

RESEARCH ARTICLE

Reaction Engineering, Kinetics and Catalysis

Comprehensive reaction kinetics model of CO₂ absorption into 1-dimethylamino-2-propanol solutionHelei Liu^{1,2,3}  | Xiaotong Jiang¹ | Raphael Idem²  | Shoulong Dong¹  | Paitoon Tontiwachwuthikul² ¹International Innovation Institute of Carbon Capture and Utilization (I3CCU), School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing, People's Republic of China²The Clean Energy Technologies Research Institute (CETRI), University of Regina, Regina, Saskatchewan, Canada³Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, British Columbia, Canada

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Abstract

In the present work, the kinetics of the reactive absorption of CO₂ in 1-dimethylamino-2-propanol (1DMA2P) solution were experimentally measured using a laminar jet absorber over a temperature range of 298–313 K, 1DMA2P concentration range of 0.5–2.0 mol/L, and CO₂ loading range of 0–0.06 mol CO₂/mol amine. The measured kinetics data were then used to develop a comprehensive numerical kinetics model using a FEM-based COMSOL software. The reaction rate model of the CO₂ absorption into 1DMA2P solution were then validated by comparing model rates with the experimental rates. An excellent agreement of model data with experimental data was achieved with an absolute average deviation (AAD) of 6.5%. In addition, vapor–liquid equilibrium plots of all ions in the 1DMA2P-H₂O-CO₂ system were also developed. Further, this work has provided an effective criterion for evaluating CO₂ absorption, that can be used for both the conventional amines and alternative amines for the purpose of providing guidelines or information on how to effectively screen solvents.

KEYWORDS

absorption, amines, CO₂, reaction kinetics

1 | INTRODUCTION

The current climate crisis, one of the greatest challenges of our times, has drawn considerable international effort aimed at tackling the issue. The 26th Conference of the Parties (COP26) of the United Nations Framework Convention on Climate Change has indicated that strengthening of global collaboration and action on greenhouse gas emissions must be put into force based on the foundation of the 2015 Paris Agreement.^{1,2} Carbon capture, utilization, and storage (CCUS) from fossil fuel has commonly been considered to play an increasingly significant role in reducing CO₂ emissions, especially in power stations

and heavy industries such as for the manufacture of steel, cement, and chemicals.³ Direct air capture with carbon capture and storage (DACCS) also provides the potential for eliminating carbon emissions.⁴ In addition, the deployment of bioenergy with carbon capture and storage (BECCS) could also provide the potential technology for negative carbon emissions to accelerate the process of net zero carbon emissions.⁵ As one of the main carbon capture technologies, post combustion carbon capture (PCCC) from flue gases generated from fossil fuel power plants is vital for deployment to mitigate CO₂ emissions since PCCC could easily be integrated and implemented into both existing and new industrial plants (i.e., cement plants, steel

plants, etc.) and power stations such as natural gas fired power stations.⁶ Meanwhile, PCCC could offer a lower technology risk and a higher operational flexibility in comparison with other competing technologies.⁷ PCCC with chemical absorption based mainly on amines has been considered to be a commercially feasible as well as most suitable way to treat large volumes of flue gases containing low concentrations of CO₂ due to its advantages of high reactivity and high absorption capacity.⁸ However, this PCCC technology based on amines suffers from some critical disadvantages of high energy requirements for amine regeneration and amine degradation.⁹

To reduce energy consumption, many researchers working in this field have proposed different innovative techniques including precipitating solvent,^{10,11} biphasic solvent,^{12,13} process optimization,¹⁴ etc. Modeling and simulation are helpful approaches to screening potential solvents, process configurations, process intensification, and process optimization. For example, Moioli et al.^{10,15} employed ASPEN Plus to compare amino acid-based solvent with traditional amine solvent processes for CO₂ removal and to model the methyldiethanolamine-piperazine (MDEA-PZ) scrubbing system for CO₂ removal.

More importantly, one of the techniques that can help to address the issue of energy consumption is to develop efficient amine solvents with high capacity, fast absorption rate, and low heat duty.¹⁶ A fundamental consideration when selecting an amine for PCCC is the performance of the amine across both the absorption and desorption regimes.¹⁷ For the absorption process, the absorption kinetics is a vital factor as it directly correlates with the required physical size of the absorber; thus, an amine that reacts fast with CO₂ is advantageous. In addition, the energy requirement for the stripping process is important, as the cost of steam often accounts for over half of the running cost of the plant.¹⁸ However, the traditional primary/secondary amines (e.g., MEA) cannot meet the above-mentioned criteria. Many efforts have been spent on exploring novel tertiary amines, which can be mixed with primary/secondary amines to achieve the benefit of fast reaction kinetics with low regeneration energy requirements and high absorption capacity. New solvents that have been screened include: 4-(diethylamino)-2-butanol (DEAB) by Sema et al.,¹⁹ 1-dimethyl-amino-2-propanol (DMA2P) by Kadiwala et al.,²⁰ 2-(1-piperazinyl)-ethylamine (PZEA) by Paul et al.,²¹ 3-diethylamino-1,2-propanediol (DEA-1,2-PD) by Chowdhury et al.,²² and 1-diethylamino-2-propanol (1DEA2P) by Liu et al.²³ All these amines were reported to exhibit good performance for CO₂ capture with respect to CO₂ solubility, kinetics, mass transfer, and regeneration heat.

Recently, a new tertiary amine, 1-dimethylamino-2-propanol (1DMA2P), has drawn significant attention for its good performance in capturing CO₂.²⁰ Chowdhury et al.²² also presented the CO₂ cyclic capacities and the absorption rates of 1DMA2P, which were much higher than those of MDEA. Liang et al.²⁴ reported that 1DMA2P shows much better mass transfer performance than MDEA. In order to develop a reliable and systematic design of PCCC systems using any potential solvents, knowledge of the absorption/desorption parameters of the solvent for CO₂ capture (e.g., CO₂ absorption kinetics, CO₂ solubility, heat of CO₂ absorption, and mass transfer characteristics) is required. This implies that for 1DMA2P to be evaluated

for its potential as an alternative solvent, such parameters must be evaluated. In addition, the knowledge of these parameters can be used to judge if 1DMA2P can be a standalone alternative solvent or a component in a blended solvent.

