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Optimized CO_2-flue gas separation model for a coal fired power plant

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Abstract
The detailed description of the CO_2 removal process using mono-ethylamine (MEA) as a solvent for coal-fired power plant is present in this paper. The rate based Electrolyte NRTL activity coefficient model was used in the Aspen Plus. The complete removal process with re-circulating solvent back to the absorber was implemented with the sequential modular method in Aspen Plus. The most significant cost related to CO_2 capture is the energy requirement for re-generating solvent, i.e. re-boiler duty. Parameters' effects on re-boiler duty were studied, resulting decreased re-boiler duty with the packing height and absorber packing diameter, absorber pressure, solvent temperature, stripper packing height and diameter. On the other hand, with the flue gas temperature, re-boiler duty is increased. The temperature profiles and CO_2 loading profiles were used to check the model behavior.

Keywords: Carbon dioxide capture; Coal fired power plant; Parameters effect; Re-boiler duty.

1. Introduction

Due to the large number of fossil fuel based power plants, the bulk amount of CO_2 is releasing to the atmosphere. In order to maintain the atmospheric green house gases, mitigation technologies have to be developed. Post combustion capture technologies are the best and widely used method for CO_2 recovery process. CO_2 capture by absorption and stripping process is currently considered as the most feasible option for CO_2 removal from fossil fuel fired power plants. The main drawback of this technology is energy consumption and the capital cost. Post combustion CO_2 capture technology with amine solvent is a reactive system. Hence, mass transfer of CO_2 from the bulk vapor to the liquid solvent and chemical reactions between amine and flue gas are the main two phenomena to be considered.

In the chemical absorption, flue gas enters the absorber at the bottom whilst the solvent enters at the top. The reactions start between MEA and CO_2 while flowing through the column (packing bed). An un-reacted gas leaves the column at the top, while the CO_2 rich solvent discharges at the bottom. The rich solvent goes through the heat exchanger to increase the temperature before sending it to the stripper section. The heated rich MEA stream then goes to the stripper at the top. In the stripper, steam is used for the regeneration process. Finally, separated acid gases leave the stripper at the top. The lean MEA then leaves the system at the bottom of the stripper and goes through the heat exchanger. The MEA and water are added to the lean MEA stream to balance the component before recycled back to the absorber unit.

The main problem with installing capture plant to the fossil fuel fired power industry is operating cost. Installation of capture plant increases the electricity unit cost. The main point that requires considering operating cost is the energy requirement to run the carbon capture process. Therefore, it is necessary to perform research on this topic to reduce the operating cost and to improve the existing technologies to capture the CO_2. This paper primarily focuses on developing the model for gas treating plant of CO_2 from the coal-fired power plant flue gas and simulates the adaptable model to reduce the re-boiler duty.

2. Model development

A simulation of a 500MW coal-fired power plant flue gas is considered. The flue gas composition and inlet conditions are extracted from the literatures [1]. The comprehensive flow sheet is developed in Aspen Plus for three different CO_2 removal models with 85, 90 and 95% efficiency.

The suitable operating conditions are selected from previous studies, and sensitivity analysis is performed to check the validity of the parameters. A simplified flow sheet of the implemented model which employs CO_2 capture by absorption/stripping with an aqueous amine solution is shown in Figure 1.

