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Simulation of carbon dioxide capture for industrial applications

S.P.R. Arachchige Udara*, Rasenthiran Kohilan, M.A.L. Lakshan, M.K. Lakshitha Madalagama, P.R. Prabhath Pathirana, P.W. Sakuna Sandupama

Faculty of Technology , University of Sri Jayewardenepura, Nugegoda, Sri Lanka

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Abstract

Carbon dioxide emissions to the atmosphere are drastically increased due to fossil fuel-based power plants and different kinds of industrial processes. Carbon capture is essential to maintain a better environment. Flue gas emissions from the coal-fired power plant, gas-fired power plant, cement manufacturing industry as well as the aluminium production industry are considered for the present study. Carbon dioxide capture model is developed and implemented in Aspen Plus to calculate the regeneration energy requirement. The regeneration energy requirement in the stripping process in the carbon capture is calculated as 3634, 3781, 3229 and 3085 kJ/kg respectively for coal, gas, cement, and aluminium production process flue gas treating.

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Keywords: Carbon capture; Aspen plus; Simulation; Regeneration energy; Flue gas

1. Introduction

Carbon dioxide (CO_2) is known as a greenhouse gas (GHG) which absorb and emit thermal radiation. The CO_2 concentration in the atmosphere has rapidly risen after the industrial revolution [1]. CO_2 is the main anthropogenic contributor for greenhouse gas effect as a result of a major contribution to the temperature rising. CO_2 is produced in large quantities by many industries which can be mainly naming as coal and gas-fired power plants, steel production, cement production, chemical and petrochemical production, etc. [2]. There are several methods that have been suggested by the scientists, including switching to the green energy (wind power, solar power), improving process efficiency of the power plants, and capturing CO_2 emissions of the power plants and industries [3]. However, the most realistic option will remain as the carbon capture and storage (CCS) for several decades to maintain the green environment [4]. CCS technology is not widely applicable due to the high energy consumption of the regeneration process. The main idea behind this research study is to develop and implement a CO_2 capture process model to minimize the regeneration energy requirement in the CO_2 mitigation process.

* Corresponding author.
E-mail address: udara@sjp.ac.lk (S.P.R.A. Udara).

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The post-combustion chemical absorption process is the most viable technique to capture flue gas carbon dioxide. The acid gas mainly CO_2 can be chemically captured with amine solvents by the post-combustion process. The captured CO_2 with amine solvent can be regenerated to collect as purified CO_2 suing steam as the medium for the regeneration process. However, with the current situation, the main drawback of the technology is the high amount of energy requirement in the regeneration process. Therefore, reduction of energy requirement in the carbon capture process is necessary to be implemented in the industries and power plants to achieve a green environment.

2. Model development

The carbon capture model is developed for flue gas stream from 500 MW coal and gas-fired power plants, Cement industry as well as for aluminium production industry. The conditions of the flue gas stream are given in Table 1, which is taken from the literature coal-fired power plant [5], Gas fired power plant [6], Cement industry [7], and Aluminium industry [1].

Aspen Plus rate based model is used to develop the comprehensive process flow sheet (Fig. 1).

The process flow diagram is developed to capture 85% of CO_2 from the flue gas stream. Absorber and stripper are considered as the main two-unit operation blocks in the capture process. Inlet flue gas and the solvent are supplied at 313 K, and absorption process is performed at 1 bar pressure for optimum operation. The rich solvent leaving the bottom of the absorber column is heated up to 382 K using a heat exchanger unit before sending it to the stripper section. The stripper is operating at 2 bar absolute pressure. The solvent stream is selected based on previous studies [8]. The solvent stream condition which is used to perform the simulation studies is given in Table 2.

The amine-based carbon capture process is implemented in Aspen Plus process simulation software as shown in Fig. 1. Monoethanolamine (MEA) is considered as the solvent which is used for the absorption process. The main drawback of the MEA based carbon capture process is a high amount of energy requirement in the regeneration process, that is the re-boiler duty in the stripper column. Hence, the optimization of the capture plant is required

Table 1. Flue gas composition and parameters.

