

# Optimized Carbon Dioxide Removal Model for Gas Fired Power Plant

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## Abstract

The carbon capture process model was developed for 500MW gas-fired power plant flue gas treating. Three different efficiencies, 85%, 90%, and 95%, were used to implement the model in Aspen Plus. The electrolyte NRTL rate base model was used to develop the model. The selected solvent properties were used to develop and implemented model is used for further simulations. The implemented open loop base case model of 85% removal efficiency is used to check the parameters' effect on removal efficiency and re-boiler duty. Absorber packing height and diameter, absorber pressure, solvent and flue gas temperatures are positively affected on CO<sub>2</sub> removal efficiency. The packing height of absorber and stripper, solvent temperature and absorber pressure are negatively effects on re-boiler duty. The energy requirement in the re-generation process (re-boiler duty) are 3781, 4050, and 4240 kJ/kg CO<sub>2</sub> for 85%, 90%, and 95% capture models respectively. Parameter optimization is important to implement the carbon capture process in real industries to get higher removal efficiency and lowest re-boiler duty.

**Keywords:** Gas fired power plant, Carbon capture, Parameters effect, Re-boiler duty, Aspen Plus

## 1. Introduction

The green house gas emissions from the exhaust gases of the fossil fuel fired power plants (coal and natural gas) account for the global warming and climate change. Carbon dioxide (CO<sub>2</sub>) is the main green house gas causes for most of the environmental problems. Emission reduction technologies with high efficiencies are important in near future to avoid the problems. Carbon capture and sequestration (CCS) is the best available option for the power plant flue gas mitigation. The post combustion chemical absorption process is considered as the most viable option today.

The main advantage of amine scrubbing for post combustion carbon capture process is, it can be installed to the existing power plants without major modifications. Apart from that, it can be used with low partial pressure of CO<sub>2</sub> streams as it used to be with flue gases.

This research study will focus on improving existing carbon capture process with solvent improvements. Monoethanolamine (MEA) solvent is considered for model development in the present study. Here, an improvement of solvent concentration and lean loading is used to optimize the model. According to the previous studies [1], solvent concentration and lean loading is selected for gas-fired power plant flue gas treating process. Increasing solvent concentration will lead to reduce the required solution circulation and therefore, the plant operating cost [1].

## 2. Case Studies

### 2.1. Flue Gas and Solvent Properties

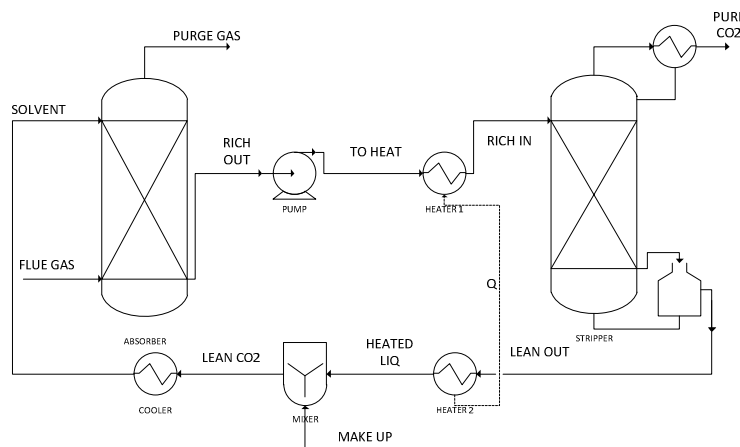
The carbon capture model is developed for 500MW gas-fired power plant flue gas stream. The conditions of the flue gas stream are given in Table 1, which is taken from the literature [2]. Aspen Plus rate based model is used to develop the comprehensive process flow sheet (Figure 1). Three different efficiencies, 85%, 90%, and 95%, are used to implement the model.

**Table 1:** Flue gas stream conditions [2]

Parameter	Value
Flow rate [kg/s]	793.9
Temperature [K]	313
Pressure [bar]	1.1
Major Composition	mol%
H <sub>2</sub> O	8.00
N <sub>2</sub>	76.00
CO <sub>2</sub>	4.00
O <sub>2</sub>	12.00

The process flow diagram consists of several unit operation blocks, such as absorber and stripper, pumps, heat exchanger, cooler and make up unit. For absorber and stripper, Rad-frac unit operation block is selected from the Aspen Plus model bank.