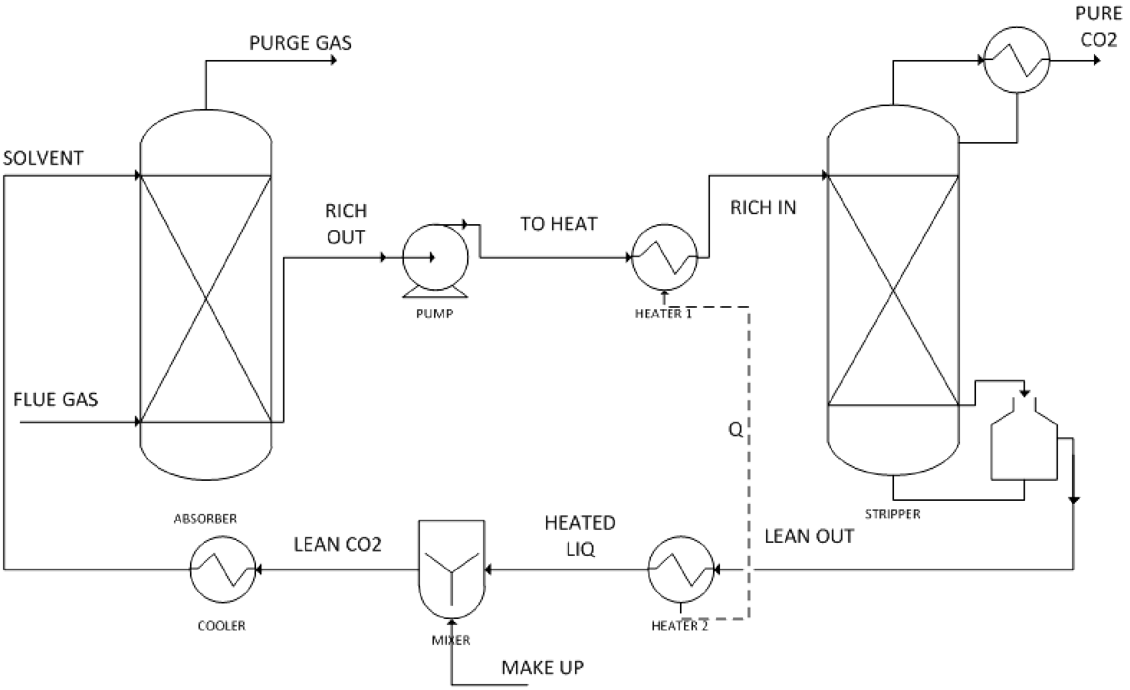


Figure 1. Process flow diagram

2.1 Operating conditions

The process flow diagram is developed to capture 85, 90 and 95% of CO_2 from coal-fired power plant flue gas. Absorber and stripper are the main two-unit operation blocks in the capture process. Inlet flue gas and solvent stream are supplied at 313K, and absorber is operating at 1bar absolute pressure. The rich solvent stream is heated up to 382K using a heat exchanger unit before sending it to stripper section for maximum performance. The stripper is operating at 2 bar absolute pressure and reflux ratio (fraction of the condensed is coming back to the stripper section) and distillate rate (flow rate of the PURE CO2 line) are used to implement the stripper unit. The inlet flue gas stream data are selected from Alie, 2004 [1] and tabulated in Table 1 and selected solvent conditions from simulation studies are given in Table 2.

The main component in the pure gas stream of the stripper (PURE CO2 in Figure 1) is CO_2, and the rest of that is MEA and water. High temperature (393K) steam (produce in the re-boiler) is used to remove the CO_2 from the solvent. Steam is produced in the re-boiler and main energy requirement in the process is related to re-boiler duty. Therefore, the CO_2 capture model is implemented to reduce the re-boiler duty so that energy requirement can be minimized. The operating conditions of absorber and stripper section are tabulated in Table 3. Due to several reasons Aspen Plus Rad-Frac model is selected for absorber and stripper:

- It is the active unit operation model for vapour- liquid absorption and stripping section.
- The simulation time is faster for Rad-Frac column in comparison with other available options.
- Fewer convergence problems compared to other available options in Aspen Plus with high accuracy.

