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Effect of Flue Gas Composition on the Design of a CO₂ Capture Plant

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Abstract

According to studies conducted by the International Energy Agency, the energy sector is the biggest producer of greenhouse gas emissions (CO_2), having important environmental consequences. Various alternatives have been sought to reduce CO_2 emissions during electric production, highlighting as an alternative, the implementation of CO_2 capture and storage plants. In this work, it is shown the global optimization of a coupling CO_2 capture plant to an electric power plant, having as objective function minimize the energetic requirements of the process. For this study, it was considered four different fuels in the power plant; biogas, coal, non- associated natural gas, and associated natural gas. Two operating scenarios are considered: in the first, generate the same combustion gas flow for all the proposed fuels and in second, obtain the same energy demand with the 4 fuels. For the design and simulation, the software ASPEN Plus simulator was used.

Keywords: CO₂ Capture plant, biogas, coal, non-associated natural gas.

1. Introduction

In recent years demand for electricity has been rapidly increased, the International Energy Agency reported that 65% of the energy produced worldwide was obtained from the burning of fossil fuels, which are the main sources of CO₂ emissions, generating climate change as the main consequence (IEA, 2018). From 37.1 trillion tonnes of CO₂ produced in 2018, 35 trillion tonnes are related to the energy sector (EIA,2019), in that way, the production of energy by fossil fuels is considered unsustainable processes in accordance with the principles of green chemistry and circular economy. Considering the aforementioned, the production of greenhouse gases and their relationship with the energy sector is of significant importance. Understanding a thermoelectric generator (TEG) as an apparatus that produces electricity from waste heat. There are several ways to produce electricity, the first of them is by a conventional thermal power plant that works with a simple thermal cycle, with a yield of 33%, the rest of the energy is dissipated in the form of heat. On the other hand, there are combined cycle thermoelectric plants where electric and thermal energy is produced simultaneously from the same fuel. The advantage of these over conventional plants is that they take better advantage of the energy produced, thus achieving greater efficiencies and in turn have lower CO2 emissions. Globally, 836 Romero-García et al.

several alternative solutions have been sought to reduce CO_2 emissions turning electricity production into cost-effective and sustainable processes. To achieve this goal, some authors propose different possibilities to reduce CO_2 emissions: 1) reduce the intensity of energy; 2) reduce the intensity of coal; for example, the use of carbon-free fuel; and 3) improve CO_2 capture. highlighting the implement of CO_2 Capture and Storage plants (CCS). Where post-combustion CO_2 capture is the most feasible technology than other alternatives; by reacting with alkanolamines as solvents, post-combustion capture technology is the best choice for CO_2 separation, because it has high efficiency, low cost, and facility to be adapted to existing power plants.

In order to have a positive environmental impact on CO_2 capture processes, it is necessary to highlight the technical challenges involved in the separation method of CO_2 due to the use of amine aqueous solutions, as well as consider using new ionic liquids solvents to CO_2 separation. To achieve high efficiency, low environmental impact and the best operating cost, it is important to consider two different aspects: first is needed to have a high concentration of CO_2 which depends on the type of fuel used in the power plant and second the election of the solvent used to CO_2 capture so as its proportions.

As discussed in Nagy and Mizey (2013), changing flue gases conditions significantly influence the optimal operation of the capture process, particularly the solvent and energy requiments. These authors evaluated the influence of type and flowrate of seven fuels (including 3 coals, 2 gasses, and one biomass) during capture process by means of a parametric study. Their findings indicate that different ratios absorbent/gas are required in order to operate the capture plant in optimum conditions. According to their results, the optimal L/G ratio shows a linear correlation with the $\rm CO_2$ content of the flue gas.

In this work, we present a global optimization for the design of a CO₂ capture process coupled to a power generation plant (see Figure 1). The use of four different fuels in the power plant was considered; biogas, coal, non-associated natural gas, and associated natural gas. Two operating scenarios were considered; in the first, the same fuel flow was considered for all the plants and in the second, the same energy demand was specified. The design and simulation of the process plants were developed through the use of the ASPEN Plus simulator. Study Cases and Methodology: for the simulation of the power plant and the CO₂ capture plant, the ASPEN PLUS process simulator is used. In order to model the thermodynamic properties involved in the power generation plant, the Peng-Robinson method is used according to the reported by Hasan et al. (2012). For the combustion chamber, a RGibbs type reactor was selected, considering a molar ratio of air to the fuel of 30: 1 and a fuel flow of 1000kmol/h for all analyzed cases. Table 1 shows the mass percentages of the fuels used for the simulation. For the CO₂ capture process, it was considered a chemical absorption using as solvent an aqueous solution of monoethanolamine (MEA) with a weight of 30% in a RadFrac equilibrium stage block for the absorber and regenerator. The reactions involved in the CO₂ capture process are shown below from Eq. (1) to Eq. (5).

