NUMERICAL SIMULATION OF CO₂ ABSORPTION BY AMP SOLUTION IN STRUCTURED PACKING WITH DIFFERENT PARAMETER CONDITION

by

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The FLUENT software is utilized in this research to simulate the CO₂ absorption process by 2-amino-2-methyl-1-propyl (AMP) alcohol through numerical simulation. A mathematical model is established to represent the mass transfer process between the AMP alcohol solution and CO₂. Various operating parameters, such as the molar fraction of the solution, gas mass fraction, pressure, and gas-flow velocity, are investigated to calculate the absorption efficiency of CO₂ under different conditions. The distribution of the product reveals that the AMP alcohol carbamate product more readily infiltrates the surface of the unit model when the gas phase velocity is relatively low. In contrast, the product AMP alcohol carbamate tends to accumulate in the upper half of the unit model when the gas phase velocity is relatively high. Sixteen simulation conditions are summarized to determine the optimal parameters. These optimal parameters include a AMP alcohol molar fraction of 0.4, atmospheric pressure, a flue gas-flow velocity of 0.0737 m/s, and a CO_2 mass fraction of 0.12. This research serves as a valuable reference for engineering applications related to CO₂ absorption using AMP alcohol solutions, providing essential technical support in the fight against climate change.

Key words: *AMP*, numerical simulation, CO₂ absorption, chemisorption, carbon emission reduction

Introduction

In recent years, with the aggravation of the GHG, global temperatures have continued to rise, and the emission of GHG CO_2 has garnered increasing concern. Industrial production relies on coal, petroleum, natural gas, and other sources as energy [1], making them the primary sources of CO_2 emissions in industrial processes following combustion and usage. Globally, coal is the main fuel for power generation, with its share reaching 36.4% in [2]. For the cement industry, CO_2 emissions account for about 7-8% of total global CO_2 emissions [3]. It is therefore, important to limit and sanction anthropogenic greenhouse gas and related sectoral CO_2 emissions.

Given the current development landscape, the thermal power and cement industries employ three main methods to reduce carbon emissions: substituting traditional fuels with low carbon alternatives, enhancing unit heat efficiency, and implementing carbon capture and storage (CCS) technology [4]. In practical production, the availability of fuel sources for cement plants in

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each area, theoretical heat consumption limits for mineral products, and cement kiln clinker without viable alternatives, as well as potential disruptions to the cement production process by these methods, can impact the quality of the produced cement. Consequently, there is a growing interest in CCS technology that can be applied in the thermal power and cement industries.

Within the realm of CCS technology, post-combustion carbon capture technology and oxygen-enriched combustion technology are considered to be particularly well-suited for industrial applications. Oxygen-enriched combustion produces exhaust with a high CO₂ concentration, which is advantageous for the subsequent CO₂ capture process after water condensation [5]. Post-combustion carbon capture technology involves the enrichment and purification of CO₂ in post-combustion flue gas using absorbents and the reutilization of purified CO₂ in industrial production after compression and liquefaction [6]. The CO₂ absorption entails the flow of gas and chemical absorbents in a vertical tower (such as a packed tower) in a countercurrent mode, ensuring thorough mixing of gas and liquid through tower structures to maximize contact and ensure efficient gas absorption [7]. Presently, organic amine solutions are the most widely used in the industry.

Ethanolamine (MEA) was among the first amines used as an absorbent in the industry. However, in practical applications, several drawbacks were identified. The MEA as an absorbent requires relatively high temperatures, increasing energy consumption and leading to more severe equipment corrosion [8]. As a result, current research is focused on reducing the energy consumption during MEA regeneration in the desorption process [9].

Benamor and Aroua [10] used a laboratory stirred reactor and analyzed the experimental data for the determination of CO_2 uptake at different concentrations of methyl diethanolamine (DETA) at different temperatures and calculated the kinetic parameters related to the reaction, such as the number of reaction stages and the reaction rate constant. Feng *et al.* [11] and Kierzkowska-Pawlak *et al.* [12] found that in terms of uptake rate, CO_2 uptake by *n*-methyldiethanolamine (MDEA) was slower. Consequently, Ahmady [13] and colleagues proposed mixed CO_2 absorption using an ionic liquid, [bmim][BF4], in combination with MDEA. Their research on the absorption kinetics of CO_2 in MDEA + [bmim][BF4] water solutions at different temperatures and ionic solution concentrations, using a stirring tank reactor, confirmed that the amount of CO_2 absorbed in the solution steadily increased as the ionic liquid concentration rose. Also, Glazyrin *et al.* [14] have shown that by reacting wastewater with flue gas components, solutions with regenerative properties are generated and used for the regeneration of ion exchangers for water treatment and flue gas purification.

