

Computer Simulation and Process Improvement of CO₂ Capture by Chemical Absorption

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By means of computer simulation, we improved the chemical-based CO₂ capture system with Monoethanolamide (MEA) absorbent on the PRO/II software platform. The research results of the capture process provides suggested optimal process parameters for large-scale flue gas CO₂ capture projects, in an attempt to reduce the cost of capture, reduce energy consumption and increase the rate of CO₂ recovery. The chemical-based CO₂ adsorption model was established in this paper, with which we analysed the effects of various absorption solution parameters (volume flow rate, temperature, concentration, etc.) on CO₂ absorption rate, obtaining optimum process parameter.

1. Introduction

Since the industrial revolution, carbon dioxide emissions have increased, and the greenhouse effect has been greatly enhanced. Coal-fired CO₂ capture and storage (CCS) is an effective way to control CO₂ emissions (Mathias et al., 2010; Dong et al., 2015; Wang et al., 2016; Carotenuto et al., 2016). Among all the CO₂ capture technologies, the chemical absorption method receives widespread application because of its high absorption efficiency, large handling capacity, good removal effect, and coming-of-age technology. MEA solvent has been successfully applied to the absorption of CO₂ in flue gas (Niu et al., 2012; Schneider and Górak, 2001).

Most of previous studies are experimental approaches to the influence of parameters (such as absorption solution temperature and flue gas CO₂ concentration) on CO₂ absorptivity (Ömer et al., 2012; Zhang et al., 2016; Park and Kang, 1995). However, they lack the comprehensive consideration of parameters influencing CO₂ absorption rate, and require high cost and sophisticated process (Gebicke et al., 1993; Gebicke et al., 1993). The alternative of chemical process simulation provides an access to computer simulation of flue gas CO₂ capture, which overcomes the above shortages but instead obtains reliable simulation results, capable of guiding industrial applications. (Chen et al., 2014)

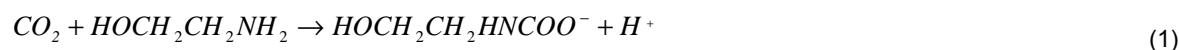
In this paper, from the perspective of industrial application, by analyzing the change of MEA absorbance under various absorption conditions, we monitored the response of CO₂ absorption effects to absorption condition. Meanwhile, some suggestions were proposed according to the simulation results, which provides a reference for industrial application.

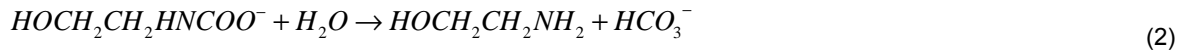
2. The process of using chemical absorption method to capture CO₂

2.1 The principle of CO₂ being absorbed by MEA

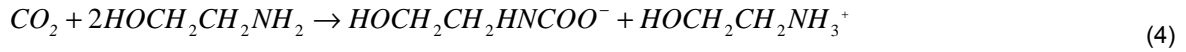
MEA solution is weakly alkaline. When contacting acid flue gas (CO₂), MEA reacts with it to generate unstable salts in the process of gas-liquid mass transfer in the absorption equipment. In the conditions of heating and air stripping, the product will be decomposed to release CO₂, which regenerates the absorption liquid.

The reaction between MEA and CO₂ is as follows:





The complete chemical reaction is:



The reaction is a reversible exothermic reaction, which allows CO₂ to be desorbed from the MEA solution by heating, while the MEA solution is regenerated. According to the total reaction formula, it can be said that the ideal maximum load of CO₂ absorbed by MEA solution is 0.5molCO₂ / mol MEA (Mudhasakul et al., 2013).

2.2 A brief description of the process

The typical process of recovering flue gas by the MEA method is shown in Figure 1.