Table 1. Flue gas composition and parameters [1]

Parameter	Coal Fired
Flow rate [kg/s]	673.4
Temperature [K]	313
Pressure [bar]	1.1
Major Composition	Mol%
H_2O	8.18
N_2	72.86
CO_2	13.58
O_2	3.54
H_2S	0.05

Table 2. Solvent stream parameters

Specification	85% Removal Efficiency	90% Removal Efficiency	95% Removal Efficiency
Coal fired power plant CO_2 capture			
MEA concentration [w/w%]	40	40	40
CO_2 lean loading [mole CO_2/mole MEA]	0.27	0.27	0.25
Solvent flow rate [kg/s]	2212	2422	2483

Table 3. Absorber and stripper column specifications

Specification	Coal fired flue gas	
	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 method [2]	Bravo et al. (1985)	Bravo et al. (1985)
Interfacial area method [2]	Bravo et al. (1985)	Bravo et al. (1985)
Interfacial area factor	1.5	2
Heat transfer coefficient method	Chilton and Colburn	Chilton and Colburn
Holdup correlation [3]	Billet and Schultes (1993)	Billet and Schultes (1993)
Film resistance	Discrxn for liquid film and Film for vapour film	Discrxn for liquid film and Film for vapour film
Flow model	Mixed	Mixed

Packed columns are used for the model development and the type of the packing is selected to get better operating conditions. The packing height, section diameter, packing factor and material are important factors and tabulated (Table 3). The number of stages is selected to obtain high accuracy. The input conditions and model specifications used for model development in the absorber, and stripper are shown in Table 3. The specifications are recommended for rate based model of the CO_2 capture process by Aspen Tech [4].

2.2 Property method selection

A property method is defined as a collection of property calculation routes. Each unit operation model requires property method to perform the calculation [5]. Mainly, four different property methods are available for CO_2+ MEA system:

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 vapor 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 and electrolyte wizard is used to develop the simulation kinetics and reactions. The ELECNRTL is the most versatile electrolyte property method as it can handle both very low and high concentrations of aqueous and mixed solvent systems. The solubility of gases can be modeled with Henry's law and required coefficients are available in databanks. For the calculation of vapor phase properties, the Redlich-Kwong equation of state is used.

2.3 Thermodynamic behavior

The acid gases in the flue gas are weak acid electrolytes, and amines are weak organic base electrolytes. Combination of those two forms partially ionizes or partially dissociates aqueous solution in reacting system. The reacting system (1-7) can be expressed as dissociation of components as below [6].

Water: $2H_2O \leftrightarrow OH^- + H_3O^+$ (1)

Hydrogen sulfide: $H_2O + H_2S \leftrightarrow HS^- + H_3O^+$ (2)

Hydrogen bisulfide: $H_2O + HS^- \leftrightarrow S^{2-} + H_3O^+$ (3)

Carbon dioxide: $CO_2 + 2H_2O \leftrightarrow HCO_3^- + H_3O^+$ (4)

Bicarbonate: $HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{2-}$ (5)

Protonated alkanolamine: $MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+$ (6)

Hydrolysis reaction: $MEACOO^- + H_2O \leftrightarrow MEA + HCO_3^-$ (7)

Equilibrium constants are required for each of the above equations to continue their vapour/liquid mole fraction calculations. It can be calculated by,

$$\ln K_j = A_j + \frac{B_j}{T} + C_j \ln T + D_j T \tag{8}$$

where K_j is representing equilibrium constant for thermodynamic model, T is temperature in (K), and constants are given by A_j, B_j, C_j, and D_j. Equilibrium constant values are imported from the literature sources [7] and tabulated in Table 4.

Table 4. Values of equilibrium constant equations [7]

Reaction number	A_j	B_j	C_j	D_j
Reaction 1	132.89	-13445.9	-22.47	0
Reaction 2	214.58	-12995.4	-33.55	0
Reaction 3	-9.74	-8585.47	0	0
Reaction 4	231.46	-12092.1	-36.78	0
Reaction 5	216.05	-12431.7	-35.48	0
Reaction 6	-3.038	-7008.3	0	-0.00313
Reaction 7	-0.52	-2545.53	0	0

It is important to understand the kinetics of the reactions. The reactions (4) and (7) are replaced by kinetic reactions (9), (10) and reverse reactions (11), (12) for rate model.