Reaction kinetics, which is considered to be a key factor in the performance evaluation of a new solvent, has a vital significance for process simulation and design of a CO₂ capture plant. Several devices (e.g., a stirred cell reactor, wetted wall column, laminar jet absorber, wetted sphere absorber, and stopped-flow apparatus) could be used to determine the kinetic behavior of amine solution absorption of CO₂.²⁵ In comparison with other experimental setup, the laminar jet absorber is one of the most commonly used equipment for kinetics studies of CO₂ absorption because of its several advantages. The liquid phase contacts gas in a short time due to its high speed, the interfacial area could be known accurately, and the physical absorption rates can match well with penetration theory predictions.²⁶ Thus, it is appropriate to intensify the CO₂ absorption process of mixed amine systems. It can be used not only to determine the reaction kinetics, but also in testing mass transfer performance.²⁷ However, the disadvantage of this technique is that turbulent liquid may appear. By using the laminar jet absorber, Iden et al.²⁸ studied the comprehensive kinetics models of CO₂ absorption into blended amine systems. In the work of Edali et al.,²⁹ a comprehensive kinetics models of MDEA-PZ absorption of CO₂ was developed by coupling the chemical equilibrium, mass transfer, and all the chemical reactions into the developed model. In order to develop a comprehensive kinetics model of CO₂ absorption into amines, the partial differential equations involved in the systems need to be solved. For solving those partial differential equations, there are two different numerical methods: the finite difference method (FDM) on the basis of Barakat-Clark scheme and finite element method (FEM) on the basis of COMSOL. FDM is an in-house coded program, which was used to estimate the Jacobian. In this program, a double precision calculation was used to get an accurate Jacobian to arrive at the exact roots of the equations. By employing this technique, the convergence for the solution could be obtained even when the initial guesses are not close to the solution.²⁹ The FDM is a commercial package based on the software, COMSOL, which eliminates the extra effort of coding the program to solve the partial differential equations.²⁹ Based on the results from the reference 29, both the FDM and FEM methods could be used to represent the comprehensive kinetics model of CO₂ absorption into amines, which provide good predication of experimental CO₂ absorption rate.

In the present work, the reaction kinetics data of 1DMA2P were experimentally measured using the laminar jet absorber over a temperature range of 298–313 K, 1DMA2P concentration range of 0.5–2.0 mol/L, and CO₂ loading range of 0–0.06 mol CO₂/mol amine. The measured kinetics results were then described using a comprehensive numerical kinetics model developed using a FEM approach based on COMSOL software. The reaction kinetics behavior of CO₂ absorption into 1DMA2P solution was represented by a second order reaction rate constant. In addition, vapor–liquid equilibrium (VLE) plots of all ions in the 1DMA2P-H₂O-CO₂ system were also developed in this work. The absorption parameters obtained in this work could be

analyzed and used for both conventional amines and this alternative amine for the purpose of providing guidelines or information on how to effectively screen solvents.

2 | EXPERIMENTAL SECTION

2.1 | Chemicals

Reagent grade 1DMA2P and MEA with purity of ≥ 99 wt% was obtained from Sigma-Aldrich. The amine solutions were prepared to the desired concentrations using deionized water. Carbon dioxide (CO_2) and nitrogen (N_2) with purities of 99.9% were obtained from Praxair Inc., Regina, SK.

2.2 | Absorption rate of CO_2

The apparatus used to determine the CO_2 absorption rate was the laminar jet absorber shown in Figure 1. A brief description of experimental procedure is provided as follows: Initially, the amine solution with the desired concentration was degassed for 20 minutes by using an ultrasonic bath (VWR model 75D, VWR international, ON). Then, the degassed amine solution was introduced into the solution tank, which was connected to the vacuum pump. The solution in the tank was vacuumed using the vacuum pump for

30 minutes in order to remove the gas from the amine solution. After that, the 2 L degassed solution was pumped to a constant head system through the two flow meters, which were used to make sure constant head system to maintain a constant liquid level. The solution in the constant head system was introduced into the jet chamber through a water jacket in order to reach the desired temperature. The jet chamber was made up of two 6.4-mm diameter tubes. One was located at the bottom as the receiver. Another delivery nozzle was installed at the top, which one could slide vertically to change the jet length. The jet chamber was constructed from a 250 mm long and 50-mm diameter acrylic cylinder which was enclosed in a constant-temperature jacket constructed from a 250-mm long and 150-mm diameter acrylic cylinder. The temperature of the water jacket was controlled by the water bath. The flow rate of solution injected into the jet chamber was controlled by the flow meter. The solution was then passed through the jet nozzle in the chamber in order to obtain a smooth-surfaced rod-like jet. Once the jet was stable, a 200 ml amine solution was collected and recorded by a stopwatch to obtain a real liquid flow rate. The CO_2 gas which was made to pass through the soap-film meter was injected into jet chamber. The CO_2 absorption rate (R_A ; mol/s) was measured by a soap-film meter (ranging from 0.1 to 10 ml/min with $\pm 1\%$ accuracy). The height (h ; mm) and diameter (d ; mm) of the liquid jet was measured by employing a two-dimensional traveling microscope, which was used to measure the jet-length within 0.01 mm and the jet-diameter to within 0.001 mm.