$$MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+$$
 (1)

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

$$HCO_3^- + H_2O \leftrightarrow CO_3^{2-} + H_3O^+$$
 (3)

$$OH^{-} + CO_{2} \xleftarrow{k_{1}} HCO_{3}^{-}$$

$$\tag{4}$$

$$MEA + CO_2 + H_2O \longleftrightarrow MEACOO^- + HCO_3^-$$
 (5)

Table 1. Fuel composition

	Natural Gas	Associated Gas	Biogas	Coal
CH ₄	96.00	87.20	60.00	-
C_2H_6	1.80	4.50	-	-
C_3H_8	0.40	4.40	-	-
$i-C_4H_{10}$	0.15	1.20	-	-
N_2	0.70	2.70	2.00	-
CO_2	0.95	-	38.00	-
\mathbf{C}	-	-	-	78.20
H	-	-	-	5.20
O	-	-	-	13.60
N	-	-	-	1.30
\mathbf{S}	-	-	-	1.70

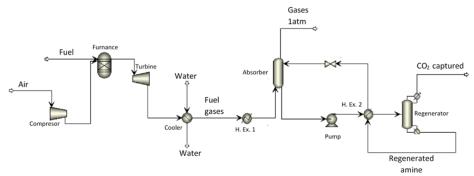


Figure 1. Representation of a thermoelectric power plant and the CO2 capture plant in postcombustion using chemical absorption with monoethanolamine

Because of the components present in the absorption are dissociate, it is necessary to achieve a CO_2 recovery in the gas output stream of the same equipment. In the case of the regenerator, the distillate flow and the reflux ratio were manipulated to capture the greatest amount of CO_2 from the flue gas stream from the thermoelectric plant and thus reduce CO_2 emissions into the atmosphere and the environmental impact that they generate For this reason, in all the cases analyzed, they were standardized to a purity of 99 mol% CO_2 and recovery of at least 95% of CO_2

2. Global Optimization

Once the Aspen Plus simulation is completed, a multi-objective optimization technique is employed having as objective function the minimization of energy requirement as

reboiler heat duty. The minimization of this objective was subject to the required recoveries and purities in each product stream (Eq. 6).

$$Min(Q) = f(N_m, N_{fn}, R_m, D_{rf}, F_{rn})$$
 (6)

Where N_{tn} is the total number of column stages, N_{fn} is the feed stage in the column, R_{rn} is the reflux ratio, F_{rn} is the distillate/bottoms flux, and D_{cn} is the column diameter. This minimization considered 10 continuous and discrete variables.

To optimize the process route for CO₂ capture, a stochastic optimization method, Differential Evolution with Tabu List (DETL) was used, which has shown being robust to optimize intensified separation systems. This technique works as a combined system between the biological evolution from Differential Evolution technique and the random search method from the Tabu search technique. Sharma & Rangaiah, (2007) showed that the use of some concepts of the metaheuristic tabu could improve the performance of DE algorithm. The implementation of this optimization approach was made using a hybrid platform where the DETL method was coded using Microsoft Excel (ME). Initially, the method proposes a vector which is sent to Aspen Plus by means of dynamic data exchange (DDE). In there the separation process was rigorously simulated. For the optimization of process routes analyzed in this study, the following parameters for DETL method were used: 200 individuals, 500 generations, a tabu list of 50% of total individuals, a tabu radius of 0.0000025, 0.80 and 0.6 for crossover and mutation fractions, respectively.

3. Results

In this section, it is presented the results of the study cases where the operating conditions were varied for both constant fuel flow and energy demand. Both cases were analyzed for four different fuels. It is important to remark that the selection of fuel is very important because it has a direct impact not only on energy production but also on the fuel gas composition that is obtained (Nagy and Misey, 2013). Besides the concentration of the gases obtained will have a direct impact on the energy and solvent requirements used for the CO_2 capture plant. When it is presented the lower concentration of gases the capture efficiency will decrease, then the energy and solvent requirements for the capture will increase.

After the optimization process for reducing energy demand in the capture process, the optimum designs of absorber and desorber colums for Case 1 are presented in Table 2. For Case 2 the columns structure remains close to that obtained in Case 1, the operating parameters, however, shown important differences. The optimum operating parameters for both scenarios are shown in Table 3. For both cases, the CO_2 generated by GJ of energy produced in the power plant (CO_{2GEN}/E_{PP}) is larger when burning mineral coal and biogas than for the natural gasses. This is more noticeable for the scenario in which energy demand is specified, since it is necessary to adjust the feed flows of each fuel in order to reach the specified demand. It is important to highlight that CO_2 concentration in flue gases coming from burning mineral coal and biogas have lower values in the first scenario, but it significantly increases in the second case, which directly influences the capture effectiveness.