The MEA and DETA aforementioned are commonly used alkanolamines in the industry. They have the capability to form stable carbamic acid esters, which possess the activity to facilitate rapid chemical reactions. However, it's important to note that the formation of stable carbamic acid esters can result in significantly high regeneration costs [15]. Except for currently widely used amine solution absorbents, sterically hindered amines have been gaining attention due to their relatively higher efficiency in CO_2 absorption. Furthermore, the steric hindrance effect significantly impacts the stability of the generated carbamic acid ester, resulting in low stability and easy hydrolysis into bicarbonate ions [16]. Sterically hindered amines also possess favorable thermodynamic properties, resistance to degradation, and high absorptivity, among other advantages [17].

Sartori and Savage [18] were among the first to propose two types of sterically hindered amines:

 first amine is classified as a secondary amine wherein the amino group is attached to at least one secondary or tertiary carbon and - primary amines with an amino group connected to a tertiary carbon.

Various sterically hindered amines have been identified, including 2-piperidinol (2-PE), 2-piperinol (2-PM), 2-amino-2-ethyl-1,3-propanediol (AEPD), 2-amino-2-hydroxymethyl-1,3-propanediol (AHPD), and AMP. According to Khan *et al.* [19], the regeneration performance of AMP was experimented with for two amine loaded solvents in a temperature range and vacuum, and it was found that the CO₂ loading capacity of AMP was higher than the MEA value, and AMP had a better regeneration efficiency of 97.85% than MEA. At a regeneration temperature of 382 K, the regeneration efficiency was 85.4%. The energy intensity of AMP regeneration was found to be 41.7% lower than MEA in terms of reboiler heat load. Challenges in actual operation, such as high temperatures, high pressure, toxic substances, and complex equipment, have led to difficulties in conducting relevant experiments in factories.

With advancements in computer technology, carbon capture using CFD has emerged as a novel research method [20]. Compared to experimental methods, CFD simulations require less time, can be easily repeated for verification and to test varying conditions, and offer greater flexibility in changing parameters. The combination of CFD technology and practical production provides valuable insights for the application of CO₂ absorption in industrial settings. This paper primarily focuses on researching the influencing factors and absorption rules for CO_2 absorption using AMP as an absorbent.

The 3-D modelling utilizes the unit filler in the Mellapak 250Y-type filler, and CFD technology simulates the process of AMP solution and CO₂ within the unit filler. Calculations are conducted to explore CO₂ absorption by AMP in the unit model, considering different AMP molar fractions, CO₂ mass fractions, various pressures, and gas-liquid-flow velocities. A multifactor analysis is employed to determine the optimal ratios of each factor, facilitating a better understanding of fluid distribution and mixing in the absorption process. This study utilizes AMP solutions for efficient absorption of CO₂ to mitigate climate change and GHG emissions. Through simulations using FLUENT software, we were able to accurately analyze the kinetics of CO₂ absorption in solution, mass transfer characteristics, and the effects of various parameters in the solution, which opens up new possibilities for low energy carbon capture technologies. Secondly, this technology is practically feasible for CO₂ capture in industrial emissions, which is expected to help companies achieve their emission reduction targets and meet the urgent global need for climate protection. For industrial applications, we have considered the integration of CO₂ absorption from AMP solutions into existing industrial production processes to minimize carbon emissions. The successful application of this technology will have a positive impact on the sustainable development of the industry and will drive further innovations in environmental protection technologies.

Numerical simulation

Physical model and boundary condition

After a comparative study with other common fillers, it has been determined that the Mellapak 250Y-type filler exhibits high surface area, low pressure drop, even distribution, pollution resistance, and corrosion resistance. These characteristics contribute to the outstanding performance of the Mellapak 250Y-type filler in gas-liquid mass transfer. Consequently, the Mellapak 250Y-type filler is employed, with the filler plate's dop angle set at 45°. The specific geometric parameters of the filler are provided in tab. 1. To create a 3-D model of the filler layer, the unit structure is simulated using ICEM CFD software, as depicted in fig. 1(a).

