps, blowers, and compressors

CO2 capture recovery is considered as an optimization variable with its corresponding lower and upper bounds (90% and 98%, respectively). According to the proposed objective function, the optimal value of the CO2 capture recovery should reach its lower bound. As expected and will be presented later, this is confirmed in all optimization results.

Table 3. Numerical Values of the Parameters Assumed for the CO2 Capture Plant

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of capture trains</td>
<td></td>
<td>6</td>
</tr>
<tr>
<td>minimum CO2 capture target</td>
<td>%</td>
<td>90</td>
</tr>
<tr>
<td>fresh amine composition</td>
<td>% w/w</td>
<td>30</td>
</tr>
<tr>
<td>fresh amine temperature</td>
<td>K</td>
<td>298.15</td>
</tr>
<tr>
<td>reboiler pressure</td>
<td>kPa</td>
<td>200</td>
</tr>
<tr>
<td>compression pressure</td>
<td>MPa</td>
<td>8.6</td>
</tr>
<tr>
<td>CO2 pumping pressure</td>
<td>MPa</td>
<td>14</td>
</tr>
<tr>
<td>minimum cold flue gas temperature</td>
<td>K</td>
<td>313.15</td>
</tr>
<tr>
<td>Packing Properties</td>
<td>Intalox saddles</td>
<td></td>
</tr>
<tr>
<td>specific area</td>
<td>m²/m³</td>
<td>118</td>
</tr>
<tr>
<td>nominal packing size</td>
<td>m</td>
<td>0.05</td>
</tr>
<tr>
<td>critical surface tension</td>
<td>N/m</td>
<td>0.061</td>
</tr>
<tr>
<td>void fraction</td>
<td>%</td>
<td>79</td>
</tr>
<tr>
<td>dry packing factor</td>
<td>m²/m³</td>
<td>121.4</td>
</tr>
<tr>
<td>Overall heat transfer coefficients</td>
<td></td>
<td></td>
</tr>
<tr>
<td>economizer</td>
<td>W/m² K</td>
<td>760.8</td>
</tr>
<tr>
<td>condenser</td>
<td>W/m² K</td>
<td>320.2</td>
</tr>
<tr>
<td>reboiler</td>
<td>W/m² K</td>
<td>1360.3</td>
</tr>
<tr>
<td>MEA cooler</td>
<td>W/m² K</td>
<td>1005</td>
</tr>
<tr>
<td>interstage coolers</td>
<td>W/m² K</td>
<td>277.7</td>
</tr>
</tbody>
</table>

Table 4. Numerical Values of the Parameters Assumed for NGCC

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>net electricity production (minimum)</td>
<td>MW</td>
<td>700</td>
</tr>
<tr>
<td>number of gas turbines/HRSGs</td>
<td></td>
<td>2/2</td>
</tr>
<tr>
<td>fuel LHV</td>
<td>kJ/kmol</td>
<td>802.518</td>
</tr>
<tr>
<td>fuel composition (CH₄)</td>
<td>%</td>
<td>100</td>
</tr>
<tr>
<td>fuel temperature</td>
<td>K</td>
<td>298.15</td>
</tr>
<tr>
<td>maximum fuel pressure</td>
<td>kPa</td>
<td>1215.9</td>
</tr>
<tr>
<td>pressure ratio</td>
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<td>18.2</td>
</tr>
<tr>
<td>isentropic efficiency of compressors</td>
<td></td>
<td>0.95</td>
</tr>
<tr>
<td>isentropic efficiency of turbines</td>
<td></td>
<td>0.863</td>
</tr>
<tr>
<td>maximum inlet temperature in GT</td>
<td>K</td>
<td>1500</td>
</tr>
<tr>
<td>minimum air excess (mole basic)</td>
<td>%</td>
<td>220</td>
</tr>
<tr>
<td>air inlet (ISO condition)</td>
<td>kPa/K</td>
<td>101.3/288.15</td>
</tr>
<tr>
<td>isentropic efficiency of steam turbines</td>
<td></td>
<td>0.9</td>
</tr>
<tr>
<td>minimum pinch point</td>
<td>K</td>
<td>15</td>
</tr>
<tr>
<td>approach point</td>
<td>K</td>
<td>5</td>
</tr>
<tr>
<td>minimum heat transfer temperature difference</td>
<td>K</td>
<td>15</td>
</tr>
<tr>
<td>minimum feedwater temperature at HRSG</td>
<td>K</td>
<td>333.15</td>
</tr>
<tr>
<td>overall heat transfer coefficient</td>
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<td></td>
</tr>
<tr>
<td>economizer</td>
<td>W/m² K</td>
<td>42.6</td>
</tr>
<tr>
<td>evaporator</td>
<td>W/m² K</td>
<td>43.7</td>
</tr>
<tr>
<td>superheater</td>
<td>W/m² K</td>
<td>50</td>
</tr>
</tbody>
</table>

Complete mathematical model used for the CO2 capture process was recently presented in Mores et al.34 (stand-alone process). In addition, the models used for each piece of equipment of the HRSG were presented in Manassaldi et al.5 with the only difference being that no discrete decisions are considered in the actual models. In other words, the models previously developed for the economizer, evaporator, and superheater are properly connected in order to model the HRSG configuration illustrated in Figure 1. The main model constraints of the CO2 capture plant and NGCC are presented in Appendix A. The more important assumptions used to derive the resulting models are presented below.