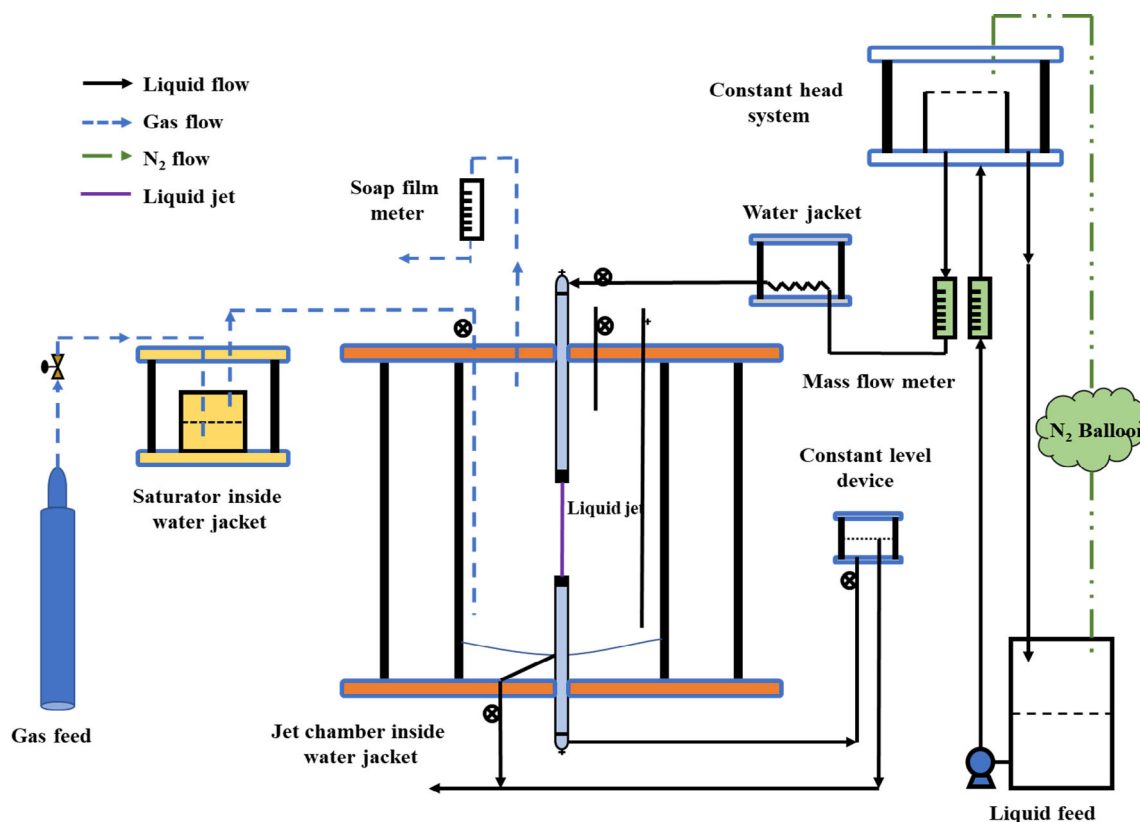


FIGURE 1 The diagram of the laminar jet absorber

2.3 | Repeatability of experimental data

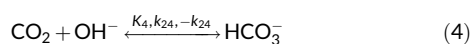
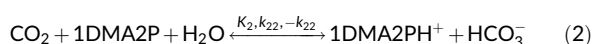
In order to obtain accurate experimental data, all experiments were repeated at least three times. The average of the obtained results was used to do data analysis. The average relative error (ARE) of each data points was less than 3%, which indicated that the experimental apparatus had good repeatability. The ARE can be defined as follows:

$$\text{ARE} = \frac{1}{n} \sum_{i=1}^n \left| \frac{x_i - \bar{x}}{\bar{x}} \right| \times 100$$

where n denotes the times repeated, x_i stands for the i th experimental data, and \bar{x} indicates the average of n experimental data.

3 | THEORETICAL BASIS FOR PARAMETERS ESTIMATION

The base-catalyzed hydration mechanism originally proposed by Donaldson and Nguyen³⁰ was employed to interpret the reaction process with respect to the reaction of tertiary amines with CO_2 . As suggested in this mechanism, the tertiary amine just acts as a base that catalyzes the hydration of CO_2 without direct reaction with CO_2 . On the base of the base catalyzed hydration mechanism, the reaction of tertiary amine- H_2O - CO_2 can be expressed in Equations (1)–(6):



where K_i are the chemical equilibrium constants for reaction i . k_{2i} are second order reaction rate constant of the reaction.

The chemical species in the 1DMA2P- H_2O - CO_2 system are CO_2 , HCO_3^- , OH^- , CO_3^{2-} , H^+ , 1DMA2P, and 1DMA2PH⁺. In order to simplify the concentration of those species, the concentration of the species were designated as follows: $C_1 = [\text{CO}_2]$, $C_2 = [\text{HCO}_3^-]$, $C_3 = [\text{OH}^-]$, $C_4 = [\text{CO}_3^{2-}]$, $C_5 = [\text{H}^+]$, $C_6 = [1\text{DMA2P}]$, and $C_7 = [1\text{DMA2PH}^+]$. In this 1DMA2P- H_2O - CO_2 system, there are several equilibrium constants for chemical reactions, which can be presented as follows:

$$K_1 = \frac{C_7}{C_5 C_6} = \frac{K_2}{K_3} \quad (7)$$

$$K_2 = \frac{C_7 C_2}{C_6 C_1} \quad (8)$$

$$K_3 = \frac{C_2 C_5}{C_1} \quad (9)$$

$$K_4 = \frac{C_2}{C_1 C_3} = \frac{K_3}{K_1 K_6} \quad (10)$$

$$K_5 = \frac{C_4 C_5}{C_2} \quad (11)$$

$$K_6 = C_3 C_5 \quad (12)$$

Based on Equations (7)–(12), there are independent correlations for four of the equilibrium constants (K_2 , K_3 , K_5 , and K_6). On the other hand, K_1 and K_4 can be obtained by using Equations (7) and (12), respectively.