**Figure 1:** Process flow diagram



The inlet solvent stream properties which is selected from the previous studies [1], is tabulated below (Table 2). Number of simulation was performed in previous studies to select the best solvent condition for specified efficiencies.

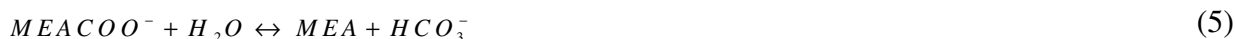
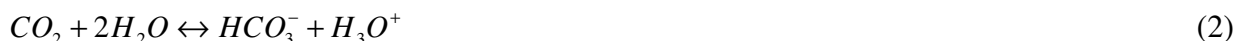
**Table 2:** Solvent stream conditions [1]

Specification	85% Removal Efficiency	90% Removal Efficiency	95% Removal Efficiency
Gas fired power plant CO <sub>2</sub> capture			
MEA concentration [w/w%]	40	35	30
Lean CO <sub>2</sub> loading [mole CO <sub>2</sub> /mole MEA]	30	25	25
Solvent flow rate [kg/s]	1048.6	895.6	1177.8

In the chemical absorption process, flue gas is counter currently passing through the solvent in a packed bed absorber column. Afterwards, rich solvent is transferred to the stripper section to regenerate the solvent by purifying the CO<sub>2</sub> using steam. Before sending it to the stripper, rich solvent stream is passing through the heat exchanger to increase the temperature to around 380K. Regenerating solvent step is the main energy-consuming part in the process, is called re-boiler duty. As it is the main drawback of this technology, process optimization is important before install in to the real industry.

## 2.2. Aspen Plus Model Parameters-Reaction Scheme

The MEA-CO<sub>2</sub> reacting system consists with several chemical reactions. The main chemical reactions involving in the carbon capture process are considered with thermodynamic and kinetic parameters. When CO<sub>2</sub> absorb into the amine solvent, following reversible chemical reactions (Eq. 1-5) are taking place [3].



The equilibrium constants for above equations can be calculated by Eq. 6 and relevant parameters are taken from the literatures (Table 3).

$$(6)$$

where:

$K_j$  is equilibrium constant for thermodynamic model;

$T$  - Temperature in K;

$A_j, B_j, C_j,$  and  $D_j$  – Constants.

**Table 3:** Constant values of equilibrium constant equation [4]

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

Kinetics of the reacting system is important to understand the model behavior. Equation 2 and 5 is replaces the kinetic reactions 7 and 8 and reverse reactions 9 and 10.





The kinetic expression is defined in equation (11) and required parameters are tabulated in Table 4.

$$(11)$$

where:

$r_j$ , is rate of reaction;

$k$  - Rate coefficient;

$T$  and  $T_0$  - temperatures in K;

$R$  - Universal gas constant;

$E$  - Activation energy.

The constant values used for the simulation in Aspen Plus for kinetic calculation are given in Table 4. The tabulated values are extracted from the Aspen Plus available databanks.

**Table 4:** Constant values for equation (11)

Parameter	Reaction 7	Reaction 8	Reaction 9	Reaction 10
$k_j$	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

### 2.3. Aspen Plus Model Parameters-Absorber and Stripper Column Parameters

The absorber and stripper column parameters used in the implemented model is tabulated in Table 5. Similar conditions are applied in all three efficiency processes (85%, 90%, and 95% removal efficiency). The model specifications used for model development in the absorber, and stripper are shown in Table 5. The selected specifications are recommended for rate based model of the CO<sub>2</sub> capture process in literatures [5].

**Table 5:** Absorber and stripper column parameters

Specification	Value	
	Absorber	Stripper
Number of stages	15	15
Operating pressure	1 bar	1.6 bar
Pressure drop	0.1 bar	0.1 bar
Re-boiler	None	Kettle
Condenser	None	Partial-vapour
Packing Type	MELLAPAK, Sulzer, Standard, 250 Y	FLEXIPAC, KOCH, METAL, 1 Y
Packing height	24m	18m
Packing Diameter	18m	12m
Mass transfer coefficient method [6]	Bravo et al. (1985)	Bravo et al. (1985)
Interfacial area method	Bravo et al. (1985)	Bravo et al. (1985)
Interfacial area factor	1.2	1.5
Heat transfer coefficient method	Chilton and Colburn	Chilton and Colburn
Holdup correlation [7]	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