3.1. Postcombustion CO2 Capture Plant. Flue gas is cooled down by a direct contact cooler (CT1) with a spray of water at 298 K. During the cooling process, water is recovered from the flue gas because of condensation. Finally, a blower (B1) increases the pressure of the cooled flue gas to a pressure above the atmospheric level, to balance the pressure losses in the capture plant. In the CO2 postcombustion capture process based on amine scrubbing, the CO2 of the flue gas is chemically absorbed by a 30% MEA solution in an absorption tower (ABS). The resulting rich solvent is regenerated in a stripper unit (STP1) by means of its associated reboiler (R1), while the lean solvent is thermally conditioned (AC1, EC4) and sent back again to the absorption process within a closed loop; the stripping gas is condensed (C2) and refluxed to the regeneration column, and the CO2 concentrated gas stream is divided into “z” units (model parameter) which allow one to compute profiles of temperatures, flow rates, and compositions along columns by means of mass and energy balances and considering mass transfer with chemical reaction phenomena conforming to a rate-based model. On the other hand, condenser and reboiler are modeled as equilibrium stages.
(2) The CO$_2$ contained in the exhaust flue gas stream coming from the two HRSGs reacting with a 30% (w/w) MEA solution with the following scheme of reactions R1−R7:

\[
\begin{align*}
2\text{H}_2\text{O} & \leftrightarrow \text{H}_2\text{O}^+ + \text{OH}^- \\
2\text{H}_2\text{O} + \text{CO}_2 & \leftrightarrow \text{H}_2\text{O}^+ + \text{HCO}_3^- \\
\text{H}_2\text{O} + \text{HCO}_3^- & \leftrightarrow \text{H}_2\text{O}^+ + \text{CO}_3^{2-} \\
\text{H}_2\text{O} + \text{MEA}^+ & \leftrightarrow \text{H}_2\text{O}^+ + \text{MEA} \\
\text{MEACOO}^- + \text{H}_2\text{O} & \leftrightarrow \text{MEA} + \text{HCO}_3^- \\
\text{MEA} + \text{CO}_2 + \text{H}_2\text{O} & \leftrightarrow \text{MEACOO}^- + \text{H}_2\text{O}^+ \\
\text{CO}_2 + \text{OH}^- & \leftrightarrow \text{HCO}_3^- 
\end{align*}
\]

(R1–R7)

R1−R5 are equilibrium reactions. R6 and R7 are considered as pseudo first order reactions with the aim to compute the effect of kinetic reaction on the mass transfer phenomena through the enhancement factor.

(3) The superficial gas velocity is limited between 70% and 80% of the flooding velocity in order to compute the diameter of absorber and stripper columns. The number of transfer units (NTU)-transfer unit height (HTU) concept is employed to compute column heights.

(4) On the basis of a maximum column diameter of 12.8 m, six parallel capture trains (model parameter) are assumed in this paper in order to treat the NGCC exhaust combustion gases.

(5) The maximum reboiler temperature, to avoid amine degradation and equipment corrosion, is 393 K.

(6) Dependence of solubilities, densities, viscosities, diffusivities, fugacity coefficients, and enthalpies with the temperature and composition, pressure drops along the absorber and regenerator units, and liquid and mass transfer coefficients, among others, are computed by using the state-of-the-art correlations listed in Table 1.

(7) The compression stage design is based on a 450 K maximum temperature limit and a maximum compression ratio of 3. It is assumed that the stages have equal compression ratios, which are optimization variables. In this way, a train with four intercooled centrifugal compressors (model parameter) is necessary to achieve the CO$_2$ compression pressure (8.6 MPa). Then, the dense phase stream is pumped up to 14 MPa to allow an efficient transportation. Water is removed during the cooling process and is sent back to the capture plant to diminish water losses.

(8) Regarding the computation of heat transfer areas, the following hypotheses are considered: (1) the overall heat transfer coefficients are constant throughout the exchanger; (2) heat losses and pressure drops are negligible; and (3) geometry and fouling are not taken into account.

3.2. Natural Gas Combined Cycle Plant. The following are the main hypotheses corresponding to the NGCC plant: (1) Pure methane is assumed as fuel. (2) The pressure ratio in the air compressors and the expander of the gas turbines are fixed. (3) Correlations taken from Poling et al. are used to describe the dependence of the thermodynamic properties of ideal gases with temperature and pressure. (4) Complete
combustion with excess of air is assumed; thus CO₂, H₂O, O₂, and N₂ are the components of the combustion gases stream. (5) Regarding the HRSG design, the following assumptions are considered: (a) unfired equipment; (b) constant overall heat transfer coefficients; (c) pressure drops in the water or steam sides are neglected; (d) geometry and fouling are not taken into account; (e) Chen approximation⁴⁷ is used to compute heat transfer areas; (f) correlations taken from IPWS 97⁴⁸ are used to compute the thermodynamic properties of steam and water. (6) A single deareator is considered. It may be fired by the following three alternatives: steam (stream #33) and/or by hot water streams (stream #15).

On the basis of the assumptions described, the mathematical model has been proposed. Table 2 lists the main optimization variables for both plants. The complete mathematical model involves approximately 3600 variables and 3750 constraints (equality and inequality constraints). It was implemented in the General Algebraic Modeling System (GAMS⁴⁹) which is a high-level modeling system for mathematical programming and optimization. The generalized reduced gradient algorithm CONOPT 3.0 was here used as the NLP solver.⁵⁰