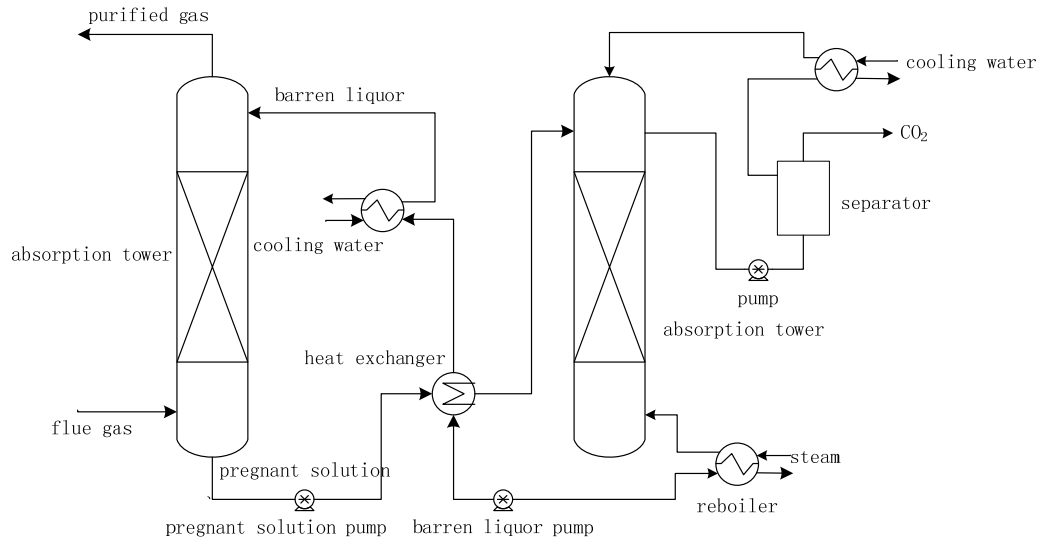


Figure 1: Process flow diagram of absorption and desorption for CO₂ capture

During the absorption process, the absorption solution flows downward from the top of the absorption tower, transfers mass with flue gas on each tray, absorbs flue gas CO₂ and converts from CO₂-lean solution to CO₂-rich solution. The CO₂-rich liquid flows into the desorption tower where the CO₂ is desorbed and the absorption solution is regenerated.

CO₂ load is used to represent the amount of CO₂ to be dissolved per mole of absorbent in the absorption liquid. In the absorption process, CO₂ load in the absorption solution should be increased as much as possible to approach CO₂-saturated state, so that helping reduce the circulation volume of the absorption fluid.

$$CO_2 \text{ load} = \frac{\text{The } CO_2 \text{ amount in the absorption liquid (kmol / m}^3\text{)}}{\text{The absorbent amount in the absorption liquid (kmol / m}^3\text{)}} \quad (5)$$

The flue gas entering the capture system contains a variety of ingredients: mostly N₂, CO₂ and O₂, and a small amount of water vapor and inert gas. In order to facilitate the simulation, the flue gas composition is simplified, and the simplified simulated flue gas composition, proportion and molar flow rate are shown in Table 1.

Table 1: The Composition and Molar flow rate of simulative flue gas

Flue gas compositions	Proportion (%)	Molar flow rate kmol/h
N ₂	81	115.451
CO ₂	14.5	644.935
O ₂	4.5	35.829

3. Process parameters simulation optimization

On the basis of the process mechanism model, chemical process computer simulation technology describes chemical process by using mathematical methods, and performs material balance, heat balance, equipment size estimation, energy analysis, and evaluation on the environment and economy (De et al., 2013; Geraili et al., 2014; Volesky, 2003). In recent years, chemical process computer simulation technology has developed continuously, with Pro / II software as the representative (Özel and Altan, 2000; Pantelides, 1998).

3.1 Absorption process modeling

In the practical application of flue gas CO₂ stripping, the flue gas flow is large and fluctuates up and down within a certain range, but the absorption solution flow needs to be adjusted according to the fluctuation of the gas phase. Therefore, it is necessary to select the appropriate bubble cap tray to respond effectively to the change of gas load and fluid load. Pro/II software is used to simulate the process, in which we import the simulation data of the composition and proportion of flue gas fed through the inlet of the tower bottom, as shown in Figure 2.

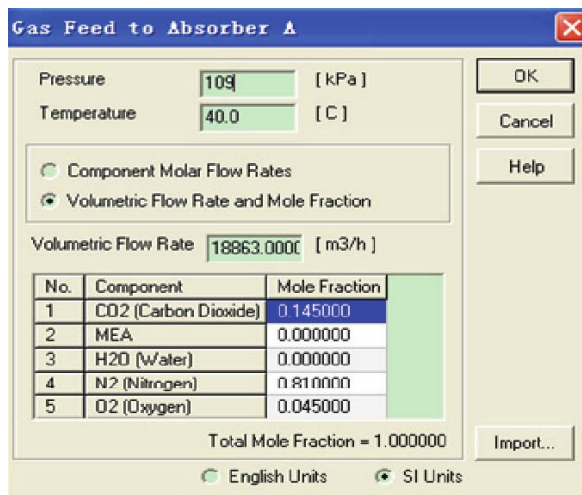


Figure 2: Interface of flue gas feed

Figure 3 shows the interface of absorber data input:

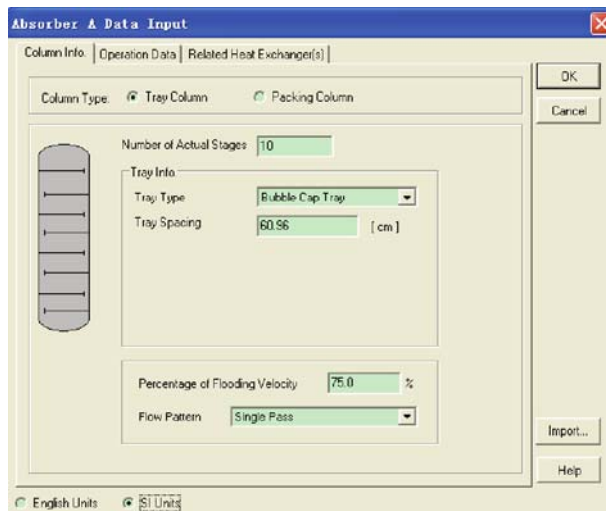


Figure 3: Interface of absorber data input

3.2 Study on Absorption Characteristics of MEA Solution

3.2.1 The Effect of Absorption Flow Rate on Absorption Rate

The MEA solutions with the mass fractions of respective 10%, 20% and 30% were used as the absorption solution to simulate the absorption process. The effect of the absorption solution volumetric flow rate on absorptivity was investigated in this paper, and their relationship curves are plotted in Figure 4.

It can be seen from Fig. 4 that when the concentration of MEA in the absorption solution is low, CO₂ absorptivity gradually increases with the increase of the absorption solution volumetric flow rate, albeit smaller in magnitudes. When the absorption solution volumetric flow rate is small, the MEA molar flow rate is not high enough to absorb CO₂ in most of the flue gas. Afterwards, CO₂ absorptivity increases slowly. This is because the driving force of gas-liquid mass transfer is reduced, and an extra amount of absorption solution is added, which continues to lower down CO₂ concentration. Nevertheless, the flue gas CO₂ cannot be absorbed completely no matter how much CO₂-lean solution is added, because the minimum size of CO₂ pressure in purified gas is no less than the equilibrium partial pressure in the absorption solution and the theoretical number of trays is not infinite. In this case, not only cannot the CO₂ absorptivity be enhanced effectively, but the system operation cost will increase with the increase of the circulation volume of absorption solution. Therefore, when the absorbent in the absorption solution is sufficient, on the premise of suitable liquid-gas ratio, the absorption solution volumetric flow rate should be reduced as much as possible to reduce CO₂ capture cost.

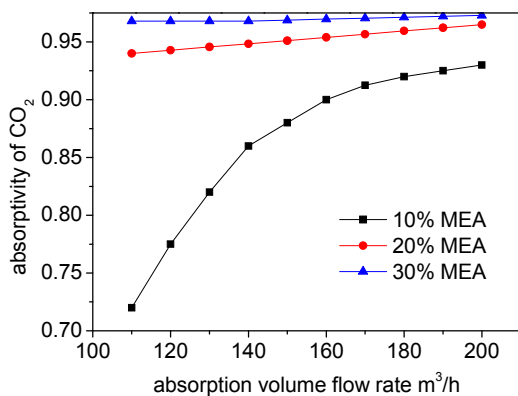


Figure 4: Effects of absorption solution volumetric flow rate on CO₂ absorptivity

3.2.2 Effects of absorption solution temperature on CO₂ absorptivity

The MEA solutions with the mass fractions of respective 10%, 20% and 30% were used as the absorption solution to simulate the absorption process. We assumed absorption solution volumetric flow rate as 130m³/h, and accordingly conducted a computer simulation on the effect of absorption solution temperature in the tower inlet on absorptivity. Their relationship curves are plotted in Figure 5.