## 2.4. Parameters Effect on Removal Process

At the beginning, open loop process is developed in Aspen Plus to get the exact efficiency which is specified in stripper column. The base case models are developed for 85%, 90% and 95% removal efficiencies. The selected solvent properties are used to develop the model and implemented model is used for further simulations. The implemented open loop 85% removal efficiency base case model is used to check the parameters' effect on removal efficiency and re-boiler duty. Main important parameters, such as absorber packing height and diameter, absorber pressure, flue gas and solvent stream temperature, are used to perform the parameters' effect on CO<sub>2</sub> removal efficiency. Similarly, in addition to above parameters, stripper packing height and diameter also varied to check the parameters' effect on re-boiler energy requirement. In order to study the effect of one parameter, other parameters are kept constant. Base case parameter values and range of the parameters are varied for sensitivity analysis is given in Table 6.

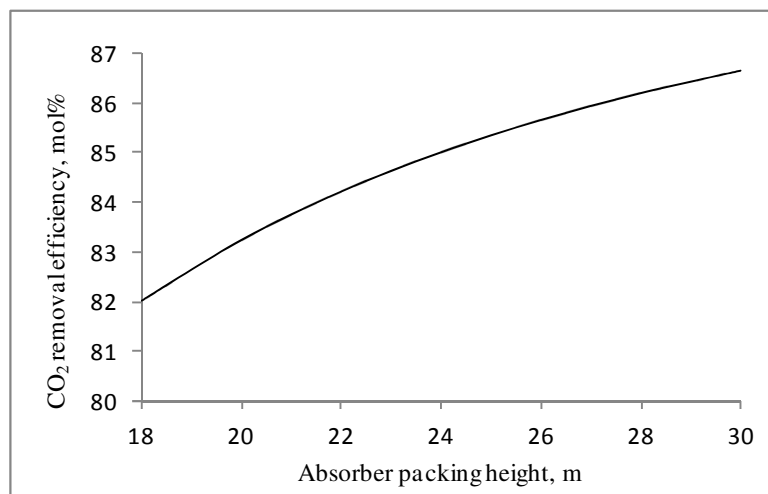
**Table 6:** Main input parameters considered for sensitivity analysis

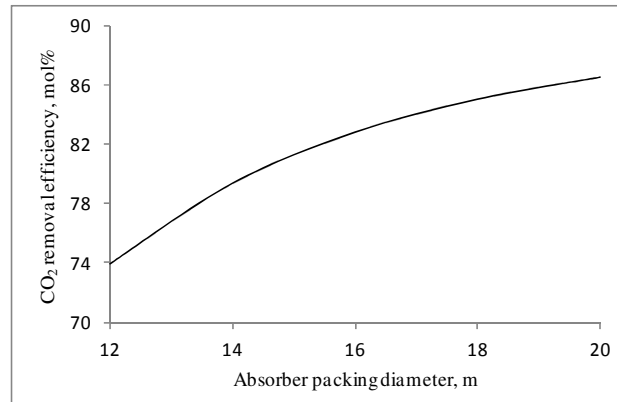
Input parameter	Base case value	Range of the parameter varied
Absorber packing height (m)	24	18-30
Absorber packing diameter(m)	18	12-20
Absorber operating pressure (bar)	1	0.8-1.2
Flue gas temperature (K)	313	303-313
Solvent temperature (K)	313	307-319
Stripper packing height (m)	18	14-24
Stripper packing diameter (m)	12	10-18

## 2.5. Parameters' Effect on Removal Efficiency

The removal efficiency variation with different parameters such as, absorber packing height and diameter, absorber pressure, flue gas and solvent stream temperature, are analyzed for the implemented base case model. Figure 2 and 3 shows how the CO<sub>2</sub> capture efficiency variation with the absorber packing height and diameter. Absorber packing height is varied from 18-30 m, and diameter is varied from 12-20 m to check the removal efficiency variation. Removal efficiency is increasing with packing height and diameter. Reason for that is, solution contact area is increasing with the increase of packing height and diameter. Therefore, residence time for reacting system is increased and removal efficiency increased. The results of the parameters' effect on removal efficiency are compared with the literatures to validate the sensitivity analysis [8].

**Figure 2:** CO<sub>2</sub> removal efficiency variation with absorber packing height



**Figure 3:** CO<sub>2</sub> removal efficiency variation with absorber packing diameter

The CO<sub>2</sub> removal efficiency variation with absorber column operating pressure is shown in Figure 4. Removal efficiency is increasing with the increase of absorber pressure.