Zuo, X., *et al.*: Numerical Simulation of CO₂ Absorption by AMP Solution ... THERMAL SCIENCE: Year 2024, Vol. 28, No. 4B, pp. 3293-3305

Table 1. Mellapak250Y packing layer geometric parameters

Specific surface area [m ² m ⁻³]	Porosity [%]	Bevel length [m]	Tilt angle [°]
250	97	0.0135	45

The unit model does not have a smooth wall surface; instead, it contains multiple bends. As a result, unstructured meshing is adopted, and the grid chart is displayed in fig. 1(b).



Figure 1. Model; (a) geometry and (b) mesh model



Figure 2. The CO₂ absorption rate at different grid numbers



In this research, the independence of the computational grid is taken into account. Figure 2 shows the CO_2 uptake rate for different numbers of grids.

The trend chart in fig. 2 reveals that as the number of grids increases, the CO_2 yield also rises. When the number of grids reaches 656772, the CO_2 yield stabilizes. Therefore, the adoption of 656772 units for the number of grids in this research has a minimal impact on the research results.

The boundary conditions are obtained from Huaneng carbon capture test research [21].

Table 2. Boundary conditions				
The kind of boundary condition	Specific settings			
Gas phase inlet	Using a speed inlet. The flue gas is set to CO_2 (16% mass fraction) and N_2 (84% mass fraction)			
Liquid phase inlet	Using a speed inlet. The imported components are AMP (1% molar fraction) and water (90% molar fraction)			
Chemical reaction	Using a component transport model and a general finite rate model, the operating temperature is 313 K, and the operating pressure is one standard atmospheric pressure (101325 Pa)			

3296

As depicted in fig. 1(a), the top of the model serves as the liquid phase inlet, the bottom as the gas phase inlet, and both the left and right sides act as pressure outlets. The gas phase is designated as the dominant phase, while the liquid phase is considered the secondary phase. The basic pressure is set to 1 standard atmospheric pressure (101325 Pa). Taking gravity into account, the gravitational acceleration is set at 9.8 m/s², acting in the negative y-axis direction. The specific boundary conditions are outlined in tab. 2.

Fundamental equations and turbulence model

Assuming that CO_2 behaves as an ideal gas, the AMP solution is an incompressible fluid, the transient reaction is established, and the ambient temperature remains constant throughout the entire reaction process, the mass conservation equation:

$$\frac{\partial (\alpha_k \rho_k)}{\partial t} + \nabla (\alpha_k \rho_k u_k) = S_k \tag{1}$$

The momentum conservation equation:

$$\frac{\partial (\alpha_k \rho_k u_k)}{\partial t} + \nabla (\alpha_k \rho_k u_k u_k) = -\alpha_k \nabla p + \nabla^2 (\alpha_k u_k \mu_k) + \alpha_k \rho_k g + F_k$$
(2)

The energy conservation equation:

$$\frac{\partial (\alpha_k \rho_k h_k)}{\partial t} + \nabla (\alpha_k \rho_k u_k h_k) = \alpha_k \frac{\partial p}{\partial t} + \nabla (\lambda_k \nabla T_k) + Q_k + S_{e,k}$$
(3)

In the FLUENT, the standard k- ε model is selected:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial k u_i}{\partial x_i} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\eta_t}{\sigma_k} \right) \frac{\partial k}{\partial x} \right] + G_k - \rho \varepsilon$$
(4)

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho\varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} + \left[\left(\mu + \frac{\mu_i}{\sigma_{\varepsilon}} \right) \frac{\partial\varepsilon}{\partial x_j} \right] + \frac{C_{1\varepsilon}\varepsilon}{k} G_k - C_{2\varepsilon}\rho \frac{\varepsilon^2}{k}$$
(5)

