

# Simulation and Optimization Study on Aqueous MEA-Based CO<sub>2</sub> Capture Process

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Chemical absorption with monoethanolamine (MEA) is the most common technology used in the CO<sub>2</sub> removal unit for a power plant. However, the application is hindered by its high energy consumption for absorbent regeneration. In this study, a rate-based model of the typical MEA-based CO<sub>2</sub> capture process was built for a power plant with Aspen Plus software. The thermodynamic model of ENRTL-RK was adopted. Temperature fields and the flow rates changes of components in absorber and stripper were obtained. And process analysis using the equilibrium stage model was performed to investigate the effects of operation parameters (CO<sub>2</sub> loading in lean solution and stripper pressure) on the regeneration energy consumption. With heat pump technology adopted to assist lean solution regeneration, two processes were proposed and the reboiler duties decreased to 2.77 GJ/t CO<sub>2</sub> and 2.38 GJ/t CO<sub>2</sub>, respectively, owing to the recovery of latent heat and part of sensible heat. Moreover, condenser duties were reduced obviously.

## 1. Introduction

A large increase in CO<sub>2</sub> concentration in the atmosphere is believed to be a chief factor that has caused the greenhouse effect and global climate change, which has aroused global concern (Bryce et al., 2015). The combustion of fossil fuels in generating station is one of the primary contributors. And in the near future, fossil fuels will continue to play a main role in the energy supply. CO<sub>2</sub> capture technology was proposed as one of promising ways to reduce and control CO<sub>2</sub> emission (Ding et al., 2016). As the simple process flow and operation, chemical absorption technology is considered as an ideal method. However, the wide application of solvent-based post-combustion CO<sub>2</sub> capture technology is hindered by its high energy consumption for absorbent regeneration and capital cost. According to literature data, installing a capture process for an existing coal-fired power plant would raise the generating cost by 80% and decrease generating capacity by 30% (DOE/NETL, 2010).

To reduce the energy consumption and the electric efficiency penalty, many efforts on solvent-based CO<sub>2</sub> capture technology have been made. One of the focuses is developing novel absorbents that possess more efficient capture performance and are more energy-saving than monoethanolamine (MEA), such as mixed amine solution (Mehassouel et al., 2016), ionic liquids (Jing et al., 2018), and porous liquid (James, 2016). But MEA solution has been regarded as a common solvent in practical industrial application due to its low cost, fast reaction rate and rich industrial experience. In addition, the optimization of operational parameters and process configuration for CO<sub>2</sub> capture system also attracts the attention of researchers. Based the conventional amine-based CO<sub>2</sub> capture configuration, a 0.4 GJ/t CO<sub>2</sub> decrease of reboiler duty was obtained after the optimization of operational parameters, such as CO<sub>2</sub> loading in lean solution, temperature of lean solution and stripper pressure, and economic evaluation was carried out (Li et al., 2016). A thermodynamic model of the CO<sub>2</sub> capture process was derived by Zhang et al. (2015) to analyse the mechanism and potential of energy saving. By comparing with a reboiler based stripper, an interheated stripper and a flash stripper, Lin et al. (2014) obtained the best energy performance from the stripper with a warm rich bypass and a rich exchanger bypass. Heat pump system is an economical and efficient way to realize heat recovery (Walmsley et al., 2017). The utilization of heat pump for CO<sub>2</sub> capture would reduce effectively regeneration energy consumption (Kansha et al., 2009).