$$CO_2 + OH^- \rightarrow HCO_3^- \tag{9}$$

$$MEA + CO_2 + H_2O \rightarrow MEACOO^- + H_3O^+ \tag{10}$$

$$HCO_3^- \rightarrow CO_2 + OH^- \tag{11}$$

$$MEACOO^- + H_3O^+ \rightarrow MEA + CO_2 + H_2O \tag{12}$$

The kinetic expression is defined in Aspen Plus and given below in (13) with constant values. Parameters used in (13) are, *rj* rate of reaction, *kj* rate coefficient, *T* and T_0 are operating and absolute temperatures in (K), *R* is universal gas constant and *E* is activation energy.

$$r_j = k_j \left(\frac{T}{T_0} \right)^{n_j} exp\left[-\frac{E_j}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \tag{8}$$

Table 5 presents the constant values taken for the simulation in Aspen Plus for kinetic calculation. The given values are extracted from the Aspen Plus available databanks and checked with literatures to confirm the accuracy.

Table 5. Rate constant values

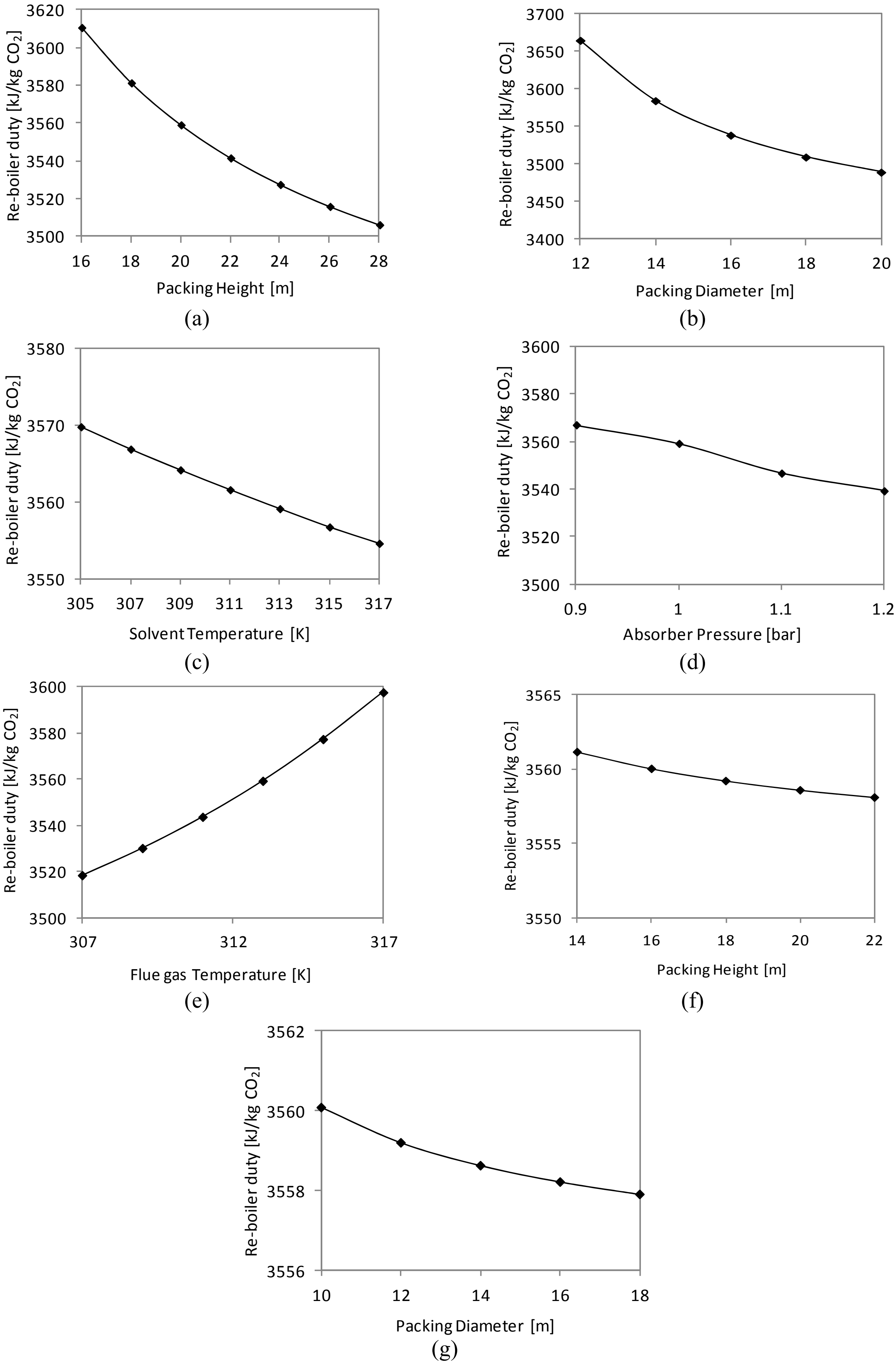
Parameter	Reaction 9	Reaction 10	Reaction 11	Reaction 12
k_j	4.32e+13	9.77e+10	2.38e+17	2.7963e+20
n_j	0	0	0	0
E_j (J/mol)	55433	41236	123222	72089
T_0 (K)	298	298	298	298