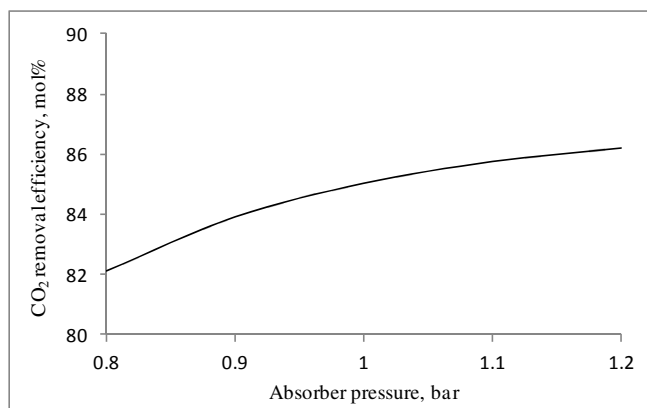
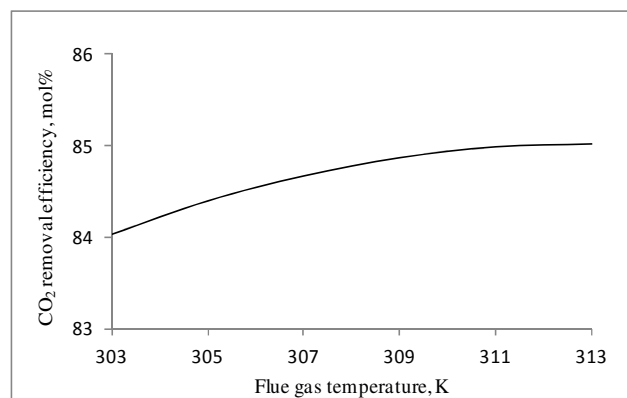
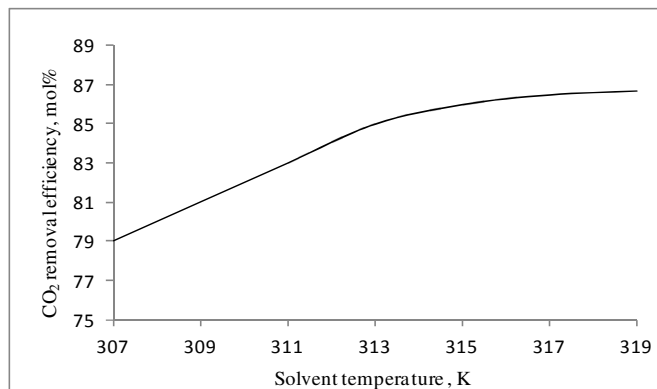
**Figure 4:** CO<sub>2</sub> removal efficiency variation with absorber pressure

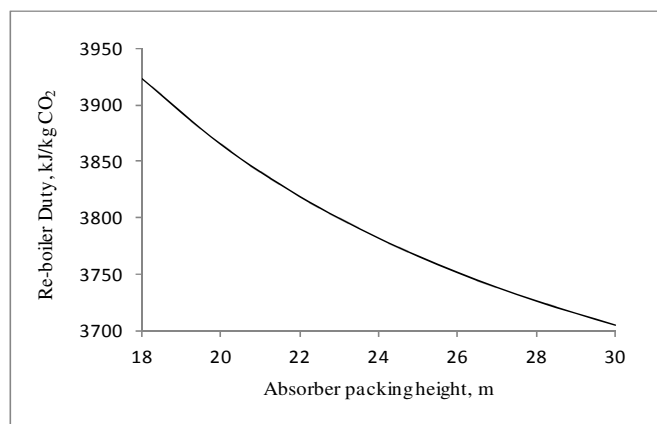
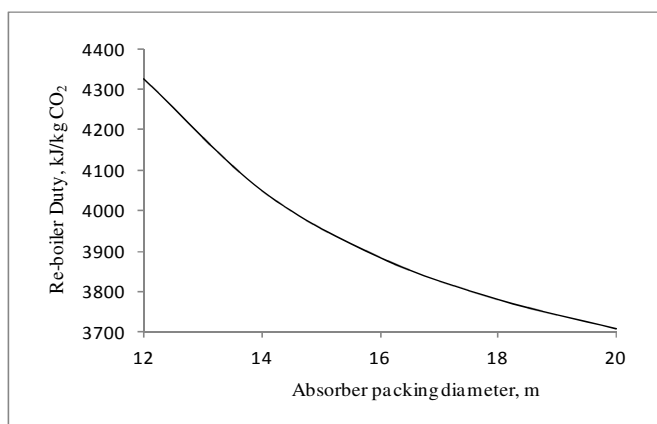
Figure 5 and 6 is presenting removal efficiency variation with flue gas and solvent temperature. The effect of flue gas temperature on removal efficiency is negligible. However, the removal efficiency is slightly increasing with the flue gas temperature. The simulations are carried out in solvent temperature range from 307-319 K. The removal efficiency is increasing with the increase of solvent temperature in the range of studied. As the solvent temperature increases, rate of reaction and diffusivity increase and efficiency of the CO<sub>2</sub> removal is increased.