The physical solubility of CO_2 in 1DMA2P solution could be expressed by using Henry's law as follows:

$$P_{\text{CO}_2} = \text{He}_{\text{CO}_2} [\text{CO}_{2(\text{aq})}] \quad (13)$$

where P_{CO_2} is the CO_2 partial pressure in gas phase, He_{CO_2} represents the Henry's law constant of CO_2 in 1DMA2P solution, which could be obtained from our previous work.³¹

The values of K_3 , K_5 , and K_6 for 1DMA2P- H_2O - CO_2 system can be obtained from the literature.^{32–34}

In addition, there are several balance equations that exist in the 1DMA2P- H_2O - CO_2 system, which can be represented as follows:

Mass balance of 1DMA2P:

$$[1\text{DMA2P}]_0 = C_6 + C_7 \quad (14)$$

Mass balance of carbon:

$$\alpha [1\text{DMA2P}]_0 = C_1 + C_2 + C_5 \quad (15)$$

Charge balance:

$$C_5 + C_7 = C_2 + C_3 + 2C_4 \quad (16)$$

where $[1\text{DMA2P}]_0$ is the initial 1DMA2P concentration (mol/L) and α represents the CO_2 loading (mol CO_2 /mol amine).

3.1 | VLE Model

The concentrations of all chemical species in the amine- H_2O - CO_2 system are necessary to analyze and understand the kinetics data. The concentrations of ion species (Amine, AmineH⁺, HCO_3^- , and CO_3^{2-}) in the solution of the tertiary amine obtained from the computational method combining equilibrium constants (K_2 , K_5 , and K_6), and

Equations (13)–(16) are provided in this study. The FEM model from COMSOL with OD stationary solver was employed to solve eight equation by inputting the initial guess for eight unknowns in order to obtain the unknown of C_1 – C_7 and P_{CO_2} of the 1DMA2P–H₂O–CO₂ system. The process was continued until the deviation of the results of unknown of P_{CO_2} and experimental results of P_{CO_2} was less than 0.01%. For different CO₂ loadings, the concentration of all chemical species were obtained using the same procedure. As a result, the ion speciation plot were developed as function of CO₂ loading.

3.2 | Reaction kinetics model

In this work, the absorption rate data of CO₂ in aqueous 1DMA2P solutions were interpreted by using a comprehensive CO₂ absorption rate model. For this model, all the coupling of chemical equilibrium, mass transfer, and reaction kinetics of all possible chemical reactions were taken into account, which could be used to represent the CO₂ absorption performance into amine solution as well as the enhancement factor of the amine reaction with CO₂. In addition, this comprehensive model could be used to correlate the experimental CO₂ absorption results to obtain reaction kinetics of CO₂ into amine.

This comprehensive model could be derived from a full 3D cylindrical coordinate system. This cylindrical coordinate system could be presented by the full shape of cylindrical liquid jet, which was obtained in the laminar absorber. As shown in Figure 2, the gas–liquid interface parallel to the symmetry axis located at the outer boundary, which results in a radial diffusion of gas. In this work, the absorption of CO₂ into amine solution with constant diffusivity and density is presented by using the molecular transport equation, which could be expressed as in Equation (17).³⁵ Based on Equation (17), the molecular

transport of CO₂ into liquid is made up of convection, accumulation ($\frac{\partial C}{\partial t}$), and reaction rate (R).

$$D\nabla^2 C = u \cdot \nabla C + \frac{\partial C}{\partial t} + R \quad (17)$$

where u is velocity (m/s), D is diffusion coefficient (m²/s).

Equation 17 could be expanded as in the following Equation (18):

$$D \left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} + \frac{1}{r^2} \frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2} \right] = \left[v_r \frac{\partial C}{\partial r} + \frac{v_\theta}{r} \frac{\partial C}{\partial \theta} + v_z \frac{\partial C}{\partial z} \right] + \frac{\partial C}{\partial t} + R \quad (18)$$

In a laminar jet absorber, the assumption of constant diffusivity and density is acceptable. The change of concentration does not lead to a substantial variation in the mole-fraction of the diffusion as the contact time is short.²⁷ In addition, there are some assumptions in this system: (1) penetration theory applies for the transport gas into liquid where absorption takes place by unsteady molecular diffusion in the liquid. (2) The depth of penetration for the absorbed gas is much smaller than the jet diameter as the contact time is very short. (3) The diffusion in the z axial is negligible. (4) The effect of convection movements on the absorbed gas transport was eliminated because of quiescent liquid. Based on the hydrodynamics conditions of the laminar jet and the above assumptions, Equation (18) could be simplified to the diffusion equation of Equation (19). The 3D cylindrical coordinate system could be simplified 1D system, which could be shown in Figure 3.

$$D \frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} + R \quad (19)$$

This equation governs the variation in time and space of the concentration of all reactants and products in the liquid phase.

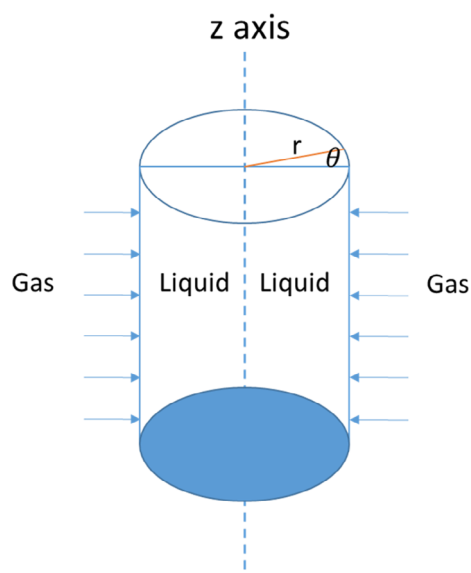


FIGURE 2 The diagram of the gas transportation to liquid in the laminar jet absorber

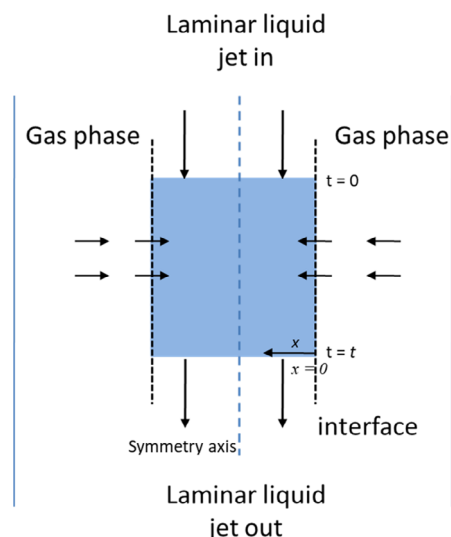


FIGURE 3 The simplified diagram of the gas transport to liquid in the laminar jet absorber