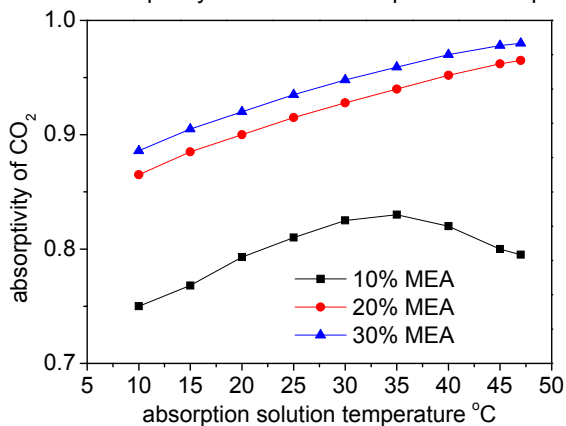


Figure 5: Effects of absorption solution temperature on CO₂ absorption rate

It can be seen from the figure that when the concentration of MEA in the absorbing liquid is small, the CO₂ absorption increases first and then decreases with the increase of the absorption liquid temperature. When the MEA mass fraction is small, the activity of MEA is enhanced with the increase of the temperature of the absorbing liquid. As a result, the reaction rate between MEA and CO₂ is accelerated, and the CO₂ absorbability is enhanced. When the temperature of the absorption liquid continues to rise, desorption reaction occurs, reducing CO₂ absorption rate. When the MEA mass fraction is large, the reaction rate of MEA and CO₂ increases, rendering CO₂ desorption more difficult, and thus CO₂ absorption rate is increasing continuously.

In engineering applications, if the MEA concentration of an absorption solution is high, the higher temperature the absorption liquid have, the higher rate of CO₂ absorption it has. It is possible to reduce the degradation rate of MEA by adding a small amount of antioxidant to the absorbing liquid, and to appropriately increase the absorbing liquid temperature, which is advantageous for reducing the consumption of cooling water required in the lean liquid cooler. Generally, the temperature of the absorption liquid is controlled at about 40°C.

3.2.3 The relationship between absorption solution volumetric flow rate and CO₂ load

The MEA solutions with the mass fractions of respective 10%, 20% and 30% were used as the absorption solution to simulate the absorption process. We assumed the absorption solution's volumetric flow rate as 130m³/h and its temperature as 40°C, and accordingly conducted a computer simulation on the relationship between absorption solution volumetric flow rate and CO₂ load. Their relationship curves are plotted in Figure 6.

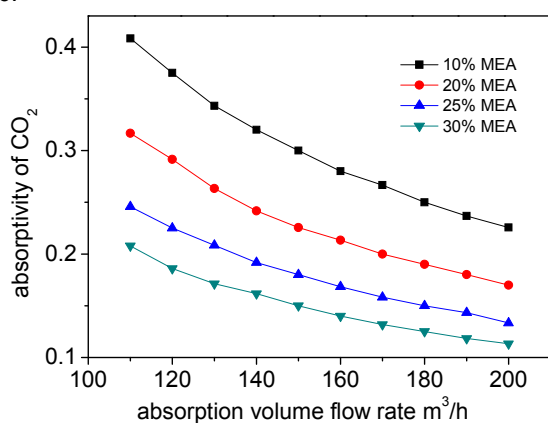


Figure 6: The relationship between absorption solution volumetric flow rate and CO₂ load

The simulation results show that when the concentration of absorption solution is fixed, CO₂ load in CO₂-rich fluid will be increasingly smaller with the increase in absorption solution volumetric flow rate, and the CO₂-rich solution will be farther and farther away from CO₂-saturated state. The dissolved amount of the absorption solution will not be utilized to the fullest degree. At a given absorbed liquid volumetric rate, the smaller the CO₂ load in the CO₂-rich liquid is, the more difficult it is to desorb CO₂ in the desorption tower.

4. Conclusion

With computer simulation, the process of MEA-based CO₂ capture was studied by using Pro/II software. Through our research into the effects of parameters such as absorption solution's volumetric flow rate and its temperature on CO₂ absorptivity and CO₂ load, we drew the following conclusions:

- (1) When the MEA content in the solution is insufficient, the CO₂ absorptivity increases with the increase of the absorption solution's volumetric flow rate. When the amount of MEA in the solution is sufficient, the absorption solution volumetric flow rate has little effect on CO₂ absorptivity. For flue gas with low CO₂ volumetric fraction, CO₂ absorption should be done at the minimum volumetric flow rate, so as to reduce the operating cost of the CO₂ capture system.
- (2) For MEA solution with low mass fraction and insufficient MEA, CO₂ absorptivity increases first and then decreases with the increase of absorption solution temperature. For MEA solution with high mass fraction and sufficient MEA, CO₂ absorptivity increases at a relatively small magnitude with the increase of absorption solution temperature. The absorption liquid temperature should be controlled, and generally the temperature is controlled at about 40°C.
- (3) The higher the absorption solution volumetric flow rate is, the smaller the CO₂ load in the outlet of the CO₂-rich liquid is; the higher MEA concentration the absorption liquid has, the smaller the CO₂ load in the outlet of

the CO₂-rich liquid is. As the absorption solution flows down, its CO₂ load gradually increases at an increasingly enlarged magnitude.

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