**Figure 5:** CO<sub>2</sub> removal efficiency variation with flue gas temperature

**Figure 6:** CO<sub>2</sub> removal efficiency variation with solvent temperature

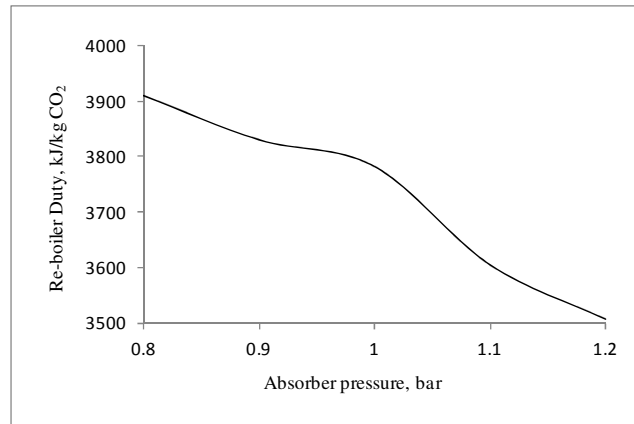
## 2.6. Parameters' Effect on Re-boiler Duty

Parameters' effect on re-boiler duty is analyzed to implement the removal process. Initially, open loop model is used to check the parameters' effect. Similarly, in addition to above parameters, stripper packing height and diameter also varied to check the parameters' effect on re-boiler energy requirement. For this sensitivity analysis, 85% of removal model is used. Figure 7-13 is shown re-boiler duty variation with above mentioned parameters. Regeneration energy requirement mainly can be categorized in to three parts: energy required to release the CO<sub>2</sub>, energy required to evaporate the water and energy needed for heat up the solvent in the stripper.

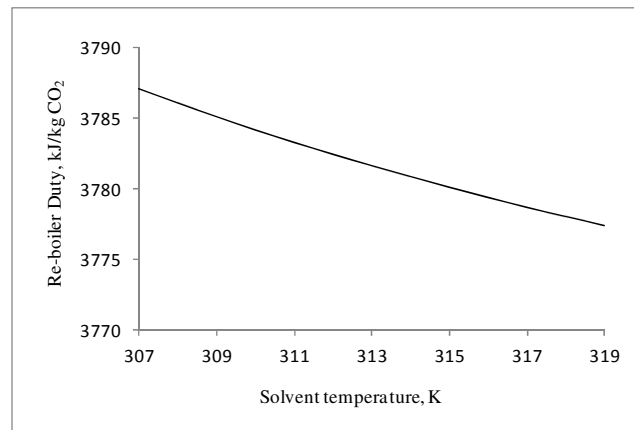
**Figure 7:** Re-boiler duty variation with absorber packing height**Figure 8:** Re-boiler duty variation with absorber packing diameter

As can be seen from Figure 7 and 8, re-boiler duty is drastically decreasing with the absorber packing height and diameter. When the absorber packing height and diameters increase, contacting surface area for the reaction medium is increase. This means that, amount of solvent required to react with CO<sub>2</sub> is reduced. As a result, required energy to heat the solvent in stripper is reduced. Therefore, regeneration energy is decreased in the re-boiler with packing height and diameter. The re-boiler duty variation with absorber pressure is given in Figure 9 and solvent and flue gas temperature effect on re-boiler duty is shown in Figure 10 and 11 respectively.