2.4 Parameter selection

In the amine-H_2S-CO_2-H_2O system, where the amine is MEA and eight ionic species ($OH^-, H_3O^+, HS^-, S^{2-}, HCO_3^-, CO_3^{2-}, MEAH^+, MEACOO^-$) and four molecular species (H_2O, H_2S, CO_2, MEA) are present in the liquid phase. Therefore, pure component parameters, binary parameters as well as electrolyte parameters have to be introduced in order to implement the process model. If any of the parameters are missing, it can be estimated with molecular structure, or using regression with experimental data. The Aspen Plus physical property system contains built in parameters for the electrolyte NRTL model. The databank contains energy parameters and other electrolyte parameters for molecular-electrolyte and electrolyte-electrolyte systems.

3. Results and discussion

Sensitivity analysis is performed to understand the parameters' effect on re-boiler duty. Therefore, initially, open loop model was developed for the simulation, and absorber packing height, diameter of the packing bed, absorber pressure, solvent and flue gas temperatures, stripper packing height, and diameter are varied to check the effect on re-boiler duty. For this sensitivity analysis, only 85% removal efficiency is considered. In order to study the effect of one parameter on energy consumption in the re-boiler, other parameters of the model are kept constant. Figure 2 represents the re-boiler duty variation with listed parameters.



(a) (b) (c) (d) (e) (f) (g)

Figure 2. Re-boiler duty variation with model parameters; (a) absorber packing height, (b) absorber packing diameter, (c) solvent temperature, (d) absorber pressure, (e) flue gas temperature, (f) stripper packing height, (g) stripper packing diameter