Chemical reaction for CO₂ absorption by AMP alcohol

The AMP solution is employed to capture CO_2 using two approaches: physical dissolution and chemical reaction. When the solution absorbs CO_2 , several sequential reaction steps occur. The first thing that will be generated is the 2-amino-2-methyl-1-propyl alcohol carbamate (AMPCOO⁻) and the combination of the protonated AMP(AMPH⁺) [22]:

$$CO_2 + 2AMP \rightarrow AMPCOO^- + AMPH^+$$
 (6)

Due to its poor stability, the generated carbamic acid ester readily undergoes hydrolysis, yielding alcohol, amine, and bicarbonate ions:

$$AMPCOO^{-} + H_2O \rightarrow AMP + H_2CO_3 \tag{7}$$

So, the total equation:

$$CO_2 + AMP + H_2O \rightarrow AMPH^+ + H_2CO_3$$
 (8)

The reaction equation indicates that the sterically hindered adhesive could theoretically absorb 1 mol of CO_2 per mole of sterically hindered amines after a specific CO_2 chemical dose. The process by which AMP absorbs CO_2 is relatively complex. Assuming that achieving this absorption is a secondary irreversible reaction during the simulation in FLUENT, the total equation can be simplified:

$$CO_2 + 2AMP + H_2O \xrightarrow{\lambda_2} AMPCOO^- + AMPH^+$$
(9)

The diffusion coefficient of CO_2 in AMP solution was calculated according to the method proposed by Saha [23] and Versteeg *et al.* [24]. Simultaneously, the method proposed by Sherman *et al.* [25] was used to determine the diffusion coefficient of AMP. Furthermore, through the experimental work of Kim *et al.* [26], it was possible to calculate the solubility of CO_2 .

Mass transfer model

In the contact process between AMP and CO_2 , the gas phase and liquid phase come into contact with each other in a highly turbulent state. During this phase, there is no stable phase interface. Higbie [27] proposed the penetration theory, which treats interphase mass transfer as a dynamic process and describes the unsteady mass transfer process between the two-phases. Consequently, the unsteady diffusion model is adopted in FLUENT for simulation purposes.

The solute undergoes a 1-D unsteady diffusion process within the fluid unit. When it diffuses to the gas-liquid interface, CO_2 is involved in a secondary chemical reaction. The rate of generation for CO_2 and AMP:

$$r_{\rm CO_2} = -k_2 c_{\rm CO_2} c_{\rm AMP} \tag{10}$$

$$r_{\rm AMP} = -2k_2 c_{\rm CO_2} c_{\rm AMP} \tag{11}$$

The mass transfer differential equation of CO₂ could be expressed:

$$D_{\rm CO_2}^{\rm solution} \frac{\partial_{c_{\rm CO_2}}^2}{\partial v^2} = \frac{\partial_{c_{\rm CO_2}}}{\partial t} - r_{\rm CO_2}$$
(12)

This reaction can be categorized as an instantaneous reaction with a high reaction rate, allowing us to consider their diffusion coefficients as consistent. According to the solute permeability theory, mass transfer coefficient can be calculated:

$$k_{\rm L,CO_2} = \left(1 + \frac{c_{AMP}}{2c_{\rm CO_2,i}}\right) \left(\frac{4D_{\rm CO_2}}{\pi\theta_c}\right)$$
(13)

The mass transfer coefficient is substituted into the mass source item, S_k :

$$S_{k} = \frac{Mk_{L,CO_{2}}AC_{L}(c_{CO_{2},i} - c_{CO_{2},0})}{V}$$
(14)

Simulation results of CO₂ absorption by AMP alcohol

Distribution condition of internal components of the unit model at different times

The CO_2 is introduced into the model from the bottom, facilitating its interaction with the AMP solution flowing in from the top. During this reaction process, there is mass transfer between the gas and liquid phases, where the gaseous CO_2 is absorbed into the liquid phase and reacts. Based on the overall reaction eq. (1) mole of CO_2 generates 1 mole of AMPCOO⁻ after

the reaction. Consequently, the CO_2 absorption efficiency can be assessed on the basis of the production of AMPCOO⁻. The conversion rate of CO_2 is approximately equal to the molar fraction of ammonium bicarbonate on the filler's surface at steady-state, divided by the molar fraction of CO_2 .

At a gas-flow velocity of 0.5526 m/s, the internal distribution of AMP and CO₂ within the model at 0.5 seconds, 1.0 seconds, and 1.5 seconds can be observed, as depicted in figs. 3-5.