Using flash evaporation and thermal vapor compression to reduce heat consumption of CO<sub>2</sub> capture processes, Zhang et al. (2014) indicated that the proposed CO<sub>2</sub> capture system reduced the specific heat consumption from 4.421 GJ/t CO<sub>2</sub> to 4.161 GJ/t CO<sub>2</sub>. An innovative process proposed by Yu et al. (2009) recovered the waste heat of flue gas and inter-stage compression, with the energy consumption decreasing to 2.75 GJ/t CO<sub>2</sub>. However, although various CO<sub>2</sub> capture processes have been presented and optimized aiming to minimize the heat energy penalty, most of them still belong to energy intensive processes due to solvent regeneration and there is still a long way to the target of 2 MJ/kg CO<sub>2</sub> (Song et al., 2017). Moreover, cooling duty is relatively less considered in the previous studies. Therefore, more work should be carried out on process optimization. The objective of this study is to design a novel CO<sub>2</sub> capture process with heat integration considering both heat and cooling energy consumptions. In this study, a rigorous and rate-based model of aqueous MEA-based CO<sub>2</sub> capture process was built in Aspen Plus software, and the effect of various important operation parameters on reboiler duty was investigated using sensitivity analysis. Considering both cooling energy consumption and heat consumption, two different configurations with heat pump were proposed and the improvement performances on energy demand were compared.

## 2. Methodology

### 2.1 Primary process flow

As shown in Figure 1, a conventional post-combustion CO<sub>2</sub> capture process was adopted for process simulation. Flue gases containing CO<sub>2</sub> were fed into absorber at the bottom and flow upward. The lean amine solution regenerated from stripper entered absorber at the top and contacted with the flue gases flowing in the counter-current direction to chemically react with CO<sub>2</sub>. The rich amine solution left the column bottom and entered to the top of the stripper through a lean/rich heat exchanger. And the amine absorbent heated by steam in the reboiler was regenerated and recycled back to the absorber. The produced CO<sub>2</sub> gas left from stripper at the top after condensation.

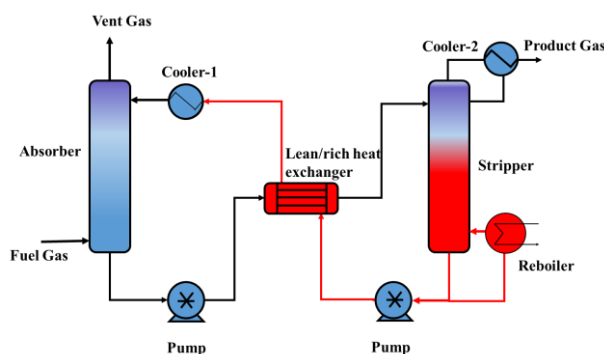


Figure 1: Flow sheets of a conventional amine-based post-combustion capture process.

According to the data of a 650 MW power plant with a 38.9 % net efficiency (EIA, 2013), the flow rate of flue gases was chosen to be 3,100 t/h. Supposing NO<sub>x</sub> and SO<sub>x</sub> were removed completely before they enter the CO<sub>2</sub> capture system, the flue gases fed into the absorber were assumed to be at 40 °C and 1.1 bar (Oh et al., 2016) containing 12 % CO<sub>2</sub>, 78 % N<sub>2</sub>, and 10 % H<sub>2</sub>O (Wang et al., 2011).

### 2.2 Thermodynamics

For thermodynamic properties of the CO<sub>2</sub>-MEA-H<sub>2</sub>O system, the unsymmetric electrolyte NRTL property method (ENRTL-RK) was used in the amines property package of Aspen Plus (Li et al., 2016). As shown in Table 1, reactions 1-5 were used to assume that all the ionic reactions were in equilibrium. For reaction models of Absorber/Stripper, instantaneous reactions (1, 3 and 5) and finite rate reactions 6-10 were consisted, and the following power law expression was used for rate-controlled reactions:

$$r = k \exp\left(-\frac{E}{RT}\right) \prod_{i=1}^N (X_i Y_i)^{Z_i} \quad (1)$$

Where  $r$  is the rate of reaction;  $k$ ,  $E$ ,  $T$  are the pre-exponential factor, activation energy (cal/mol) and absolute temperature (K), respectively;  $R$  is the universal gas constant, cal/(mol K);  $N$  is the number of components in the reaction;  $X_i$  is the mole fraction of component  $i$ ;  $Y_i$  and  $Z_i$  are the activity coefficient and the stoichiometric coefficient of component  $i$  in the reaction equation, respectively. And parameters were provided in Table 1.