<table>
<thead>
<tr>
<th>unit</th>
<th>ref-Case</th>
<th>OPTIM</th>
<th>ref-Case1</th>
<th>SUB-OPT1</th>
<th>ref-Case2</th>
<th>SUB-OPT2</th>
<th>SUB-OPT3</th>
</tr>
</thead>
<tbody>
<tr>
<td>thermal efficiency</td>
<td>%</td>
<td>60.1</td>
<td>51.7</td>
<td>59.3</td>
<td>50.9</td>
<td>59.5</td>
<td>48.7</td>
</tr>
<tr>
<td>net power output</td>
<td>MW</td>
<td>875.6</td>
<td>752.5</td>
<td>862.6</td>
<td>741.6</td>
<td>866.8</td>
<td>708.9</td>
</tr>
<tr>
<td>total electricity produced in GT</td>
<td>MW</td>
<td>1109</td>
<td>752.5</td>
<td>862.6</td>
<td>741.6</td>
<td>866.8</td>
<td>708.9</td>
</tr>
<tr>
<td>total electricity produced in ST</td>
<td>MW</td>
<td>238.2</td>
<td>222.0</td>
<td>285.8</td>
<td>211.2</td>
<td>288.5</td>
<td>179.5</td>
</tr>
<tr>
<td>electricity required in NGCC</td>
<td>MW</td>
<td>531.4</td>
<td>531.9</td>
<td>532.0</td>
<td>532.1</td>
<td>530.5</td>
<td>530.9</td>
</tr>
<tr>
<td>electricity required in capture plant</td>
<td>MW</td>
<td>0</td>
<td>46.39</td>
<td>0</td>
<td>46.36</td>
<td>0</td>
<td>48.57</td>
</tr>
<tr>
<td>total heat transfer area in HRSG (10³)</td>
<td>m²</td>
<td>4.14</td>
<td>4.02</td>
<td>3.77</td>
<td>3.48</td>
<td>3.66</td>
<td>2.30</td>
</tr>
<tr>
<td>total heat duty in HRSG</td>
<td>MW</td>
<td>351.6</td>
<td>340.9</td>
<td>333.4</td>
<td>348.8</td>
<td>346.2</td>
<td>362.9</td>
</tr>
<tr>
<td>fuel consumption</td>
<td>kmol/s</td>
<td>1.81</td>
<td>=</td>
<td>=</td>
<td>=</td>
<td>=</td>
<td>=</td>
</tr>
<tr>
<td>steam used in CO₂ capture plant</td>
<td>kg/s</td>
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<td>0</td>
<td>144.7</td>
<td>0</td>
<td>143.2</td>
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<tr>
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<td>28.35</td>
<td>1.02</td>
<td>28.94</td>
<td>1.45</td>
<td>26.03</td>
</tr>
<tr>
<td>number of iterations</td>
<td></td>
<td>191</td>
<td>4884</td>
<td>190</td>
<td>5012</td>
<td>230</td>
<td>4794</td>
</tr>
</tbody>
</table>

⁴⁷, same value that corresponds to the ref-Case.
In general, mathematical programming environments such as GAMS and AMPL have shown to be powerful tools, especially when the optimization problem is large, combinatorial, and highly nonlinear. Thus, the benefits of the mathematical programming techniques (equation-oriented modeling tools) are here exploited for the simultaneous optimization of not only the operating conditions and sizes of process units but also the process arrangement.

One of the main advantages of the resulting model is that it does not involve integer variables. Certainly, the flow-sheet proposed in Figure 1 is modeled as a NLP model instead of a MINLP model.

4. DISCUSSION OF RESULTS

The numerical values of all parameters used in all optimization runs for the CO$_2$ capture plant and NGCC are listed in Tables 3 and 4, respectively.

First, the mathematical model is solved to find the best configuration that integrates both processes in such a way that maximizes the overall thermal efficiency. As a result, not only is the best configuration obtained but also the optimal operating conditions and size of each one of the pieces of equipment. This configuration will be hereafter denoted as OPTIM. The model is then used to solve the same optimization problem but for different configurations in comparison to the OPTIM. This will allow one to perform qualitative and quantitative comparisons between suboptimal solutions which will be hereafter denoted as SUB-OPT1, SUB-OPT2, and SUB-OPT3. In addition, for a more complete presentation of results, optimal designs and operating conditions of a NGCC plant without carbon capture are used as reference cases and are compared to the corresponding integrated plants (NGCC plants with carbon capture). Precisely, the following three reference cases are included: (1) ref-Case to be compared with OPTIM. Thus, ref-Case involves the same configuration of NGCC obtained in OPTIM but without CO$_2$ capture; (2) ref-Case1 to be compared with SUB-OPT1; and (3) ref-Case2 to be compared with SUB-OPT2 and SUB-OPT3.

Before proceeding to discuss the results, it is opportune to point out that the obtained results reveal that, for given levels of CO$_2$ recovery and electricity demands, the operating conditions and sizes of process units of the NGCC plant vary much more than those of the CO$_2$ capture plant. In other words, despite the fact that the mathematical model of the CO$_2$ capture process involves many optimization variables, the flow rate of the exhaust gases and the steam required in the amine regeneration process, which are the main variables that couple both processes, do not vary significantly with different types of NGCC configurations, for given levels of CO$_2$ recovery and electricity generation. For this reason, the discussion of the results puts more emphasis on the NGCC than on the CO$_2$ capture process. However, numerical values of the main variables of the CO$_2$ capture system are also presented and analyzed.

Figure 2 shows the optimal configuration (OPTIM) indicating how both processes should be integrated in order to maximize the overall thermal efficiency. Also, Figure 2 includes the numerical values of flow rate, pressure, and...
temperature per stream, as well as the heat transfer area in each economizer, evaporator, and superheater and the amount of electricity produced in each one of the turbines (gas and steam turbines). For comparison purposes, the reference case (ref-Case) that corresponds to OPTIM is presented in Figure 3.