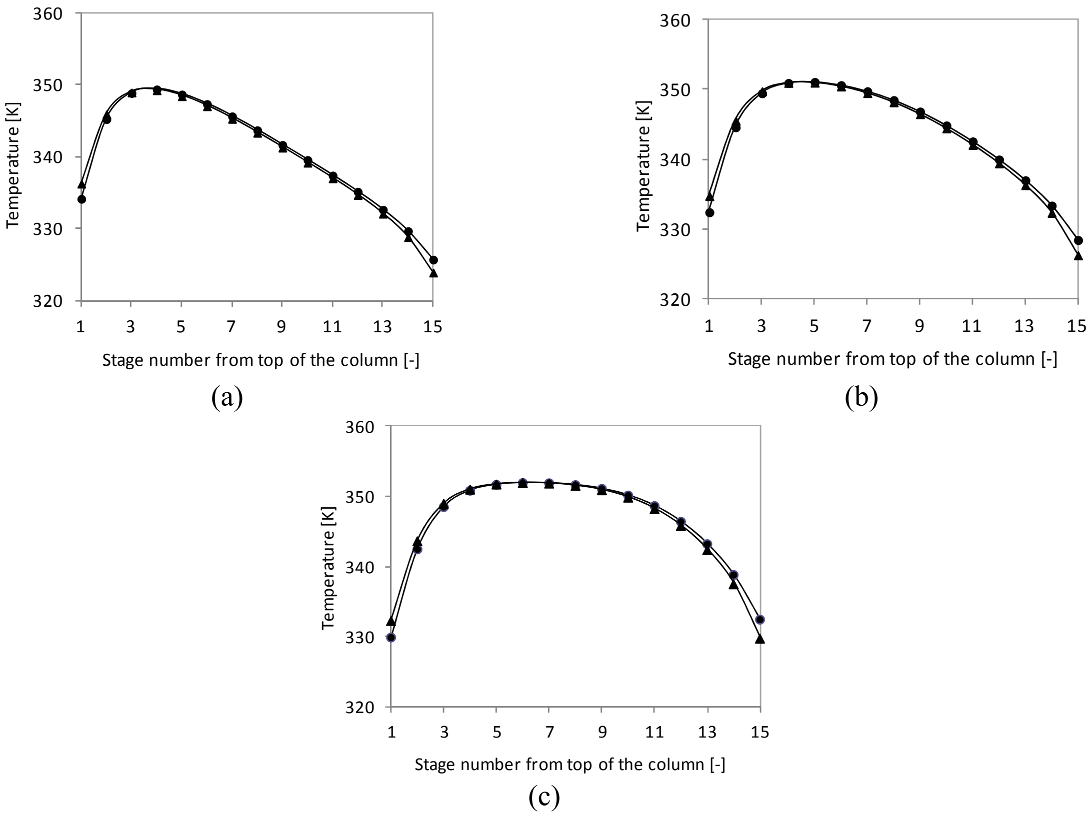
The re-boiler duty is decreasing with the increase of absorber packing height, packing diameter, absorber pressure, solvent temperature, stripper packing height, and packing diameter. The attained rich loading increased with the increase in the absorber packing height and packing diameter. Hence, required solvent flow rate is decreased and the amount of the liquid solvent process in the stripper is reduced. Therefore, the re-boiler duty to process unit mass of CO_2 is reduced and the total energy requirement decreased. Similarly, re-boiler duty decreased with the increase of absorber pressure due to higher CO_2 removal efficiency with high absorber operating pressure. Re-boiler duty decreased with the increase of solvent temperature. Reverse is applicable to flue gas temperature effect. The effect of stripper packing parameters on re-boiler duty is negligible.

The efficiency of the CO_2 removal (85%, 90%, and 95%) is achieved with distillate rate (vapour stream of the stripper outlet) variation in the stripper. However, before lean MEA stream recycled back to the absorber, rest of the CO_2 (15%, 10%, and 5%) remained in the system has to be removed from the system to get material balances. The CO_2 removal amount in the purge gas stream is calculated. Exact amount of remaining CO_2 can be removed by adjusting the open-loop MEA inlet flow rate to the absorber. Amount of MEA and H2O losses during the process are added to the make-up stream to balance the system and lean MEA stream is recycled back to the absorber (Table 6).