Table 1: Parameters  $k$  and  $E$  in the finite rate reactions (Li et al., 2016)

No	Type	Reactions	$k$	$E$ (cal/mol)
1	Equilibrium	$2\text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{OH}^-$	-	-
2	Equilibrium	$\text{CO}_2 + 2\text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{HCO}_3^-$	-	-
3	Equilibrium	$\text{HCO}_3^- + \text{H}_2\text{O} \leftrightarrow \text{CO}_3^{2-} + \text{H}_3\text{O}^+$	-	-
4	Equilibrium	$\text{MEA}\text{H}^+ + \text{H}_2\text{O} \leftrightarrow \text{MEA} + \text{H}_3\text{O}^+$	-	-
5	Equilibrium	$\text{MEACOO}^- + \text{H}_2\text{O} \leftrightarrow \text{MEA} + \text{HCO}_3^-$	-	-
6	Kinetic	$\text{CO}_2 + \text{OH}^- \rightarrow \text{HCO}_3^-$	$1.33\text{e}+17$	13,249
7	Kinetic	$\text{HCO}_3^- \rightarrow \text{CO}_2 + \text{OH}^-$	$6.63\text{e}+16$	25,656
8	Kinetic	$\text{MEA} + \text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{MEACOO}^- + \text{H}_3\text{O}^+$	$3.02\text{e}+14$	9,855.8
9	Kinetic	$\text{MEACOO}^- + \text{H}_3\text{O}^+ \rightarrow \text{MEA} + \text{CO}_2 + \text{H}_2\text{O}$ (Absorber)	$5.52\text{e}+23$	16,518
10	Kinetic	$\text{MEACOO}^- + \text{H}_3\text{O}^+ \rightarrow \text{MEA} + \text{CO}_2 + \text{H}_2\text{O}$ (Stripper)	$6.50\text{e}+27$	22,782

### 3. Results and discussion

#### 3.1 Based case CO<sub>2</sub> capture process

A general regenerative Absorber/Stripper flowsheet was adopted as the based case design for MEA-based CO<sub>2</sub> capture process. Due to a large amount of flue gas for a 650MW power plant, four parallel process trains were adopted, and the flue gas of 775 t/h was treated by each process train containing an absorber column with packing of Ø12 m × H8 m and a stripper column with packing of Ø7.5 m × H8 m. The primary operation parameters for the based case were shown in Table 2.

Table 2: Primary operation parameters of the based case

CO <sub>2</sub> removal ratio	P <sub>abs</sub>	P <sub>strip</sub>
85 %	1.06 bar	2 bar
MEA concentration	Temperature of lean liquid, T <sub>lean</sub>	CO <sub>2</sub> load of lean liquid, α <sub>lean</sub>
30 wt. %	40 °C	0.25

For the based case, the temperature fields and gas phase compositions in the columns were discussed. As shown in Figure 2, the temperatures of both liquid and gas phase increased and then decreased in their flow direction, and the maximum temperatures occurred at the 4th stage. When lean solution with more MEA entered the absorber at the 1st stage, the streams were heated rapidly by large absorption heat released owing to chemical reaction. Then liquid was cooled by the upward gas phase, resulting in a large temperature difference at the bottom of absorber. However, a smaller temperature difference between liquid and gas was found in the stripper.