Figure 3. At 0.5 seconds; (a) distribution of AMP and (b) CO₂

At 0.5 seconds, AMP is concentrated at the top of the model, while CO_2 occupies most of the model. With the ongoing reaction and under the influence of gravity, the AMP solution starts flowing downward, as illustrated in figs. 4 and 5, resulting in a gradual reduction of the area occupied by CO_2 .

Influence of molar fractions of different AMP on the CO₂ absorptivity



Figure 4. At 1.0 seconds; (a) distribution of AMP and (b) CO₂



Figure 5. At 1.5 seconds; (a) distribution of AMP and (b) CO₂

To investigate the relationship between

the molar fraction of AMP and the absorption efficiency of a unit model, the molar fraction of AMP was adjusted without altering other boundary conditions. The flue gas rich in CO_2 had a flow velocity of 0.5526 m/s, the liquid had a flow velocity of 0.00737 m/s, and the mass fraction of CO_2 in the flue gas was 16%. The pressure was set at standard atmospheric pressure, and the temperature was set at 313 K. The AMP molar fractions were set to 0.04, 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6, respectively.

Figure 6 reveals that, within 1.6 seconds, the AMPCOO⁻ content continuously rises. Before 0.4 seconds, there is a slight increase in yield due to the necessary time for the liquid and gas phases to come into contact. After 0.4 seconds, the two-phase fluid begins to make full contact, and the reaction accelerates. However, when the AMP molar fraction is between 0.4 and 0.6, the increase in AMPCOO⁻ yield gradually slows down.

Figure 7 indicates that CO_2 absorptivity increases rapidly when the AMP molar fraction is between 0.04 and 0.4, but the absorptivity of CO_2 uptake gradually slows down at AMP molar fractions of 0.4 to 0.6. From a chemical reaction equilibrium perspective, an increase in AMP molar concentration leads to an increase in the molar ratio of AMP to CO_2 , promoting the chemical reactionwards the right and enhancing CO_2 absorptivity. From a macro perspective, the two-phase fluid reacts rapidly upon initial contact, which leads to higher mass transfer rates at the gas-liquid interface and within the liquid phase, ultimately leading to an increase in CO_2 absorptivity.



0~1.6 seconds at different AMP concentrations

Figure 7. The CO₂ absorption rate calculated at different AMP concentrations

Influence of different ambient pressures on CO₂ absorptivity

To investigate the influence of ambient pressure on the absorption efficiency of a unit model, the ambient pressure is systematically adjusted by keeping all other boundary conditions constant. The ambient pressure was varied to values of 0.2, 0.5, 1, 1.5, and 2.0 atmospheres to thoroughly explore their impact on absorption efficiency.

Analyzing fig. 8, it is evident that the entire reaction process accelerates starting at 0.3 seconds and reaches a state of stability between 1.3 and 1.6 seconds. Correlating this with fig. 9, an increase in ambient pressure corresponds to a higher AMPCOO-yield at 1.5 seconds and increased CO₂ absorptivity. This can be attributed to several factors from a chemical reaction perspective: Increased pressure shifts the chemical equilibrium towards the right, intensifying the reaction rate, allowing for more effective interactions between the absorbent and gas. On a molecular level, higher pressure equates to more gas molecules within the same volume, resulting in more frequent and effective collisions between gas and liquid, consequently speeding up the reaction rate and increasing product quantities.



0~1.6 seconds at different ambient pressures

at different ambient pressures

Influence of different gas velocities on CO₂ absorptivity

To conduct an in-depth investigation into the interrelation between air velocity and CO₂ absorptivity within a unit model, the gas-flow velocity is systematically regulated while maintaining all other boundary conditions constant. Gas-flow velocities are set at 0.0737 m/s, 0.5526 m/s, 0.8844 m/s, 1.1055 m/s, 1.2529 m/s, and 1.474 m/s, corresponding to 10, 75, 120, 150, 170, and 200 times the liquid-flow velocity.

Figure 10 reveals that the AMPCOO⁻ relatively stable trend of production increased within the 0-1.6 seconds interval. When considering fig. 11 in conjunction, it becomes apparent that as gas-flow velocity increases, the output of AMPCOO⁻ diminishes, resulting in a continuous decrease in CO_2 absorptivity.