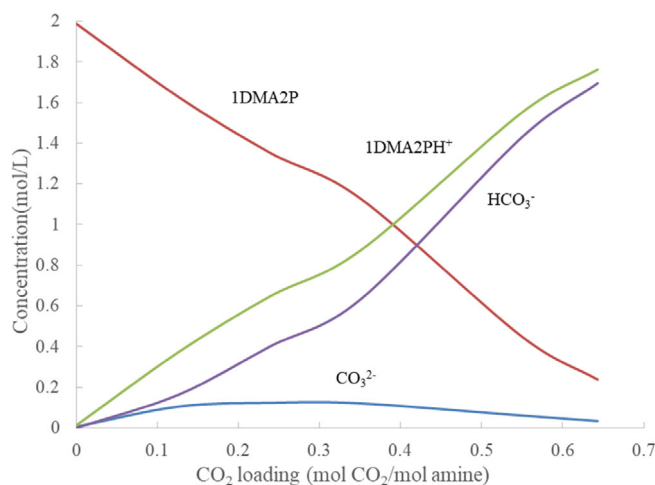


FIGURE 4 Ions speciation plot of 1DMA2P-H₂O-CO₂ system at the temperature of 298 K

Based on this equation, all the partial differential equations and nonlinear algebraic equations (Equations 1–6) for the diffusion-reaction process could be written as follows:

For CO₂ balance:

$$\frac{\partial C_1}{\partial t} = D_1 \frac{\partial^2 C_1}{\partial x^2} + R_2 + R_4 \quad (20)$$

Total carbon balance:

$$\frac{\partial C_1}{\partial t} + \frac{\partial C_2}{\partial t} + \frac{\partial C_3}{\partial t} = D_1 \frac{\partial^2 C_1}{\partial x^2} + D_2 \frac{\partial^2 C_2}{\partial x^2} + D_3 \frac{\partial^2 C_3}{\partial x^2} \quad (21)$$

Total 1DMA2P balance:

$$\frac{\partial C_6}{\partial t} + \frac{\partial C_7}{\partial t} = D_6 \frac{\partial^2 C_6}{\partial x^2} + D_7 \frac{\partial^2 C_7}{\partial x^2} \quad (22)$$

The total charge balance:

$$\frac{\partial C_2}{\partial t} + \frac{\partial C_3}{\partial t} + 2 \frac{\partial C_4}{\partial t} - \frac{\partial C_5}{\partial t} - \frac{\partial C_7}{\partial t} = D_2 \frac{\partial^2 C_2}{\partial x^2} + D_3 \frac{\partial^2 C_3}{\partial x^2} + 2D_4 \frac{\partial^2 C_4}{\partial x^2} - D_5 \frac{\partial^2 C_5}{\partial x^2} - D_7 \frac{\partial^2 C_7}{\partial x^2} \quad (23)$$

where D_i is the diffusivity of chemical species i into solution (m²/s). R_2 and R_4 are the reaction rate of Reactions (2) and (4), respectively.

For the reaction rate of Reaction (2), R_2 could be expressed as the following:

$$R_2 = -k_{1\text{DMA2P}} C_1 C_6 + \left(\frac{k_{1\text{DMA2P}}}{K_2} \right) C_2 C_7 \quad (24)$$

For the reaction of Reaction (4), R_4 could be presented as below:

TABLE 1 The enhancement factor of 1.0, 1.5, and 2.0 mol/L at 303 K in 1DMA2P solution

Concentration (mol/L)	Enhancement factor
1.0	1.82
1.5	2.43
2.0	3.14

$$R_4 = -k_{24} C_1 C_3 + \left(\frac{k_{24}}{K_4} \right) C_2 \quad (25)$$

The absorption rate constant of Equation 4 (k_{24} ; m³/kmol s) could be extracted from the equation presented in the work of Pinsent et al.,³⁶ which is shown as follows:

$$\log(k_{24}) = 13.635 - \frac{2895}{T} \quad (26)$$

All reaction are assumed to be at equilibrium. The expression of K_2 , K_3 , and K_6 are shown in Equations (2), (9), and (19).

The diffusivity of CO₂ in aqueous solution of 1DMA2P (D_1) could be extracted from the correlation obtained in our previous study.³¹ The diffusivity of 1DMA2P (D_6 ; cm²/s) can be estimated by employing the predictive correlation for diffusivity of triethanolamine (TEA) as the follows³⁷:

$$D_6 = \left(1.739 \times 10^{-9} \right) \mu^{-0.569842} T \quad (27)$$

where μ represents the viscosity of amine solution (mPa s), T is temperature (K).

For the diffusivity of HCO₃[−], OH[−], CO₃^{2−}, H⁺, and 1DMA2PH⁺, they were assumed as the same diffusivity of 1DMA2P, which is the main species in the solution.³⁸

Thus, the concentration of chemical species (C_1 – C_7) could be obtained by solving four partial differential equations and four algebraic equations. By solving those equations, the initial and boundary conditions should be included, which are provided as follows:

Initial conditions:

For all chemical species, $j = 1, 2, 3, \dots, 7$,

$$C_j(x, 0) = C_j^0 \text{ at } t = 0 \text{ and } 0 \leq x \leq \infty \quad (28)$$

Boundary conditions:

For all chemical species, $j = 1, 2, 3, \dots, 7$

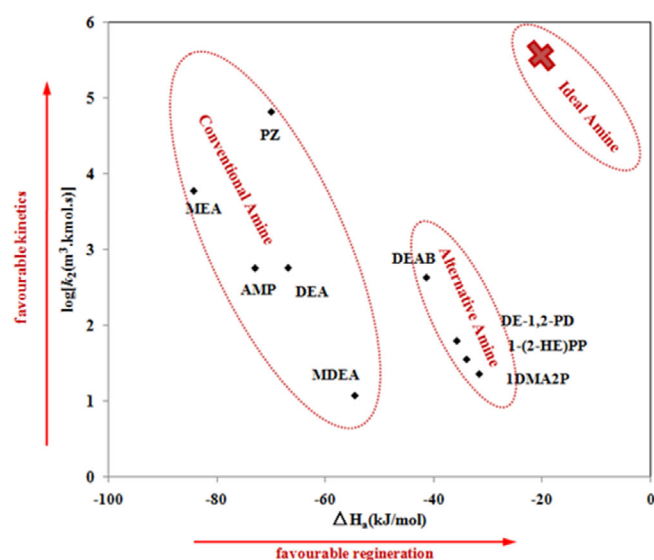
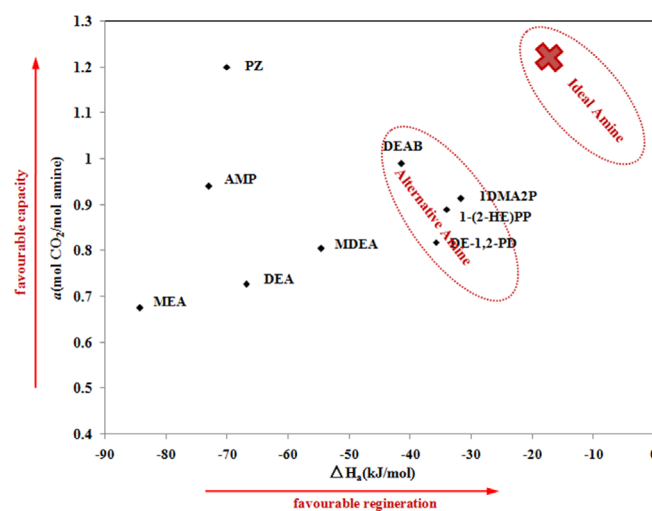
$$C_j(\infty, t) = C_j^0 \text{ at } x = \infty \text{ and } 0 \leq t \leq \infty \quad (29)$$

For volatile chemical species, $j = 1$

$$C_j(0, t) = C_j^* = \frac{P_j}{H_{ej}} \text{ at } x = 0 \text{ and } 0 \leq x \leq \tau \quad (30)$$

TABLE 2 Comparison 1DMA2P with other amines in terms of equilibrium CO₂ solubility, second order reaction constant (k_2), and CO₂ absorption heat

Amine	Equilibrium CO ₂ solubility at 2 mol/L, 313 K, and 101 kPa for CO ₂ partial pressure (a , mol CO ₂ /mol amine)	Second order reaction constant at 298 K (k_2 , m ³ kmol s)	Absorption heat (ΔH_a , kJ/mol)
MEA	0.676	5939	-84.3
DEA	0.727	576	-66.9
MDEA	0.805	12	-54.6
AMP	0.94	570	-73
PZ	1.25	65,000	-70
DEAB	0.99	429	-41.4
DE-1,2-PD	0.818	62.99	-35.8
1-(2-HE)PP	0.89	36	-34
1DMA2P	0.913	30	-31.67

**FIGURE 5** Solvent screening plot of the second order reaction constant (k_2) at 298 K, $\log(k_2)$, and CO₂ absorption heat^{42,43}**FIGURE 6** Solvent screening plot of CO₂ equilibrium solubility (a) at 2 M, 313 K, CO₂ partial pressure 101 kPa, and CO₂ absorption heat^{42,43}

where C_1^* is the CO₂ concentration at the interface of gas and liquid (kmol/m³), which is obtained by using Equation (13). C_j^0 is the bulk concentration of species j in the liquid phase (kmol/m³).

The local CO₂ absorption rate per unit area could be expressed from the CO₂ concentration profile data as:

$$N = -D_1 \left(\frac{\partial C_1}{\partial t} \right)_{x=0} \quad (31)$$

This represents the concentration gradient at the surface, which is a function of time. In order to obtain the average absorption rate per unit area of CO₂, the local CO₂ absorption rate per unit area was divided over the contact time (τ) as shown below:

$$N_{ave} = -\frac{D_1}{\tau} \int_0^\tau \frac{\partial C_1}{\partial t} (0, t) dt \quad (32)$$

The contact time (τ) was given as follows:

$$\tau = \frac{\pi d^2 h}{4L} \quad (33)$$

where d represents diameter of the liquid jet (m), h represents the height of the liquid jet, L is flow rate of liquid (m³/s).

In this work, the effect of a chemical reaction on the absorption of gas into liquid phase was presented in terms of the enhancement factor (E). The enhancement factor was defined as the ratio of the absorption rate of gas involved in chemical reaction with the

absorption rate of gas without effect of chemical reaction. This is given as follows:

$$E = \frac{N_{ave}}{k_L^0 (C_1^* - C_1^0)} \quad (34)$$

where k_L^0 is the mass transfer coefficient of liquid phase for CO_2 .

In the system of laminar jet absorber, the k_L^0 could be given as:

$$k_L^0 = 2\sqrt{\frac{D_1}{\pi\tau}} = \frac{4}{d\pi}\sqrt{\frac{DL}{h}} \quad (35)$$

In this work, the experimental enhancement factor (E) was calculated using the Equation (34) from the experimental results. In addition, the enhancement factor was calculated using Equation (35). In order to obtain the predicted enhancement factor (E_{pred}), Equations (12–15) and (20–23) were used with the 1D time-dependent mode of COMSOL Multiphysics 5.3 with the initial parameters and adjustable parameter of $k_{1\text{DMA}2\text{P}}$. For each experiment, the parameter of $k_{1\text{DMA}2\text{P}}$ was adjusted until $\left| \frac{E_{exp} - E_{pred}}{E_{exp}} \right| \leq 1\%$.