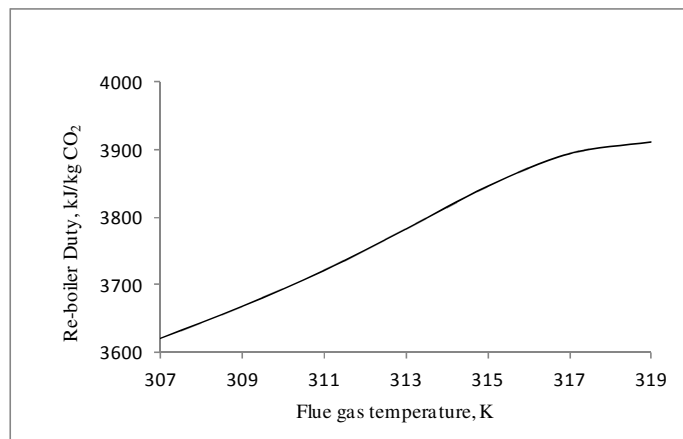
**Figure 9:** Re-boiler duty variation with absorber pressure



**Figure 10:** Re-boiler duty variation with solvent temperature



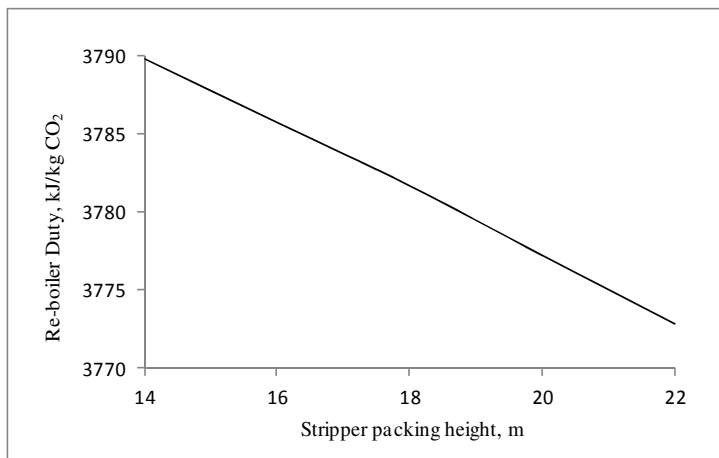
**Figure 11:** Re-boiler duty variation with flue gas temperature



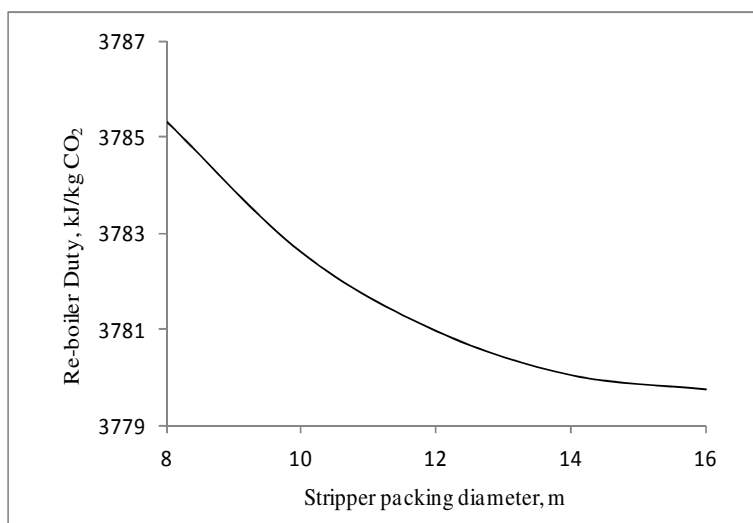


According to the Figure 11, re-boiler duty is increased with the flue gas temperature. The effect of stripper packing height and diameter is given in Figure 12 and 13. However, the effect on re-boiler duty is negligible compared to previous figures. In both cases, re-boiler duty is slightly decreasing with the packing height and diameter of stripper column.

