Meso-scale CFD Modelling of CO₂ Capture by Aqueous Ammonia Part II: Parameter Analysis

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Abstract. On the foundation of the study on the CFD modeling in the Part I, the various operating conditions including liquid inlet flow, gas inlet flow, CO₂ inlet mass fraction, ammonia concentration and pressure on CO₂ capture process are examined in this paper. The modeling results are found to be consistent with the reported experimental results on CO₂ absorption rate at different operating parameters, which verifies the feasibility of the model. Meanwhile, the comparison provides a reliable basis for the optimization of process parameters.

Introduction

Nowadays, the research on the improvement of the absorption rate has been the focus of the CO₂ capture industry, which facilitates the development of the CFD simulation of the capture process. Then the periodic packing units are widely used in the studies [1,2,3]. Based on the two-phase flow model with chemical reaction built in Part I, various operating conditions such as liquid inlet flow, gas inlet flow, CO₂ inlet mass fraction, ammonia concentration, and pressure are investigated in this paper to establish their effects on CO₂ absorption rate during the absorption process.

Parameters Analysis

To minimize the computation, single REU (Representative elementary units) model is used for parameter study, as shown in Fig. 1.

![Structured element unit](image1.png) ![Meshing unit](image2.png)

(a) Structured element unit  (b) Meshing unit

Figure 1. Single REU model.

Liquid Flow Rate

The liquid flow rate is varied from $Q_l=0.6\times10^4$ L/h to $Q_l=7.2\times10^4$ L/h. The other conditions are set as: the gas flow rate, $Q_g=3000$ m³/h; the mole fraction of $NH_3=0.05$, the mass fraction of CO₂=0.14, the operating pressure=atmospheric pressure and the temperature=300K. The CO₂ absorption rate at various liquid flow rates obtained from both the present simulation and reported experiment [4] is shown in Fig. 2. It is important to mention that the liquid flow rates in the experiment are much higher than the simulation. The same trend for CO₂ absorption rate is found in both experimental and...
simulation results. It shows that CO₂ absorption rate improves with the increase of liquid flow rate. After reaching a peak, the liquid flow rate no longer has noticeable influence on CO₂ absorption rate. This phenomenon can be explained as follows: when the liquid inlet flow is small, increasing the flow of ammonia can help increase the wetting area of packing surfaces, thus effectively increases the gas-liquid contact area, which leads to higher degree of chemical reaction; On the other hand, excessive liquid flow will reduce the gap between packing materials and gas flow areas, which could shorten the reaction time. The simulation result shows the maximum CO₂ absorption rate at the liquid flow rate \( Q_l = 6.0 \times 10^4 \text{ L/h} \).

![Figure 2. Trends of CO₂ absorption rate with different liquid inlet flow.](image)

(a) Simulation  
(b) Experiment [4]

The effective mass transfer area obtained from the present simulation with different liquid flow is shown in Fig. 3. The effective mass transfer area in packing element is defined as the interfacial area developed by the liquid phase per unit volume. It is shown from the figure that effective mass transfer area improves with the increase of liquid flow rate. This is due to fact that the higher portion of the packing surface area being wetted is available to participate in the mass transfer.

**Gas Flow Rate**

The gas flow rate is varied within the range of \( Q_g = 2400 \text{ m}^3/\text{h} \sim Q_g = 15000 \text{ m}^3/\text{h} \). The liquid flow rate is \( Q_l = 3.0 \times 10^4 \text{ L/h} \) while other boundary conditions remain the same as before. The change of CO₂ absorption rate versus gas flow rate is demonstrated in Fig. 4 for both the simulation and experimental results. Although gas flow rates between the simulation and experiment are different, the same trend
of development is observed. The CO$_2$ absorption rate decreases with the increase of gas flow rate and finally reaches a point of steady state where the gas flow rate has no further influence. This can be explained as that the higher gas flow rate reduces the gas residence time in structured packing, which means the less contact time between the gas and ammonia.

Figure 4. Trends of CO$_2$ absorption rate with different gas inlet flow.

The effective mass transfer area versus gas flow rates is plotted in Fig. 5. The results in figure show that effective mass transfer area decreases with the increase of gas flow rate. This behavior can be explained as that the lower portion of packing area being wetted due to higher gas volume fraction occupied on the packing surface, resulting the decrease of the mass transfer.

The effective mass transfer area versus gas flow rates is plotted in Fig. 5. The results in figure show that effective mass transfer area decreases with the increase of gas flow rate. This behavior can be explained as that the lower portion of packing area being wetted due to higher gas volume fraction occupied on the packing surface, resulting the decrease of the mass transfer.

Figure 5. Percentage of effective mass transfer area with different gas inlet flow.

CO$_2$ Mass Fraction

The CO$_2$ inlet mass fraction or CO$_2$ loading is varied from 0.04 to 0.16. The liquid flow rate is kept at $Q_l=3.0 \times 10^4$ L/h, the gas flow rate is $Q_g=3000$ m$^3$/h and the mole fraction of NH$_3$ is 0.05. Other boundary conditions are kept the same as before. The results in Fig. 6 demonstrate that CO$_2$ absorption rate decreases with the increase of CO$_2$ mass fraction as confirmed in both the experiment [5] and simulation. When the CO$_2$ initial concentration is increased, the molar ratio of ammonia to carbon dioxide is reduced from the perspective of chemical equilibrium, which results in the reduction of the driving force for the forward reaction and is not favorable for the absorption of CO$_2$. 

Figure 6. CO$_2$ absorption rate with different CO$_2$ mass fraction.
NH\textsubscript{3} Mole Fraction

The NH\textsubscript{3} inlet mole fraction is varied between 0.03 and 0.6. Other boundary conditions remain the same as before. The results in Fig. 7 show that CO\textsubscript{2} absorption rate increases with the increase of NH\textsubscript{3} mole fraction as confirmed by both the experiment and simulation. The increase of ammonia concentration in this case is equivalent to an increase of the molar ratio of ammonia and carbon dioxide and acts as the forward driving force of the chemical reaction to stimulate CO\textsubscript{2} absorption. However, the high concentration of ammonia used in simulation i.e., above 50% causes the decreasing trend of CO\textsubscript{2} absorption rate. This can be explained as that the high concentration of ammonia or high mole ratio of NH\textsubscript{3} to CO\textsubscript{2} can lead to precipitation of the solid in the CO\textsubscript{2} rich stream, which can reduce the CO\textsubscript{2} absorption rate. Also the higher concentration of NH\textsubscript{3} causes the volatilization of ammonia, which will directly affect the effective utilization of the absorbent. Therefore, the high concentration of ammonia is not recommended for the views of economic and practical operations.

Operating Pressure

The operating pressure is varied from 0.6 to 2.0 atms. The mole fraction of NH\textsubscript{3} is kept at 0.05 and other boundary conditions remain the same as before. The results in Fig. 8 show that the CO\textsubscript{2}
absorption rate increases with the rise of operating pressure. Given the high energy penalty and equipment costs for operations at high pressure, it is generally recommended to operate at atmospheric pressure.

![Graph](image)

Figure 8. Trends of CO2 absorption rate with different operating pressure.

**Conclusion**

A range of operating parameters including liquid flow rate, gas flow rate, CO2 mass fraction, ammonia concentration and pressure are examined for their effects on CO2 absorption rate. The results of simulation are consistent with the reported experiment by showing the same trend of variation for CO2 absorption rate at different parameters. The present work confirms the feasibility of the REU model and paves the way for further simulation of carbon capture process over a large area of packed columns.

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**References**