4 | RESULTS AND DISCUSSIONS

4.1 | Ion speciation plots of the 1DMA2P- H_2O - CO_2 system

The concentration of ionic species in 2.0 mol/L 1DMA2P solution were obtained from the procedure mentioned previously. The detailed procedure for calculating concentration of ion species can be found in Section 3.1 in this work. The ion speciation plot for the 1DMA2P- H_2O - CO_2 system at the temperature of 298 K with the CO_2 loading (mol CO_2 /mol amine) ranging from 0 to 0.87 is shown in Figure 4. It can be observed that the concentrations of 1DMA2P decreased as the CO_2 loading increased, which could be attributed to the reaction of CO_2 with 1DMA2P solution and the emergence of the protonated 1DMA2P. As a result, $1\text{DMA}2\text{PH}^+$ (protonated 1DMA2P) concentration increased gradually as the CO_2 loading increased. One of the major products, HCO_3^- , also exhibited the same increasing trend as $1\text{DMA}2\text{PH}^+$ with increasing CO_2 loading since it was formed via the reaction of CO_2 with 1DMA2P solution. However, the increase in CO_3^{2-} concentration was not straightforward; it was found to increase with CO_2 loading at low CO_2 loading, but after reaching a maximum, it then decreased as the CO_2 loading increased. This is mainly because the strongly basic solution caused by the existence of an excess amount of 1DMA2P at the low CO_2 loading led to the increase in CO_3^{2-} concentration. At higher CO_2 loading, the decrease of free 1DMA2P resulted in a weaker basic solution so that the CO_3^{2-} concentration decreased by converting to the HCO_3^- through the reverse reaction of Equation (5).

4.2 | Reaction kinetics

In this work, the CO_2 absorption rate in 1DMA2P solution were obtained over concentration of 0.5–2.0 mol/L, CO_2 loading range of 0–0.06 mol CO_2 /mol amine. All experimental data of CO_2 absorption was presented in Table S1. Based on those measured experimental results, the rate constant $k_{1\text{DMA}2\text{P}}$ was then obtained by using the procedure shown previously in the Section 3.2. All values of $k_{1\text{DMA}2\text{P}}$ for each experimental result are given in this work. The Arrhenius relationship has been generally accepted to correlate $k_{1\text{DMA}2\text{P}}$ with temperature, as shown in Equation 36.

$$k_2 = A \exp\left(-\frac{E_a}{T}\right) \quad (36)$$

where A is Arrhenius constant ($\text{m}^3/\text{mol s}$) and E_a represents the activation energy (kJ/mol).

The obtained k_2 were fitted with Equation (36). The Arrhenius equation of 1DMA2P can be expressed as:

$$k_{1\text{DMA}2\text{P}} = 7.59 \times 10^{11} \times \exp\left(-\frac{7137.3}{T}\right) \quad (37)$$

The activation energy (E_a) was determined in this work as 59.3 kJ/mol, which agrees with the reference which had 62.55 kJ/mol. By using the Equation (37), the $k_{1\text{DMA}2\text{P}}$ at the temperature of 298 K could be given the value of 30. By comparison with the value of $k_{1\text{DMA}2\text{P}}$ at 298 K extracted from the Brønsted relationship, the value of $k_{1\text{DMA}2\text{P}}$ from the experimental data shows excellent agreement.

In this work, the CO_2 absorption rate in 1DMA2P solution was also predicted in this work. All the experimental and calculated values are presented in this work. The calculated values of CO_2 absorption rate were in good accordance with experimental values with an acceptable AAD of 6.5%. This observation indicates clearly that the base-catalyzed hydration mechanism can be satisfactorily used to describe the experimental data for CO_2 absorption in 1DMA2P solution.

4.3 | Enhancement factors

The enhancement factor for CO_2 absorption in aqueous 1DMA2P solution was obtained by using Equation (34) at the temperature of 303 K over the 1DMA2P solution range of 0.5–2 mol/L. All the results are shown in Table 1. As shown in the table, the enhancement factor increases as the concentration increases. This is because an increase in the concentration of 1DMA2P leads to more molecules in the solution, which results in more chemical reaction in the system.

4.4 | Comparison with other amines in the performance of CO₂ absorption

As 1DMA2P is a new amine, it is reasonable to compare its performance in CO₂ capture with conventional amines such as MEA, DEA, MDEA, 2-amino-2-methyl-1-propanol (AMP), and PZ as well as other alternative amines such as DEAB, DE-1,2-PD, and 1-(2-HE)PP. Those results would provide a comprehensive evaluation of 1DMA2P as a promising alternative solvent for CO₂ capture. In this work, this comparison is presented in terms of the CO₂ equilibrium solubility, the reaction kinetics constant (k_2) and heat of CO₂ absorption.

The CO₂ equilibrium solubility of MEA, DEA,³⁹ MDEA,³⁹ AMP,⁴⁰ PZ,⁴¹ DEAB,⁴² DE-1,2-PD, 1-(2-HE)PP,⁴³ and 1DMA2P at concentration of 2 mol/L, temperature of 298 K, CO₂ partial pressure of 101 kPa are presented in Table 2. As Table 2 shows, the CO₂ equilibrium solubility in aqueous 1DMA2P solution was clearly higher than those in MEA, DEA, MDEA, DE-1,2-PD, and 1-(2-HE)PP, respectively, and lower than that in AMP, PZ, and DEAB. This can be ranked as: PZ > DEAB > AMP > 1DMA2P > 1-(2-HE)PP > DE-1,2-PD > MDEA > DEA > MEA.

The second order rate constant (k_2) is directly related to the reaction kinetics. A higher value of k_2 means faster reaction kinetics. The k_2 values of MEA, DEA, MDEA, AMP, PZ, DEAB, DE-1,2-PD, 1-(2-HE)PP, and 1DMA2P at temperature of 298 K are shown in Table 2.^{25,43} The table shows that the value of k_2 for 1DMA2P is lower than that for MEA, DEA, AMP, PZ, 1-(2-HE)PP, DE-1,2-PD, and DEAB, but much higher than that of MDEA. The ranking of k_2 for these amines can be represented as follows: PZ > MEA > DEA > AMP > DEAB > DE-1,2-PD > 1-(2-HE)PP > 1DMA2P > MDEA. In addition, the CO₂ absorption heats in aqueous MEA, DEA, MDEA, AMP, PZ, DEAB, DE-1,2-PD, 1-(2-HE)PP, and 1DMA2P solutions are also shown in Table 2. From the table, the heat of CO₂ absorption in aqueous 1DMA2P solution was lowest among those amines.