Figure 10. Production of AMPCOO- within 0~1.6 seconds at different gas-flow rates



Augmenting the gas-flow velocity facilitates a more rapid interaction between the gas and liquid phases, however, it also reduces the reaction time between the gas and liquid in the unit model. This increased velocity may result in some absorbents being blown out of the model by the high speed gas. Consequently, relatively lower gas velocities are favored in industrial production enhance CO_2 absorptivity. In the unit simulation, the reaction site is defined as the inner surface of the model. The higher gas-flow velocities cause the liquid to remain primarily on the upper surface of the model, preventing it from fully covering the surface of the model, resulting in insufficient CO_2 uptake.

Influence of different CO₂ mass fractions on CO₂ absorptivity

After conducting research on the influence of different AMP concentrations, ambient pressures, and gas-flowing velocities on the CO_2 absorptivity of a unit model, it is essential to further investigate the relationship between the CO_2 mass fraction and the model. The CO_2 mass fraction was set to 0.12, 0.14, 0.15, 0.16, and 0.19, respectively.

Figure 12 reveals that the content of the product AMPCOO⁻ remains nearly constant between 0-0.3 seconds for different CO_2 mass fractions. However, the difference in AMPCOO⁻ content within the range of 0.3-1.5 seconds increases gradually with varying CO_2 mass fractions. Combining this with fig. 13, it can therefore, be concluded that the absorptivity of CO_2 decreases as the CO_2 mass fraction increases.

During the reaction process, an increase in the mass fraction of CO_2 signifies a higher initial concentration of CO_2 , which in turn enhances the molar ratio of CO_2 and AMP. From the perspective of chemical reaction equilibrium, this results in a decrease in the overall reaction rate, which is unfavorable for CO_2 absorption and leads to a reduction in CO_2 absorptivity.

Additionally, an increase in CO_2 mass fraction means an elevation in the concentration of CO_2 at the unit model's gas inlet and the CO_2 partial pressure. Consequently, more CO_2 enters the AMP solution for reaction. However, this increase in the gross amount of CO_2 entering the AMP solution cannot offset the impact of the higher initial concentration of CO_2 . As a result, the overall CO_2 absorptivity decreases as the CO_2 mass fraction rises.



Figure 12. Production of AMPCOO- within 0~1.6 seconds at different CO₂ mass fractions

Figure 13. The CO₂ absorption rate calculated at different CO₂ mass fractions

Analysis of optimal parameters

The absorption of CO₂ in flue gas is analyzed under four different conditions in the aforementioned simulation. To investigate the absorption behavior of CO₂ in flue gas under the combined influence of these different conditions, the AMP mole fraction, ambient pressure, gas-flow rate, and CO₂ mass fraction are denoted by A, B, C, and D, respectively. High and low values were selected for each condition, resulting in 16 ($2^4 = 16$) distinct simulation scenarios through permutation and combination. The specific simulation scenarios and the corresponding CO₂ absorptivity are presented in tab. 3.

Number	А	B [KPa]	C [ms ⁻¹]	D [wt.%]	Absorptivity [%]	
1	0.04	20.265	0.0737	0.12	0.00382	
2	0.04	20.265	0.0737	0.19	0.00292	
3	0.04	20.265	1.474	0.12	0.00308	
4	0.04	20.265	1.474	0.19	0.00211	
5	0.04	202.65	0.0737	0.12	0.00426	
6	0.04	202.65	0.0737	0.19	0.00374	
7	0.04	202.65	1.474	0.12	0.00361	
8	0.04	202.65	1.474	0.19	0.00297	
9	0.6	20.265	0.0737	0.12	0.00628	
10	0.6	20.265	0.0737	0.19	0.00386	
11	0.6	20.265	1.474	0.12	0.00602	
12	0.6	20.265	1.474	0.19	0.00377	
13	0.6	202.65	0.0737	0.12	0.00724	
14	0.6	202.65	0.0737	0.19	0.00437	
15	0.6	202.65	1.474	0.12	0.00616	
16	0.6	202.65	1.474	0.19	0.00415	

 Table 3. Simulation results

Table 3 clearly illustrates that the highest values are chosen for Conditions A and B, leading to the maximum absorptivity obtained through simulation when lower values were chosen for Conditions C and D. When combining these findings with the analysis of absorptivity under individual conditions, it was found that the absorptivity increased insignificantly within the AMP molar fraction range of 0.4-0.6. Furthermore, the absorptivity continues to rise as the pressure increases.