Parameter	Coal fired power plant	Gas fired power plant	Cement industry	Aluminium industry
Flow rate (kg/s)	673.4	793.9	84.72	112.1
Temperature (K)	313	313	433	498
Pressure (bar)	1.1	1.1	1.013	1.1
Major Compositions	Mol%			
H_2O	8.18	8.00	7.2	1.0
N_2	72.86	76.00	68.1	75.3
CO_2	13.58	4.00	22.4	3.0
O_2	3.54	12.00	2.3	20.7

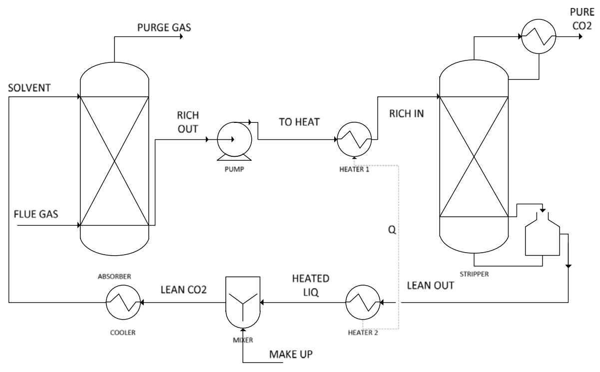

Fig. 1. Process flow diagram.

Table 2. Solvent stream parameters.

Parameter	Coal fired power plant	Gas fired power plant	Cement industry	Aluminium industry
Flow rate (kg/s)	2212	1048	612	142
CO2 lean loading [mole CO2/mole MEA]	0.27	0.30	0.30	0.30
Solvent concentration (w/w%)	40	40	40	40

Table 3. Aspen Plus model specifications of absorber and stripper column.

Specification	Parameter value	
	Absorber	Stripper
Number of stages	15	15
Operating pressure	1 bar	2 bar
Re-boiler	None	Kettle
Condenser	None	Partial-vapour
Packing type	Mellapak, Sulzer, Standard, 250Y	Flexipac, Koch, metal,1Y
Packing height	20m	18m
Packing diameter	15m	12m
Mass transfer coefficient	Bravo et al. [11]	Bravo et al. [11]
Interfacial area method	Bravo et al. [11]	Bravo et al. [11]
Interfacial area factor	1.5	2
Heat transfer coefficient method	Chilton and Colburn	Chilton and Colburn
Holdup correlation	Billet and Schultes [12]	Billet and Schultes [12]
Film resistance	Discrxn for liquid film and Film for vapour film	Discrxn for liquid film and Film for vapour film
Flow model	Mixed	Mixed

to install the carbon capture process in real industrial applications. Absorber and Stripper packing conditions and operating parameters are selected from literature to perform the simulation studies [9,10]. The most important parameters are tabulated in Table 3.

2.1. Aspen plus

There are several simulation models available in the Aspen Plus. Due to several reasons, the Aspen Plus Rad-Frac model is finally chosen as the best operating model. Rad-Frac is considered as the most active unit operation model for vapour–liquid absorption and stripping section, faster simulation in comparison with other available options. Moreover, fewer convergence problems compared to other available options in Aspen Plus with high accuracy. It is important to select the property method in Aspen Plus to perform the calculation during the simulations [1,9,13]. Each unit operation model requires a property method to perform its calculation routes. Mainly, four different property methods are available in the Aspen Plus for CO_2+MEA systems, which are:

ELECNRTL-handle both very low and high concentrations of aqueous and mixed solvent systems.

ENTRL-HF-similar to the ELECNRTL property method except that it uses the HF equation of state for vapour phase calculation model.

ENTRL-HG-similar to the ELECNRTL property method except it uses the Helgeson model for standard property calculations.

AMINES-this property method uses Kent–Eisenberg correlation for K-values and enthalpy calculation. Out of them, the ELECNRTL model is selected for the simulation of the CO_2 capture process for this study. The ELECNRTL is the most versatile electrolyte property method as it has the capability of handling both very low and high concentrations of aqueous and mixed solvent systems.