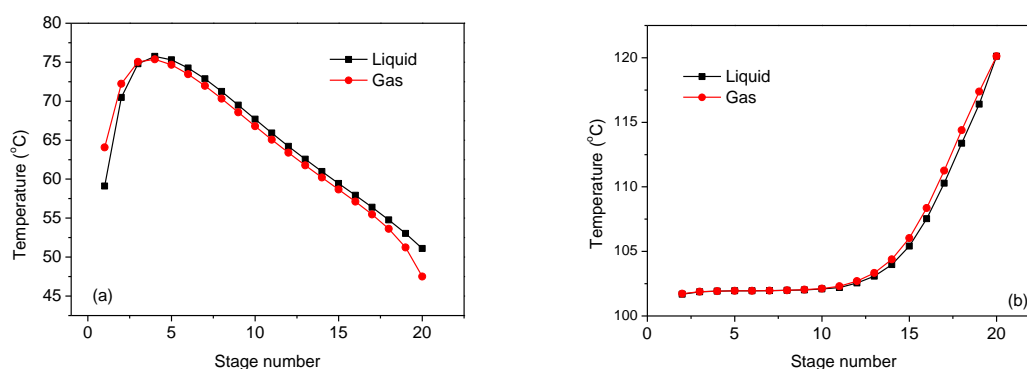


Figure 2: Temperature field of absorber (a) and stripper (b).

Then, the mass flow rates of liquid and gas phases were discussed. Figure 3a showed that a rapid change occurred for both liquid and gas at the stage 1-4, while the flow rates of H<sub>2</sub>O and CO<sub>2</sub> in gas phase had marked change according to Figure 3b. In the upper part, a high CO<sub>2</sub> absorption rate due to more free MEA and higher temperature resulted in a rapid reduction of upward carbon dioxide, and the higher temperature promoted water

evaporation into gas phase. However, both a lower CO<sub>2</sub> absorption rate and little water evaporation owing to lower temperature and saturated absorbent let to a gentle change of mass flow rates. A similar trend of flow rate of H<sub>2</sub>O in gas phase was found with the temperature field, so water vaporization could be decreased by controlling a lower temperature of lean solution entering into absorber.

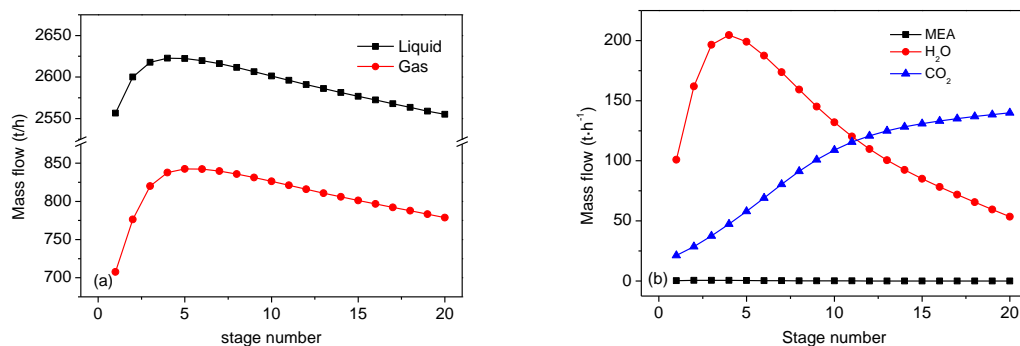


Figure 3: (a) The flow rates changes of liquid and gas phase in absorber; (b) the flow rates changes of gas components in absorber.

### 3.2 Parameter sensitivity study

Appropriate operation parameters in a CO<sub>2</sub> capture system can maintain stable operation and reduce the regeneration energy consumption. Figure 4a showed the influence of lean CO<sub>2</sub> loading and solution flow rate. With the increase of CO<sub>2</sub> loading in lean solution from 0.1 to 0.35, the flow rate of lean liquid increased from 1,465 t/h to 4,870 t/h and a rapid increase appeared at a larger lean CO<sub>2</sub> loading. However, the CO<sub>2</sub> regeneration duty presented a rapid reduction firstly and then an increase. And there was a lower value of 3.87 GJ/t CO<sub>2</sub> at the lean CO<sub>2</sub> loading of 0.2 mol CO<sub>2</sub>/mol amine. At a larger value of CO<sub>2</sub> loading, the increase of solvent circulation flow rate resulted in an increase in the sensible heat. When the lean CO<sub>2</sub> loading was below 0.2, a faster absorption was provided due to more MEA, but a larger amount of heat demand was required to regenerate solution at a low CO<sub>2</sub> loading.