Based on the CO₂ capture performance of 1DMA2P considering those CO₂ absorption parameters, the 1DMA2P could be considered as one of the alternative solvents as DEAB, AMP for mixing with the solvents with higher reaction rate and higher absorption heat (e.g., MEA and PZ).

4.5 | Solvent screening based on absorption parameters

A fundamental consideration when selecting an amine for post-combustion capture is the performance of the amine across both the absorption and desorption regimes.¹⁷ Fast absorption kinetics is a vital factor in the absorption process as it directly correlates with the required physical size of the absorber; thus, an amine that reacts quickly with CO₂ is advantageous. Also, the equilibrium CO₂ solubility is another parameter, which should be considered because it is related to the consumption of solvent in the absorption plant. In addition, the energy consumption for CO₂ stripping is another considered parameter because it makes up over half of the operating costs of the CO₂

capture plant.⁴⁴ It is generally accepted that the heat of CO₂ absorption has a close relationship to the energy requirement for regeneration of the amine in the CO₂ removal process. The information about CO₂ absorption heat (ΔH_a) in amines solution is considered to be a parameter of prime importance for designing the unit operations of CO₂ removal plant. The solvent screening therefore represented three CO₂ absorption parameters, namely, CO₂ equilibrium solubility, second order reaction constant (k_2), and CO₂ absorption heat. In this work, all the three parameters of conventional amines (MEA, DEA, MDEA, AMP, and PZ) and alternative amines (DEAB, DE-1,2-PD, 1DMA2P, and 1-(2-HE)PP) were analyzed in order to provide guidelines about an effective screening of solvents.

Figure 5 shows the relation between ΔH_a and $\log k_2$ for conventional amines (i.e., MEA, DEA, MDEA, AMP, and PZ), the alternative amines (e.g., DEAB, 1-(2-HE)PP, and DE-1,2-PD), and the new solvent (1DMA2P). Based on this figure, the primary (MEA), secondary (DEA), steric hindrance (AMP), cyclic (PZ) conventional amines exhibited fast reaction kinetics, which implies that the physical size of the absorber will be small. However, high absorption enthalpies also accompany these amines, which may result in large energy consumption in the stripper. MDEA with lower kinetics and lower absorption enthalpy will increase investment in equipment but can regenerate at a decreased desorption cost. Figure 4 shows that all solvents MEA, DEA, MDEA, AMP, and PZ are located in the conventional section, which could be considered to be first generation solvents or conventional solvents. From Figure 5, the solvents located above the first generation such as DEAB, DE-1,2-PD, 1-(2-HE)PP, and 1DMA2P show both fast kinetics and small absorption enthalpy. This means that those solvent located in the alternative section exhibit the potential for commercial application. Other solvents considered as the alternative amines should located in this section.

Figure 6 shows the relation between the equilibrium CO₂ solubility versus heat of CO₂ absorption for conventional amines (e.g., MEA, DEA, MDEA, AMP, and PZ), the alternative amines (e.g., DEAB, DE-1,2-PD, 1-(2-HE)PP) and the novel solvent (1DMA2P). The figure shows that MEA and DEA have lower CO₂ solubility and higher absorption heat, which result in both larger solvent and energy consumption. AMP and PZ show higher CO₂ solubility and heat of CO₂ absorption. However, the higher absorption enthalpy will lead to larger energy consumption. MDEA exhibits low absorption heat, which would result in low energy consumption in desorption. Based on Figure 6, DEAB, 1DMA2P, DE-1,2-PD, and 1-(2-HE)PP show higher CO₂ solubility and lower absorption heat, which would result in lower cost of CO₂ capture. This means that the solvents located in the alternative section exhibit the potential for commercial application. Any other solvents considered as alternative should be located in this section.

Both Figures 5 and 6 were developed to correlate the kinetics of CO₂ absorption with the CO₂ stripping process and CO₂ solubility with CO₂ stripping process, respectively, which would provide information about the possibility and/or capability of new solvents being useful as commercial or alternative solvents for CO₂ capture. As shown in Figures 5 and 6, 1DMA2P exhibits good performance in

CO₂ capture with fast kinetics, high CO₂ solubility, and low absorption heat. As such, 1DMA2P could be considered as one of the alternative amines to mix with MEA or PZ. In addition, Figures 5 and 6 can also provide direction for future design or screening of better or ideal amines for CO₂ capture. The ideal amine should have fast reaction, high CO₂ solubility and low absorption enthalpy. These types of amines should be located in the top right corner of the figures.

5 | CONCLUSIONS

In this work, the reaction kinetics data of 1DMA2P were experimentally measured using the laminar jet absorber under different conditions. A comprehensive reaction kinetics model for CO₂ absorption in 1DMA2P solution was developed. The reaction constant ($k_{1\text{DMA2P}}$) of CO₂ with 1DMA2P solution was as shown in the equation as: $k_{1\text{DMA2P}} = 7.59 \times 10^{11} \times \exp\left(-\frac{7137.3}{T}\right)$. In addition, the reaction rate of CO₂ absorption into 1DMA2P solution could also be predicted, which have a good agreement with the experimental with an AAD of 6.5%. On the basis of the absorption parameters provided in this work, both the conventional amines and this alternative amine were analyzed for the purpose of providing the guidelines or information on how to effectively screen solvents.

AUTHOR CONTRIBUTIONS

Xiaotong Jiang: Formal analysis (equal); methodology (supporting); writing – review and editing (equal). **Helei Liu:** Investigation (lead); methodology (lead); supervision (equal); writing – original draft (lead). **Paitoon Tontiwachwuthikul:** Conceptualization (equal); project administration (equal); supervision (equal). **Raphael Idem:** Conceptualization (equal); funding acquisition (equal); project administration (equal); supervision (equal). **Shoulong Dong:** Formal analysis (equal); validation (equal); writing – review and editing (equal).

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DATA AVAILABILITY STATEMENT

Data sharing is not applicable.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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