**Figure 12:** Re-boiler duty variation with stripper packing height



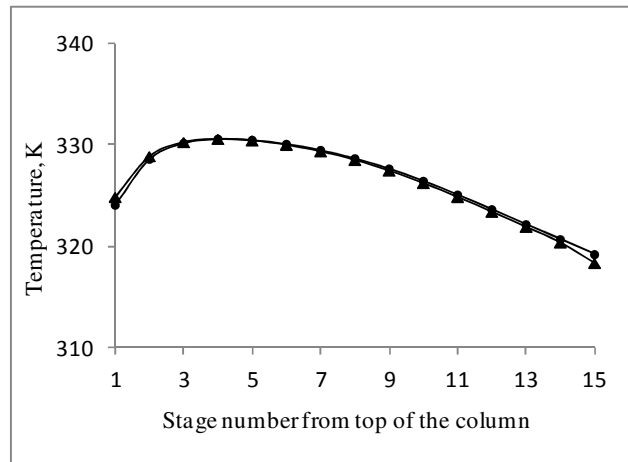
**Figure 13:** Re-boiler duty variation with stripper packing diameter



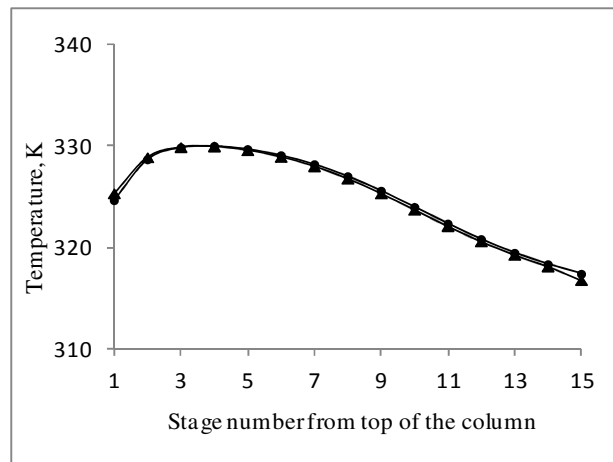
### 3. Complete CO<sub>2</sub> Removal Model

The CO<sub>2</sub> removal process models for 85%, 90%, and 95% efficiencies are implemented in Aspen Plus to check the exact re-boiler duty requirement. The closed-loop process model is developed with the recirculating lean amine stream back to the absorber unit. Make-up stream is added with MEA and water to fulfill the losses during the process. The required removal efficiency is specified in the stripper distillate stream. Finally, temperature and CO<sub>2</sub> loading profiles in absorber column is analyzed to check the model performance. The required re-boiler duties are 3781, 4050, and 4240 kJ/kg CO<sub>2</sub> for 85%, 90%, and 95% removal efficiency models respectively. Figure 14-16 is shown liquid and vapor phase temperature profiles variation in absorber column.

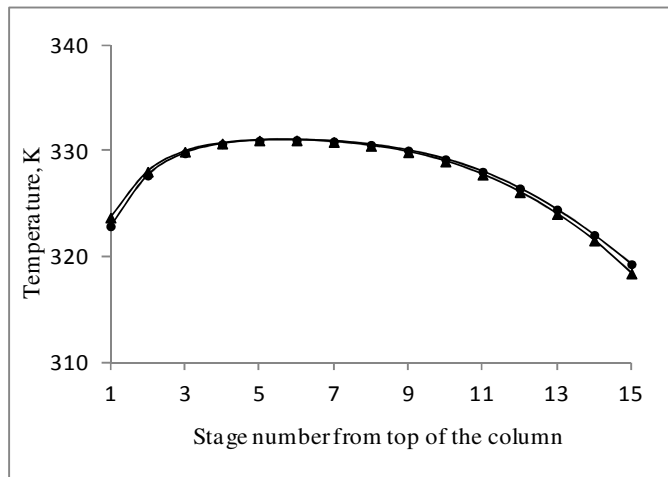
**Figure 14:** Temperature profiles in absorber for 85% removal efficiency; symbols refer to ●, Liquid phase; ▲, Vapour phase



**Figure 15:** Temperature profiles in absorber for 90% removal efficiency; symbols refer to ●, Liquid phase; ▲, Vapour phase

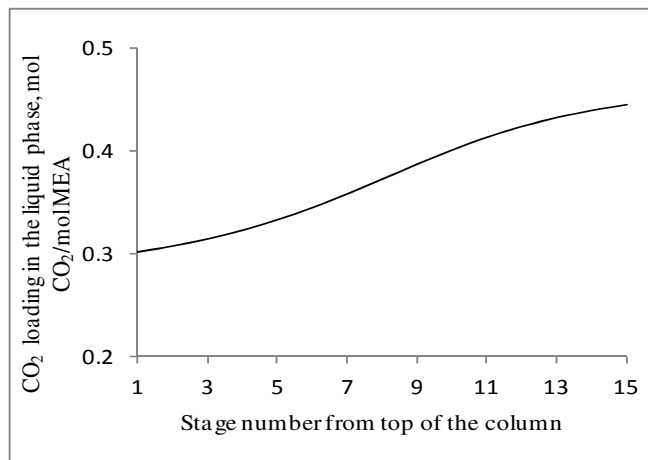


**Figure 16:** Temperature profiles in absorber for 95% removal efficiency; symbols refer to ●, Liquid phase; ▲, Vapour phase