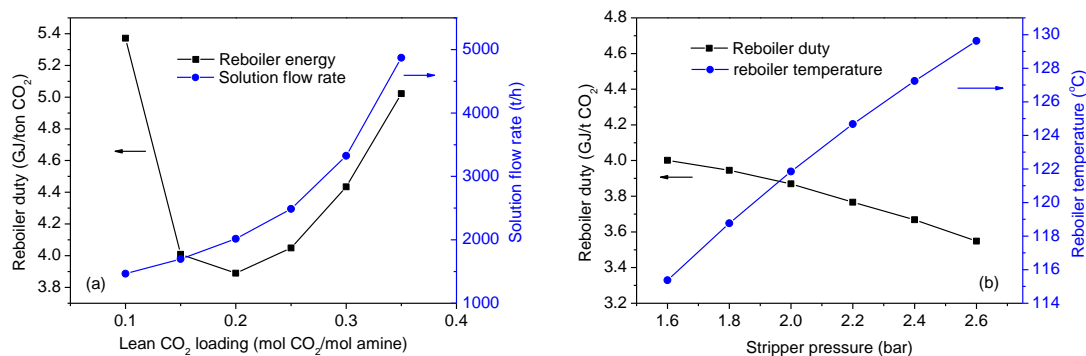


Figure 4: Effects of (a) lean CO<sub>2</sub> loading (b) stripper pressure on CO<sub>2</sub> regeneration energy.

Stripper pressure affects the partial pressure of components and the profile of temperature in stripper. Therefore, it is more meaningful for energy saving to elevate the stripper pressure. As shown in Figure 4b, obviously, a 0.45 GJ/t CO<sub>2</sub> reduction in the heat demand for MEA regeneration was presented when the stripper pressure increased from 1.6 bar to 2.6 bar. On the one hand, the water vaporization was restrained due to the increase of partial vapour pressure, and heat of water vaporization decreased. On the another hand, the higher stripper temperature promoted the CO<sub>2</sub> desorption process, and more sensible heat was recovered in lean/rich heat exchanger due to the higher temperature of lean solution from the bottom of stripper. However, the increase in stripper pressure also let to elevated reboiler temperature, which would intensify the degradation of amine and corrosion, and increase the maintenance cost and the accident risk. Meanwhile, the high pressure would increase equipment investment and preparation difficulty during the period of design and preparation. In addition, higher quality steam from vapour system was required to reach higher temperature, resulting in a lower

power plant efficiency. Therefore, in this study, 2.0 bar was chosen as a suitable pressure with reboiler temperature 121.9 °C and regeneration duty 3.87 GJ/t CO<sub>2</sub>.

### 3.3 Process Optimization

In the conventional process, CO<sub>2</sub> and vapour at a higher temperature from the top of stripper are cooled directly by a condenser and the condensed water is as the reflux back to stripper. Hence, more sensible heat and latent heat are not recovered and utilized effectively. Moreover, more cooling water is required. Based on the optimized operational parameters, two capture processes with heat pump technology were proposed and illustrated to further reduce the energy consumption.

For Configuration-1 shown in Figure 5a, the top stream of stripper (103.4 °C, 2 bar) was compressed by a compressor (isentropic efficiency: 0.85, mechanical efficiency: 0.85) to improve its energy quality. Then, the compressed stream (334.3 °C, 15 bar) exchanged heat with the lean solution from the bottom in HX-2 to a gas-liquid mixed stream (131.8 °C). Hence, the latent heat and partial sensible heat were recovered to provide regeneration energy in HX-2. Through an expander, the stream at a low pressure (2 bar) and temperature (82.2 °C) entered into a flash to separate CO<sub>2</sub> after cooled to 40 °C. Due to the heat supply from heat pump system, reboiler duty was decreased observably from 3.87GJ/t CO<sub>2</sub> to 2.77 GJ/t CO<sub>2</sub>.