The optimum ratios of absorbent to flue gas (L/G), absorbent to CO_2 recovered (L/CO₂ REC) and the reboiler duty to CO_2 recovered (Q_R/CO₂ REC), are reported in Table 2. In Case 1, the largest value for L/CO₂ REC is obtained for the mineral coal, while for the other three fuels this ratio ranges between 13 and 15. The reboiler duty in the regenerator column (desorber) highly depends on the L/G ratio, so the largest requirement is also observed

for this fuel. These results dramatically changed in Case 2, as the CO_2 concentration in the flue gas importantly increases, such that the absorbent and energy requirements during CO_2 capture diminishes.

Table 2. Optimal designs for constant fuel flow considering the best 3 fuels

Design Variables	Mineral coal	Biogas	Non associated gas	Associated gas*
	Columns Top	ology		
Stages (Absorbed)	48	20	46	19
Stages (Desorbed)	25	39	37	17
Feed flue gas stage (Absorbed)	48	20	46	19
Feed solvent stage (Absorbed)	1	1	1	1
Feed stage (Desorbed)	3	3	3	3
	Operation Speci	fications		
Top pressure (kPa)	88	88	88	88
Reflux ratio (Absorbed) Reflux	1.103	0.691	0.792	0.794
ratio (Desorbed) Heat duty	0.9006	0.809	0.839	0.796
(Desorbed) (GJ/h)	173.067	126.567	155.224	143.99
	Streams mas	s flow		
Flue gas (kg s ⁻¹)	267.68	271.055	268.25	268.78
Flue gas (kg s ⁻¹) Feed solvent (kg s ⁻¹)	251	140.49	176.950	161.88

^{*}Associated gas was taken as basis for the initial design

Table 3. Optimization results for all scenarios

Fuel type	CO _{2 GEN} /E _{PP} (Power plant)	L/G	L/CO ₂ REC	QR/CO ₂ REC	
	kg/GJ	kg/kg	kg/kg	GJ/t CO2	
	Constan fuel in power plant				
Mineral coal	55.25	0.94	27.68	5.30	
Biogas	60.13	0.58	13.93	3.09	
Non associated gas	42.91	0.68	15.50	3.65	
Associated gas	44.84	0.71	13.77	3.02	
	Constant energy in power plant				
Mineral coal	71.04	0.598	7.812	2.950	
Biogas	71.23	1.023	13.524	3.694	
Non associated gas	44.24	0.672	13.848	3.214	
Associated gas	44.88	0.705	13.773	3.017	

Nagy and Misey (2013) found optimum operating parameters for CO_2 capture plants by considering seven fuels and two operating cases (similar to those here considered). After a parametric searching, they reported L/G values ranging between 1 to 4, with Q_R/CO_2 REC close to 4. For the studied cases in this work, L/G ratio took values between 0.58 and 1.023. From the overall results, it is clear that the optimum designs obtained through a global optimization, wherein the column structures are considered, may significantly

reduce not only the energy requirement but also the absorbent flowrate. Given the interest in CO_2 capture processes as an alternative to reduce the environmental impact during the generation of electricity, the implementation of this additional objective to the optimization problem may be considered in future works, in order to identify optimum solutions beyond the techno-economic point of view.

4. Conclusions

The implementation of the CO_2 capture process in power plants has been considered so far, the most mature technology to reduce the environmental impact associated with electricity production. Most research efforts in this field have been focused on performing techno-economic analysis and optimizing the energy efficiency of the capture process. There is a clear incentive to analyze the process from a holistic point of view, considering not only the CO_2 capture as a strategy to reduce the negative effects of the power plant but also by identifying new environmental effects due to the implementation of such capture process

References

- EIA- U.S. Energy Information Administration Independent Statistics and Analysis, 2019, "U.S. Energy-Related CO2 Emissions Expected to Rise Slightly in 2018", Remain Flat in 2019, U.S. Energy Information Administration (EIA). Taken from: www.eia.gov/todayinenergy/detail.php?id=34872.
- International Energy Agency, 2018, "Electricity Information 2018 overview", International Energy Agency. Taken from: https://www.iea.org/statistics/electricity/
- M. F. Hasan, R. C., Baliban, Elia, J. A. and C.A. Floudas, 2012, "Modeling, simulation, and optimization of postcombustion CO2 capture for variable feed concentration and flow rate. 1. Chemical absorption and membrane processes", Industrial & Engineering Chemistry Research, 51, 48, 15642-15664.
- S., Sharma, and G.P. Rangaiah, 2013, "An improved multi-objective differential evolution with a termination criterion for optimizing chemical processes", Computers & Chemical Engineering 56, 155-173.
- T. Nagy and P. Mizsey, 2013, "Effect of fossil fuels on the parameters of CO2 capture", Environmental science & technology, 47, 15, 8948-8954.