3. Chemistry of the amine + CO_2 reacting system

Carbon dioxide and monoethanolamine reacting system, CO_2 is solubilized in the liquid phase either as carbamate, carbonate or bicarbonate form. The most important chemical reactions are given in Eqs. (1)–(5) [14].

Table 4. Constant values of equilibrium constant equation (6).

Parameter	Reaction 1	Reaction 2	Reaction 3	Reaction 4	Reaction 5
A_j	−0.52	231.46	216.05	−3.038	132.89
B_j	−2545.53	−12092.1	−12431.7	−7008.3	−13445.9
C_j	0	−36.78	−35.48	0	−22.47
D_j	0	0	0	−0.00313	0

Table 5. Re-boiler energy duty.

Parameter	Coal fired power plant	Gas fired power plant	Cement industry	Aluminium industry
Re-boiler duty [kJ/kg]	3634	3781	3229	3085

Hydrolysis reaction:

$$MEACOO^- + H_2O \leftrightarrow MEA + HCO_3^- \tag{1}$$

Dissociation of dissolved carbon dioxide:

$$CO_2 + 2H_2O \leftrightarrow HCO_3^- + H_3O^+ \tag{2}$$

Dissociation of bicarbonate:

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

Dissociation of protonated MEA:

$$MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+ \tag{4}$$

Ionization of water:

$$2H_2O \leftrightarrow OH^- + H_3O^+ \tag{5}$$

The mole fraction of each component is calculated using the above equations. The equilibrium constant which is required for the calculations have followed Eq. (6),

$$\ln K_j = A_j + \frac{B_j}{T} + C_j \ln T + D_j T \tag{6}$$

According to the literature [15], constants in Eq. (6) which are corresponding to Eqs. (1)–(5) are given in Table 4.

4. Results and discussion

Sensitivity analysis is performed to identify the effect of the parameters on the CO_2 removal process. The most important factor is the regeneration energy requirement in the stripping column. The required regeneration energy is calculated based on the simulation studies for different industrial application. Four major industries (coal-fired power plant, gas-fired power plant, cement industry and aluminium industry) which mainly contribute to greenhouse gas emissions were considered for present simulation studies. The required re-boiler energy duty is given in Tables 1, 2, 3, 4 and 5 separately.

The regeneration energy requirement is changing according to the total flue gas flow rate as well as with the carbon dioxide composition in the flue gas stream. The highest regeneration energy is required for the gas-fired power plant flue gas capturing process, following coal-fired flue gas capturing process, cement industry and for the aluminium production process. At the same time, simulations are performed to identify the relationship between regeneration energy requirement and CO_2 removal efficiency. It can be clearly seen that the regeneration energy requirement is increasing gradually with the removal efficiency. The main reason behind that is, when the removal efficiency is gradually increased, the required solvent flow rate is increasing. The overall regeneration energy requirement consists of mainly three parts.

- The energy needed for liberating attached CO_2 from amines.
- The energy required to increase the solvent temperature.
- The energy required for the water evaporation process.

Moreover, the solvent concentration effect on CO_2 removal process also considered. It can be clearly seen that, with the increase of solvent concentration, the required solvent flow rate is gradually decreasing, therefore required regeneration energy for a stripper is decreasing. However, higher solvent concentration believes to have corrosive effects in all sections, in the capture plant.

5. Conclusion

This research mainly has focused on process modelling and simulation of CO_2 capture with the post-combustion chemical absorption process. The carbon capture model is developed and implemented in the Aspen Plus process simulation tool. The main problem of the post-combustion chemical absorption technology is a large amount of energy requirement in the re-generating sector. Therefore, the reduction of operating cost is important to achieve the removal process in flue gas treating. The model is developed in Aspen Plus process simulation tool to optimize the removal process. The Electrolyte NRTL (ELECNRTL) property method is used to handle the chemical reacting system. There are four different case studies considered for the simulation process which are, coal-fired power plant, gas-fired power plant, cement plant as well as the aluminium industry. The required re-boiler duty was calculated for every situation. The required regeneration energy is calculated as 3634, 3781, 3229 and 3085 kJ/kg respectively for coal, gas, cement and aluminium production process flue gas treating.

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