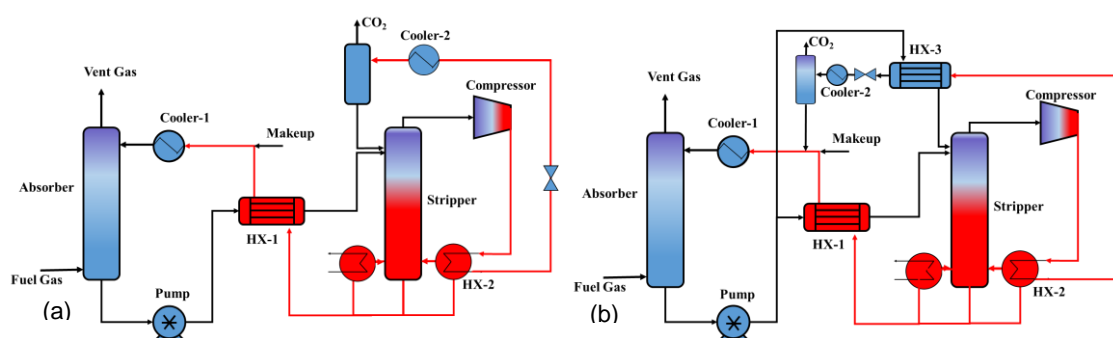


Figure 5: The proposed CO<sub>2</sub> capture processes assisted heat pump: (a) Configuration-1; (b) Configuration-2.

In Configuration-2, the compressed stream leaving from HX-2 was fed directly into HX-3 to heated part of rich solution (mass split ratio: 0.5: 9.5), and then was expanded. After cooled to 40 °C by Cooler-2, gas and liquid phase were separated, and the liquid was mixed into lean solution from the lean/rich heat exchanger (HX-1). The stream leaving stripper was heated to a higher temperature by the partial rich solution (119.3 °C) from HX-3, and a higher quality stream was obtained to assist the regeneration process. Therefore, the reboiler duty is reduced further to 2.38 GJ/t CO<sub>2</sub>.

Table 3: Performance comparison of different processes (GJ/t CO<sub>2</sub>)

	Based case	Parameter optimization	Configuration-1	Configuration-2
Cooler-1	1.66	1.27	1.27	1.30
Cooler-2	1.21	1.15	0.49	0.11
Cooling energy consumption	2.87	2.42	1.76	1.41
Reboiler	4.05	3.87	2.77	2.38
Compressor	--	--	0.50	0.58
Regeneration energy consumption	4.05	3.87	3.27	2.96

In a capture system, the energy consumption could be divided into two categories: regeneration energy consumption and cooling energy consumption. In Table 3, two kinds of energy consumption for based case, the process after parameters optimization, and two configurations with heat pump system were calculated and compared. Compared with based case, as result of effective recovery of sensible and latent heat in Configuration-2, regeneration energy consumption and cooling energy consumption were reduced by 26.9 % and 50.9 %, respectively.

#### 4. Conclusions

A typical CO<sub>2</sub> capture process using MEA as a solvent in a coal-fired power plant was simulated and designed to be less energy consumption. All simulations were performed using Aspen Plus software. The thermodynamic model of ENRTL-RK was adopted and the equilibrium stage model was used to analysis the characteristics of columns. The changes of temperatures and flow rates of all components indicated that temperature field had a large impact on absorption/desorption performance, so structuring an appropriate temperature field could help to reduce energy consumption.

The effects of two operation parameters on regeneration duty were discussed. Compared with based case, the regeneration duty decreased to 3.87 GJ/t CO<sub>2</sub> from 4.05 GJ/t CO<sub>2</sub>. Application of Heat pump system effectively recovered latent heat and partial sensible heat, and the proposed configuration reduced the system's regeneration energy requirement and cooling energy consumption by 26.9 % and 50.9 %.

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