Table 6. Composition of make-up stream

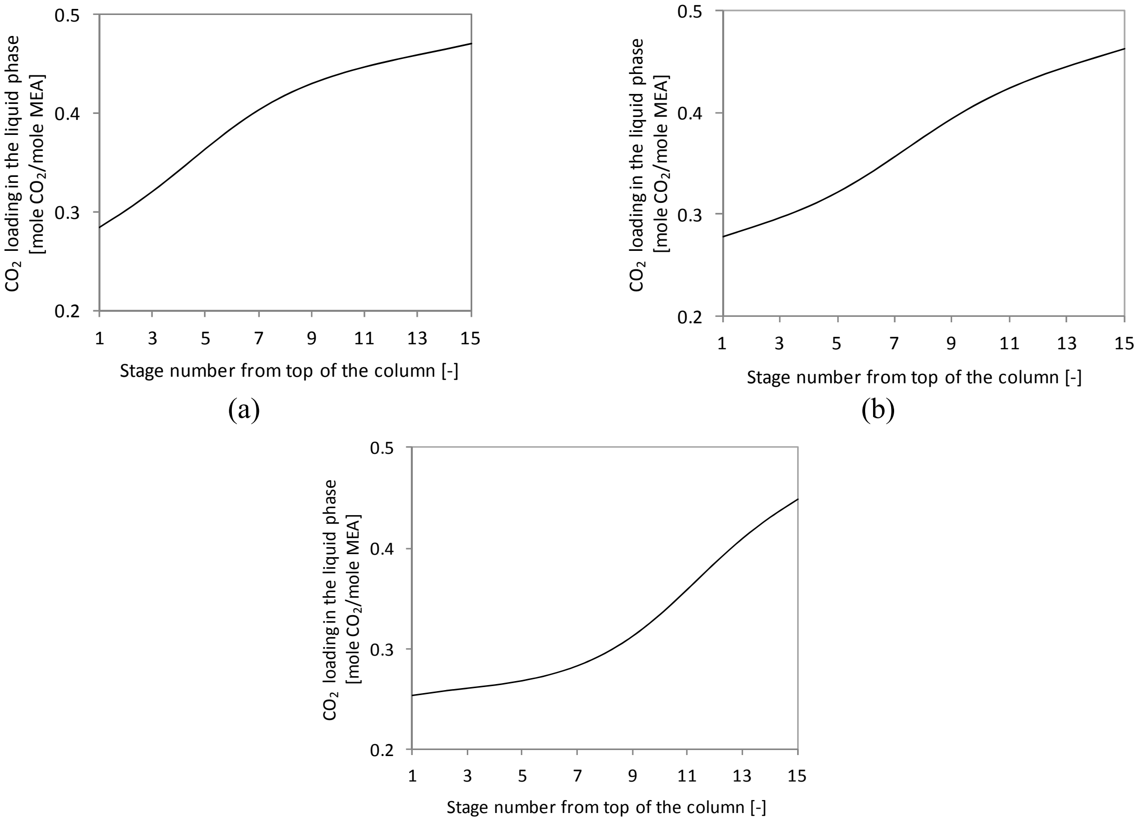
Process Model	Amount of make-up stream	
Removal Efficiency (mol %)	Water (kg/s)	MEA (kg/s)
85	42.41	0.41
90	37.85	0.38
95	29.52	0.36

Finally, the closed-loop CO_2 removal process is considered for the re-boiler duty calculation and further analyzing. Re-boiler duty is calculated as 3634.2, 3736.4, 4185.5 kJ/kg CO_2 for the 85, 90 and 95% CO_2 removal process for coal-fired power plant. Temperature profiles (Figure 3) as well as CO_2 loading profiles (Figure 4) are studied to understand the behavior of the absorber process.



(a) (b) (c)

Figure 3. Temperature profiles in absorber for (a) 85%, (b) 90% and (c) 95% removal efficiency; symbols refer to ●, Liquid phase; ▲, Vapour phase



(a)

(b)

(c)

Figure 4. CO_2 loading profiles in absorber for (a) 85%, (b) 90% and (c) 95% removal efficiency

The absorber tends to exhibit a temperature bulge at the top of the column for both liquid and vapor phase. Temperature bulge is due to highly exothermic reactions at the top of the column. The maximum temperature is reached 350K for all three models. The CO_2 loading is increasing alone the absorber and rich loading is reached to 0.4-0.5 [mole CO_2/mole MEA] for all three simulation models. The CO_2 rich loading is slightly decreasing with the increase of removal efficiency. Highest rich loading is obtained for 85% removal process.

4. Conclusion

The implemented model is properly working and converging for coal fired flue gas system. Three different models were developed with 85-95% removal efficiency. The calculated re-boiler duties are 3634.2, 3736.4, 4185.5 kJ/kg CO_2 for the 85, 90 and 95% CO_2 removal process. Temperature profiles and CO_2 loading profiles are having similar patterns for all cases.

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