However, considering that a pressurizing device is needed to increase the pressure inside the container. Therefore, it should be recommended that the AMP molar fraction be at 0.4, the pressure be at normal atmospheric levels, setting the flue gas-flow velocity be set at 0.0737 m/s, and the CO₂ mass fraction be set at 0.12.

Conclusions

In this paper, a unit model was constructed inside the absorptionwer with a grid system, and the appropriate number of grids was determined by grid independence validation. The grid model has been imported into FLUENT for simulation, and the product distribution cloud map at different gas phase velocities can be observed.

The boundary conditions were modified to simulate the CO₂ absorption conditions of the AMP solution within the unit model under different scenarios. The influencing factors were analyzed to determine CO₂ absorptivity under 16 different simulation conditions. The results indicate that absorptivity increases with higher AMP molar fractions and ambient pressure, while it decreases with higher gas phase velocities and CO₂ mass fractions. Considering the relatively challenging operation of increased pressurizing equipment, the following rational and optimal parameters were comprehensively considered: an AMP molar fraction of 0.4, ordinary pressure for the set pressure, a flue gas-flow velocity of 0.0737 m/s, and a CO₂ mass fraction of 0.12. Even though we set some parameters in our numerical simulations, we have to be honest and admit that this limitation may have some impact on our study. However, we cannot ignore the potential uncertainties that the inability to set parameters may introduce. In future studies, we plan to work on this issue and explore ways to integrate the actual operating parameters more accurately.

Nomenclature

p

A	- cell contact area, [m ²]	$r_{\rm CO_2}$	- r
C_L	- total molar concentration of	$r_{\rm AMP}$	- r
	solution, [molm ⁻³]	S_k	- n
$C_{\text{CO}_{2},i}$	- the concentration of CO ₂ on	$S_{e,k}$	– e
2	interface, [molm ⁻³]		r
$C_{\rm CO_{2},0}$	- the concentration of CO ₂ on	u_k	- V
2	liquid body, [molm ⁻³]	V	- c
F_k	- interphase interaction force, [N]	~	
G_k	- turbulence energy resulting from mean	Gree	k sy
	velocity gradient, [m ² s ⁻²]	З	- ċ
h_k	- specific enthalpy of the k^{th}	θ_c	-1
	substance, [Jmol ⁻¹]	λ_k	- t
g	- gravity volume force, [ms ⁻²]	μ_k	- ċ
$D_{CO_2}^{soluti}$	$-$ diffusion coefficient of CO_2	ρ_k	- t
2	in solution, $[m^2s^{-1}]$	σ_k	– t
k_{L,CO_2}	- mass transfer coefficient of CO ₂		I
k Î	- turbulent kinetic energy, [m ² s ⁻²]	σ_{ε}	– t
М	- the molar mass of CO ₂ , [kgmol ⁻¹]		Ċ
р	- static pressure, [Pa]		r

 O_k - interphase heat conduction intensity, [Jkg⁻¹] rate of generation for CO_2 , $[molL^{-1}s^{-1}]$

- ate of generation for AMP, [molL⁻¹s⁻¹]
- nass source term, [kgm⁻³s⁻¹]
- enthalpy source term in chemical
- reactions, [Jm⁻³s⁻¹]
- velocity vector, [ms⁻¹]
- ell volume, [m3]

ymbols

- lissipation rate, [ms⁻¹]
- ength of stay, [t]
- hermal conductivity, [Wm⁻¹K⁻¹]
- lynamic viscosity, [Nsm⁻³]
- the density of the k^{th} phase, [kgm⁻³]
- urbulent kinetic energy turbulent Planter number, [–]
- urbulent Planter number of dissipation rate ε , [–]

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3304

Zuo, X., *et al.*: Numerical Simulation of CO₂ Absorption by AMP Solution ... THERMAL SCIENCE: Year 2024, Vol. 28, No. 4B, pp. 3293-3305

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