On the other hand, Table 5 lists the corresponding values of the total electricity produced and consumed in each process as well as the required heat transfer area and fuel consumption, for both OPTIM and ref-Case solutions. The rest of the columns refer to the optimal values that correspond to the configurations of SUB-OPT1, SUB-OPT2, and SUB-OPT3 including the corresponding reference cases. Similarly, Table 6 lists the obtained values for the CO2 capture process for each one of the configurations.

As it can be seen in Figure 2, the steam required by the CO2 capture process is provided by both the evaporator EV1 of the HRSG (24.0%) and the steam turbine IP-LP ST (76.0%), and the total amount of steam extracted from both pieces of equipment are, respectively, 34.3 kg/s (17.15 kg/s each evaporator) and 110.3 kg/s. The OPTIM configuration reaches a maximal overall thermal efficiency of 51.7%, and it requires a fuel consumption of 1.81 kmol/s and 4.0 \times 10^5 m^2 of the total heat transfer area in the HRSG. The total electricity produced in the gas turbines (2) and in the steam turbine (1) are, respectively, 1109.0 and 222.0 MW while the electricity required in the NGCC and capture plant is 531.9 and 46.4 MW. The variables related to the gas turbines (temperature, fuel and air consumptions, maximum electricity generation) reach their upper bounds indicating that they operate at full loads (290 MW each one). The obtained results showed that this characteristic (full load) does apply not only for OPTIM but also for all optimization runs (suboptimal solutions and reference cases).

A comparison of the values illustrated in Figures 2 and 3 and also reported in Table 5 indicates that the overall efficiency of the NGCC with CO2 capture (OPTIM) is 8.4% lower compared to the reference case (ref-Case) (51.7% vs 60.1%). The obtained efficiencies in both cases are in accordance with values reported by other authors.44,51

As mentioned earlier, the model was also solved for three suboptimal configurations in order to perform a comparison with the OPTIM with the main objective to show how the overall thermal efficiency is affected by different electricity plant configurations. In addition, each suboptimal solution is compared with its corresponding reference cases (ref-Case1 and ref-Case2). The first suboptimal configuration proposed was SUB-OPT1 in which the total steam required by the reboiler of the CO2 capture process is only taken from the steam turbine IP/LP ST. Therefore, in order to solve the model for the SUB-OPT1 configuration, the possibility to take steam from the evaporator EV1 should be removed. For this, it was necessary to fix the value of the steam coming from EV1 at zero. Similarly, the SUB-OPT2 configuration in which the total steam required by the reboiler of the CO2 capture process is only taken from the evaporator EV1 was considered. In contrast to the previous one, the variable value related to the steam extracted from IP ST was fixed at zero. The optimal solutions corresponding to the fixed configurations of

---

**Figure 5.** Optimal solution corresponding to the reference case, ref-Case1. ∗: Optimal values that reached their lower/upper bound.
SUB-OPT1 and SUB-OPT2 including the reference cases are illustrated from Figures 4, 5, 6, and 7.

According to Table 5, the thermal efficiency of SUB-OPT1 is 50.9% which is only 0.8% lower than OPTIM. Despite the fact that in both configurations the gas turbines operate at full loads, the total net electricity generation for SUB-OPT1 is only 1.4% lower than that generated in OPTIM. However, significant differences in the flow rates, pressures, temperatures, and sizes of process units between OPTIM and SUB-OPT1 are observed. By comparing Figure 2 with Figure 4, it is possible to conclude the fact that the possibility of extracting steam from EV1 has been removed; the flow rate of the working fluid in each steam turbine HP ST and IP ST increased up to 180.7 and 227.8 kg/s, respectively, which represents an increase of 9.3% and 15.1% over that of the previous configuration (OPTIM), while the flow rate of steam in LPST decreases by 5.1%. The IP operating pressure is 80.7% lower than that in OPTIM (0.75 MPa vs 3.89 MPa) while HP and LP levels are equal, 16 and 0.29 MPa, respectively. In both cases, the operating pressure on the HP steam turbine reaches the upper bound defined on the model (16 MPa). The obtained results presented in Figures 2 and 4 and also listed in Table 5 reveal that the total electricity produced in the steam turbines in SUB-OPT1 is 211.2 MW, which is 10.8 MW lower than that produced in OPTIM. Regardless, with the total heat transfer area in the HRSG, SUB-OPT1 requires 3.5 × 10^5 m² which represents a decrease of 13.3% compared to OPTIM.

On the other hand, Figure 6 shows the results obtained for the SUB-OPT2 configuration in which the steam used as the heating utility in the CO₂ capture system is only produced and extracted from the evaporator EV1 of the HRSG. As shown, the optimal solution removes the pump (P5), economizer (EC3), evaporator (EV2), economizer (EC5), and superheater (SH1) when the possibility to extract steam from the steam turbine IP ST is avoided. The thermal efficiency of SUB-OPT2 is 48.7%, which is about 3.0% and 2.2% lower than OPTIM and SUB-OPT1, respectively. The net electricity generation for SUB-OPT2 is 5.8% lower than that for OPTIM while the energy penalty of the capture plant increases by about 4.7%. The electricity required by the NGCC remains almost constant. The total electricity generated by the HP and IP steam turbines is 37.8% lower than that generated in OPTIM because of the lower steam flow rates in the ST. Regarding the low pressure steam turbine, it is observed that, with the SUB-OPT2 arrangement, the electricity production is 46.9% greater than that with the OPTIM configuration mainly due to a better steam quality. On the other hand, in spite of the HRSG heat duty increases (6.5% compared to the OPTIM case), the heat transfer area decreases (42.7%). This can be explained due to the fact that the flue-gas temperature that leaves the HRSG is 5 K lower compared to that in the OPTIM, resulting in a higher log mean temperature difference and therefore in a lower heat transfer area. In particular, 52.7% of the total heat transfer area in each HRSG is used to generate the vapor required by the CO₂ capture plant.