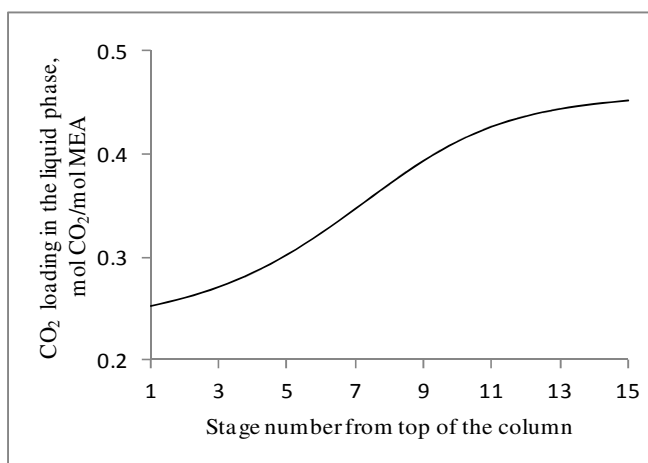


The maximum temperature is reached to 330K for both liquid and vapor phase models, and similar patterns are following in all three cases. Temperature bulge is shown in the top of the absorber column for all three models. Figure 17-19 is indicating that CO<sub>2</sub> loading profiles in absorber in liquid phase. The rich CO<sub>2</sub> loading is reached to around 0.45 mol CO<sub>2</sub>/mol MEA.

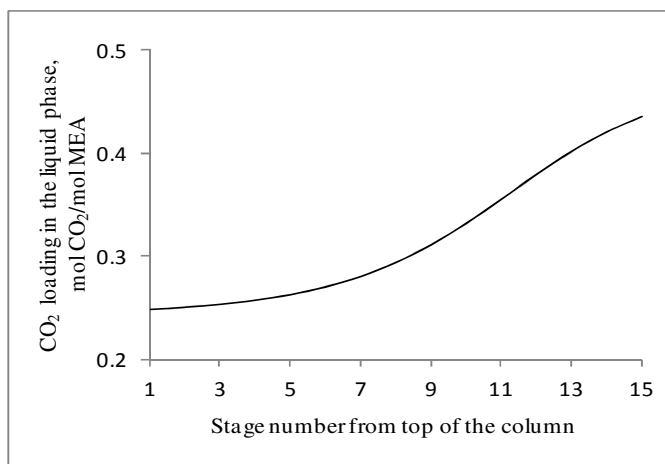
**Figure 17:** CO<sub>2</sub> loading profiles in absorber for 85% removal efficiency



**Figure 18:** CO<sub>2</sub> loading profiles in absorber for 90% removal efficiency



**Figure 19:** CO<sub>2</sub> loading profiles in absorber for 95% removal efficiency



The required make-up stream is calculated and given in Table 7 for all three models. Compare to the inlet solvent stream in an open-loop model, a small amount of make-up flow is required to continue the process with re-circulation. When the removal efficiency is increased, required amount of make-up flow also increased.

**Table 7:** Compositions of make-up stream

Process Model Removal Efficiency (mol %)	Amount of make-up stream	
	Water (kg/s)	MEA (kg/s)
85	17.90	0.22
90	25.15	0.21
95	29.52	0.36

#### 4. Conclusions

The implemented model is properly working for gas-fired power plant flue gas treating. Re-boiler duty values are given as 3781, 4050, and 4240 kJ/kg CO<sub>2</sub> for 85%, 90%, and 95% removal efficiency models respectively. Absorber packing height and diameter, absorber pressure, solvent and flue gas temperatures are positively effect on CO<sub>2</sub> removal efficiency. The packing height of absorber and stripper, solvent temperature and absorber pressure are negatively effect on re-boiler duty. The flue gas temperature has a slightly positive effect on re-boiler duty. Different types of packing materials effect on carbon capture process and regeneration energy requirement has to be analyzed in future studies.

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