Finally, a third SUB-OPT3 configuration is presented in Figure 8 in order to show how the optimal solution varies when the PS, EC3, EV2, ECS, and SH1 are included. Precisely, the
model used to obtain the SUB-OPT2 configuration is again solved but includes a lower bound (15 kg/s) in the flow rate of stream 25 (see Figure 8). As expected, the optimal value of this variable reached the imposed lower bound. As shown in Figure 8, a similar behavior to that discussed for SUB-OPT2 is observed for SUB-OPT3. Despite the fact that the thermal efficiency in both configurations remains almost constant (48.7% vs 48.4%), it is observed that the new distribution of pressures, temperatures, and flow rates leads to a decrease in the total heat transfer area in HRSG from $2.3 \times 10^5$ to $2.28 \times 10^5$ m$^2$. For instance, the temperature of the flue gas leaving the HRSG for SUB-OPT3 is 3 K cooler than that for SUB-OPT2 which increases the temperature driving force, resulting in lower heat transfer area.

According to the obtained results, SUB-OPT2 and SUB-OPT3 are the configurations with the lowest thermal efficiency and their operating conditions and sizes of the process units differ considerably from the remaining configurations. This is due to the degree-of-freedom involved in each optimization problem. In fact, the model that comprises the highest number of constraints related with the process arrangement is SUB-OPT3. In contrast to this, the model that involves the lowest number of constraints related with the process configuration is OPTIM. Thus, as expected, the thermal efficiency decreases with the increase of the number of constraints on the HRSG diagram.

The differences between SUB-OP1 with ref-Case1 and SUB-OPT2 and SUB-OPT3 with ref-Case2 can be observed by comparing Figure 4 with Figure 5 and Figure 6 with Figure 7, respectively. Table 6 lists the optimal values of the main variables of the CO2 capture plant for each NGCC configuration. As it was mentioned earlier, it can be observed that, despite the variables listed in the table are considered as optimization variables of the model, the results show that only some of them vary. Certainly, the heat duty in the reboiler, the compression work, absorber, and stripper height (and pressure drops) as well as the heat transfer areas of condenser, economizer, reboiler, and compression coolers are the main design variables that change with the type of configuration. Moreover, the amine flow rate and the CO2 loading in rich and lean solutions vary slightly, between 0.5% and 3.5%. The variation of these variables is mainly due to the change of the outlet temperature of flue gas in the HRSG and steam temperature which have an impact on the design and operation conditions of the CO2 capture plant. For instance, the comparison between SUB-OPT2 with OPTIM reveals that the decrease of the outlet temperature of the flue gas at the HRSG for SUB-OPT2 leads to a decrease of the heat duty required by the reboiler by about 2.0% while the electricity required by the compressors, pumps, and blower increases by about 4.7%. In addition, the packing volumes of absorption and regeneration columns increase, respectively, by 9.0% and 3.6%. This result reflects one of the strong trade-offs between operating conditions and dimensions.

The obtained results showed that the thermal efficiency varied from 51.7% (OPTIM) to 48.4% (SUB-OPT3). The configuration with the highest efficiency (OPTIM) involves the highest electricity production in the steam turbine as well as the lowest total electricity penalties, but it requires the highest heat transfer area. In contrast to this, the configuration with the
lowest efficiency (SUB-OPT3) involves the lowest electricity production, but it requires the lowest exchange area. However, it should be noted that, although the operating conditions and sizes of process units of OPTIM and SUB-OPT1 are quite different, their thermal efficiencies are similar. The results clearly show that the final process configuration, design, and operating conditions should be made in terms of the total investment and operating costs.

4.1. Computational Implementation Aspects. Because of the fact that the resulting model involves many non-convexities (bilinear terms in mass and energy balances), special emphasis has been put on the scaling of variables and equations. All of the constraints and variables have been scaled in such a way that their magnitudes range from $10^{-3}$ to $10^3$. In addition, a systematic and simple, but robust, initialization procedure was employed to guarantee the model convergence. From a basic set of variables, it is possible to initialize the remaining variables using the same equality constraints involved by the model. Thus, the proposed procedure minimizes the number of infeasible constraints in the first iteration and guarantees that one can find a feasible initial solution in a few number of iterations. For instance, the initialization phase can be briefly explained as follows. Equation 2 is used to calculate the enthalpy for the reheat steam ($h_1$) in terms of the pressure $P$ and temperature $T$:

\[ h_1 = RT \left( \frac{1386}{T} \right) \sum_{k=1}^{34} n_k \left( 7.1 - \frac{P}{165.5} \right)^{\frac{1386}{T} - 1.222} \]  

(2)

Once the initial values for $P$ and $T$ are provided by the user, the same eq 2 is used for the initialization of $h_1$. On the basis of the above procedure, the full variable vector of the CO2 capture plant and NGCC has been initialized. Despite the fact that different initial values were used for the basic variables involved in the initialization phase, the same optimal solutions were obtained. Thus, the proposed procedure and optimization problems were solved at a relatively low computational cost (few iterations and short computational times). Thus, they proved to be robust and flexible, achieving convergence in all the optimizations made. However, global optimal solutions cannot be guaranteed due to the nonconvex constraints involved in the mathematical model, specially the presence of bilinear terms involved in mass and energy balances.

5. CONCLUSION AND FUTURE WORK

A detailed NLP mathematical model is used to determine the optimal design and operating conditions of an integrated plant of NGCC and postcombustion CO2 capture. Precisely, it determines how the NGCC plant and CO2 capture process should be integrated to maximize the overall efficiency which is defined in terms of total electricity generated and fuel consumption. The best integration configuration is selected from three alternative arrangements, and the operating conditions and size of each process unit are determined simultaneously. As a result, it was found that the OPTIM configuration, in which the steam required in the CO2 capture process is partially extracted from an intermediate pressure steam turbine and from an evaporator of the HRSG, is
Table 6. Optimal Solutions of the CO₂ Capture Plant for Each NGCC Configuration

<table>
<thead>
<tr>
<th></th>
<th>OPTIM</th>
<th>SUB-OPT1</th>
<th>SUB-OPT2</th>
<th>SUB-OPT3</th>
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<td><strong>Flue Gas Conditions</strong></td>
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<tr>
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<td>327.8</td>
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<td>=</td>
<td>=</td>
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<td>=</td>
<td>=</td>
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<td>=</td>
<td>=</td>
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<tr>
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</table>

*Optimal values that reached their lower/upper bound. $^b$ = same value that corresponds to OPTIM.

preferred when the thermal efficiency is maximized. Optimal and suboptimal configurations were compared. One of the qualitative results reveals that the configuration with the highest efficiency (OPTIM) involves the highest electricity production and the lowest requirement of electricity required by pumps, blowers, and compressors, but it requires the highest heat transfer area. In contrast to this, the arrangements with lower efficiencies (SUB-OPT1, SUB-OPT2, and SUB-OPT3) involve lower total heat transfer area and electricity production and higher requirements of electricity to supply to mechanical devices. The numerical results clearly show that the final process configuration, design, and operating conditions should be made in terms of the total investment and operating costs.

The proposed model is being extended to include a detailed cost model in order to minimize the total annual cost. In addition, other alternative configurations are also being included. For instance, the number of NGCC (gas turbines and heat recovery steam generators) and the CO₂ capture trains will be optimization variables. This will increase the number of combinations, and it may still be possible to improve the overall thermal efficiency. The need of a MINLP model for cost minimization will depend on how the investment costs of process units are computed. For instance, if fixed costs are included, then it will be necessary to extend the proposed NLP model to a MINLP model. To the knowledge of the authors, this extension can be easily considered.

APPENDIX A: MATHEMATICAL MODEL DESCRIPTION

A1. CO₂ Capture Plant

Packed columns are considered for the CO₂ absorption and amine regeneration. For modeling purposes, both units are modeled as a cascade of non-equilibrium stages with chemical reactions, which allow one to compute profiles of temperatures, flow rates, and compositions along the column. In each stage, denoted as $z$, the gas stream goes up into stage $z$ from stage $z - 1$ and the liquid stream flows down into stage $z$ from stage $z + 1$, as can be seen in Figure A1. The total number of stages is assumed to be known (model parameter). The first stage ($z = 1$) refers to the bottom of the columns, and the last stage ($z = 10$) denotes the top of the columns.

Thus, the mass and energy balances can be described from eqs A1 to A6.

\[ m_{Lz+1} - m_{Lz} + m_{Gz-1} - m_{Gz} = 0 \]  
\[ m_{Lz+1} H_{Lz+1} - m_{Lz} H_{Lz} + m_{Gz-1} H_{Gz-1} - m_{Gz} H_{Gz} + (\Delta H_R) = 0 \]

where $m_L$, $m_G$, $H_L$, and $H_G$ refer to the liquid (amine solution) and vapor flow rates and enthalpies, respectively. \( \Delta H_R \) and \( \Delta H_L \) are the heat released by the reaction and vaporization heat of water.

\[ m_{Lz+1} x_{Lz+1} - m_{Lz} x_{Lz} + m_{Gz-1} y_{Gz-1} - m_{Gz} y_{Gz} = 0 \]
\[ \sum_j y_{Lz} = 1 \]
\[ j = CO_2, H_2O, N_2, O_2 \]
\[ \sum_i x_{Lz} = 1 \]
\[ i = CO_2, H_2O, MEA \]

\[ \text{[MEA}^+] + [\text{H}_2\text{O}] = [\text{MEACOO}^-] + [\text{HCO}_3^-] + 2[\text{CO}_3^{2-}] + [\text{OH}^-] \]

where \([i]_z\) is the molar concentration of specie “i” in stage “z”. Moreover, the liquid and gas phases are considered to be well-mixed, and consequently, there are no concentration and temperature gradients in single liquid and gas phases.

On the other hand, the Kent–Eisenberg model is used to describe the vapor–liquid equilibrium and the chemical equilibrium of the CO₂–water–MEA system. The relationships
of the equilibrium constants of reactions R1–R5 with the temperature and composition are as below:

\[
2\text{H}_2\text{O} \leftrightarrow \text{H}_2\text{O}^+ + \text{OH}^- \quad (R1)
\]

\[
2\text{H}_2\text{O} + \text{CO}_2 \leftrightarrow \text{H}_2\text{O}^+ + \text{HCO}_3^- \quad (R2)
\]

\[
\text{H}_2\text{O} + \text{HCO}_3^- \leftrightarrow \text{H}_2\text{O}^+ + \text{CO}_2^{2-} \quad (R3)
\]

\[
\text{H}_2\text{O} + \text{MEA}^+ \leftrightarrow \text{H}_2\text{O}^+ + \text{MEA} \quad (R4)
\]

\[
\text{MEACOO}^- + \text{H}_2\text{O} \leftrightarrow \text{MEA} + \text{HCO}_3^- \quad (R5)
\]

The forward constants \( k_{i,\text{CO}_2|\text{MEA}} \) and \( k_{i,\text{CO}_2|\text{OH}} \) of the parallel and kinetically controlled reactions R6 and R7 are taken from Kucka et al.\(^{56}\) and Aboudheir et al.\(^{57}\)

Regarding to column sizing, it should be mentioned that dimensions of both columns are considered as optimization variables. Certainly, the heights and diameters of both columns and the operating conditions are optimized simultaneously. The column height \( h \) is given by eq A12 using the HTU–NTU concept while the column diameter \( D \) is determined by restricting the gas velocity between 60% and 80% of gas flooding velocity \( (u_{fl}) \).

\[
h = \sum_{z=1}^{z=10} h_z = \sum_{z=1}^{z=10} \text{HTU}_z \text{NTU}_z \quad (A12)
\]

\[
\text{NTU}_z = -\ln (1 - \eta_z) \quad (A13)
\]

\[
\eta_z = \frac{m_G'y_z - m_G'y_{z-1}}{m_G'y_z - m_G'y_{z-1}} \quad (A14)
\]

\[
\text{HTU}_z = \frac{m_G'z}{RT_G'k_G'z\rho_G'z} + \lambda_z \left( \frac{m_G'z}{k_L'z\rho_L'zE_z} \right) \quad (A15)
\]

As was mentioned, the liquid and gas phases are considered to be well-mixed and, consequently, punctual efficiency can be set equal to the Murphree’s efficiency \( (\eta) \). The number of transfer units (NTU) can be computed through eq A13. The transfer unit height (HTU) is given by eq A15 where \( m_G'z \) and \( m_G'y_z \) are gas and liquid mass velocities, \( \rho_G' \) and \( \rho_L' \) are gas and liquid mass densities; \( k_G \) and \( k_L \) denote the stripping factor and the gas-side and liquid-side mass transfer coefficients, respectively. Effective interfacial area \( (a) \), computed by using Onda et al.\(^{55}\) equations, depends on packing type, operating conditions, and gas and liquid physical and chemical properties.

The diameter of the column on each stage is computed as follows:

\[
D_z^2 = \frac{4m_G'z}{u_{fl}z'\rho_G'z'} \quad (A16)
\]

\[
0.6 \leq f_z \leq 0.8 \quad (A17)
\]

\[
D_z = D_{z+1} \quad z = 1, 2, ..., 9 \quad (A18)
\]

In order to avoid the flooding problem and a bad gas–liquid distribution, the restriction on the gas velocity by using the flooding factor \( (f) \) is considered while eq A18 is used to ensure the same diameter in all stages. The flooding velocity to random packing is computed by using Leva\(^{58}\) correlations.

Pressure drop along the absorber and regenerator units is considered through eq A19.

\[
P_z = \Delta P h_z \quad (A19)
\]

where \( h_z \) is the height of the stage, which is an optimization variable, and \( \Delta P \) is the specific pressure drop \( (\text{kPa/m}) \) which is estimated by using Robbins\(^{59}\) correlation. It takes into account the pressure drop due to the dry packing and due to the liquid presence. It depends on liquid and gas flow rates, liquid and gas densities, liquid viscosity, gas velocity, and the dry packing factor.

Reboiler and condenser are considered as equilibrium stages. Thus, similar constraints previously listed are used to model both units.

Finally, transport property models (viscosity, density, diffusivity, and surface tension) among others, are required to compute column dimensions, pressure drops, mass transfer, and interfacial area correlations. These properties are computed on the basis of correlations reported in the literature and were previously listed in Table 1. The mathematical model also involves constraints related to the heat exchangers (economizer and MEA cooler and intercoolers), blowers, pumps, and compressors.
A2. NGCC Power Plant

A description of the main constraints used for modeling the NGCC power plant are presented.

A2.1. Gas Cycle. The scheme of a gas turbine unit is shown in Figure A2. Based on the hypotheses previously described in Section 3.2, the following constraints are given by eqs A23 and A24, which relate to the compressor and expander works, respectively, and LHV denotes the lower heating value of fuel.

\[ m_{G}^{38}H_{G}^{38} + W_{\text{comp}} = m_{G}^{38}H_{G}^{38} \quad \text{(A20)} \]
\[ m_{G}^{38}(H_{G}^{38} - H_{G}^{298}) = m_{G}^{38}H_{G}^{38} + m_{G}^{38} - H_{G}^{298}(1 + \text{LHV}) \quad \text{(A21)} \]
\[ m_{G}^{38}H_{G}^{38} = m_{G}^{38}H_{G}^{38} + W_{\text{exp}} \quad \text{(A22)} \]

where \( m_{G} \) and \( H_{G} \) are the mass flow rate and enthalpy of a gas stream (fuel, air, or combustion gases); \( W_{\text{comp}} \) and \( W_{\text{exp}} \) represent the compressor and expander works, respectively, and LHV denotes the lower heating value of fuel.

The compressor and expander discharge temperatures, which depend on the pressure ratio \( (P_{\text{ratio}}) \) and the isentropic efficiency \( (\eta_{\text{comp}}) \), are given by eqs A23 and A24 and denoted as \( T_{38} \) and \( T_{39} \), respectively. Finally, the net power obtained from the gas turbine \( (W_{GT}) \) is given by eq A25.

\[ T_{G}^{38} = T_{G}^{37} + \frac{T_{G}^{37}}{\eta_{\text{comp}}} \left[ (P_{\text{ratio}})^{\gamma-1} - 1 \right] \quad \text{(A23)} \]
\[ T_{G}^{39} = T_{G}^{38} - \frac{1}{\eta_{\text{exp}}} \left[ 1 - (P_{\text{ratio}})^{\gamma-1} \right] \quad \text{(A24)} \]
\[ W_{GT} = W_{\text{exp}} - W_{\text{comp}} \quad \text{(A25)} \]

A2.2. Steam Cycle. The following constraints included to model the steam turbines (Figure A3) are formulated under the assumptions listed in Section 3.2.

\[ m_{W}^{n}H_{W}^{n} = m_{W}^{o}H_{W}^{o} + W_{ST} \quad \text{(in = 1, 5, 8; out = 2, 6, 12, 7)} \quad \text{(A26)} \]
\[ H_{W}^{n} - H_{W}^{o} = \eta_{ST}(H_{W}^{n} - H_{W}^{id}) \quad \text{(A27)} \]
\[ S_{W}^{n} = S_{W}^{id} \quad \text{(A28)} \]
\[ P_{W}^{id} = P_{W}^{out} \quad \text{(A29)} \]

where \( m_{W}, H_{W}, S_{W}, \) and \( P_{W} \) are the flow rate, enthalpy, entropy, and pressure of water, respectively; the superscript id denotes the isentropic evolution of the steam turbine.

Energy balances and design constraints in each HRSG heat exchanger unit \( (HE = EC1, EC2, EC3, EV1, EV2, EV3, SH1, SH2, SH3) \) are given by eqs A30–A40 (Figure A4).

\[ Q_{HE} = (m_{W}^{o} - m_{W}^{o})_{HE} \quad \text{(A30)} \]
\[ Q_{HE} = (m_{W}^{o} - m_{W}^{o})_{HE} \quad \text{(A31)} \]
\[ \Delta T_{HE}^{\in} = (T_{G}^{in} - T_{W}^{in})_{HE} \quad \text{(A32)} \]
\[ \Delta T_{HE}^{out} = (T_{G}^{out} - T_{W}^{out})_{HE} \quad \text{(A33)} \]
\[ Q_{HE} = (UALMTD)_{HE} \quad \text{(A34)} \]

The Chen approximation \( \gamma \) (eq A35) is used to overcome numerical difficulties with the logarithmic mean temperature difference (LMTD). Moreover, with the aim to avoid a temperature cross situation and to ensure reasonable practical values of the HRSG heat transfer area, a pinch point temperature difference \( (\Delta T_{\text{pinch}}) \) is given by eq A36.

\[ \text{LMTD}_{HE} = \frac{\Delta T_{HE}^{\in} \Delta T_{HE}^{out} \left( \Delta T_{HE}^{in} + \Delta T_{HE}^{out} \right)}{2} \quad \text{(A35)} \]

\[ \Delta T_{HE}^{\in, out} \geq (\Delta T_{\text{pinch}})_{HE} \quad \text{(A36)} \]

In the evaporator’s model, the inlet water temperature \( (T_{W}^{in}) \) is given by eq A37 while the outlet \( (T_{W}^{out}) \) is the saturated steam condition (eq A38). A fixed value for the approach point \( (Ap) \) is defined in order to guarantee no water evaporation in the economizers which would cause tube erosion and other problems.

\[ (T_{W}^{in} = T_{W}^{in} - Ap)_{HE} \quad HE = EV_{1}, EV_{2}, EV_{3} \quad \text{(A37)} \]
\[ (T_{W}^{out} = T_{W}^{out} - Ap)_{HE} \quad HE = EV_{1}, EV_{2}, EV_{3} \quad \text{(A38)} \]
\[ (T_{W}^{in, out} \leq T_{W}^{in, out})_{HE} \quad HE = EC_{1}, EC_{2}, EC_{3} \quad \text{(A39)} \]
\[ (T_{W}^{in, out} \geq T_{W}^{in, out})_{HE} \quad HE = SH_{1}, SH_{2}, SH_{3} \quad \text{(A40)} \]
A3. Coupling Constraints

Finally, the modeling also includes mass and energy balances in the following integration points: (a) exhaust gas to feed the capture plant (M2), (b) steam extracted from the NGCC power plant (mixer M1 and reboiler R1), and (c) condensate returned to the deareator (D) from the reboiler.

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Notes

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■ NOMENCLATURE

\[ D \] diameter
\[ f \] flooding factor
\[ \text{GT} \] gas turbine
\[ \text{IP} \] intermediate pressure
\[ \text{LHV} \] lower heating value of fuel
\[ \text{LP} \] low pressure
\[ H \] enthalpy
\[ \text{HP} \] high pressure
\[ \text{HRSG} \] heat recovery steam generator
\[ \text{HTU} \] transfer unit height
\[ \text{LMDT} \] logarithmic mean temperature difference
\[ \text{MEA} \] monoethanolamine
\[ \dot{m}_{\text{fl}} \] fuel flow rate
\[ \text{CT} \] number of \( \text{CO}_2 \) capture trains
\[ \text{NGCC} \] natural gas combined cycle
\[ N_p \] number of pumps
\[ N_{\text{NTG}} \] number of steam turbines
\[ N_{\text{NTU}} \] number of transfer units
\[ P \] pressure
\[ \text{PSA} \] pressure swing adsorption
\[ Q \] heat load
\[ S \] entropy
\[ \text{ST} \] steam turbine
\[ \text{TSA} \] temperature swing adsorption
\[ W \] electric power

Superscripts

\[ \text{CP} \] capture plant
\[ \text{PP} \] power plant

Subscripts

\[ B \] blower
\[ \text{C} \] compressor
\[ \text{GT} \] gas turbine
\[ \text{P} \] pumps
\[ \text{ST} \] steam turbine

Greeks Symbols

\[ \eta_{\text{gen+cap}} \] thermal efficiency

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