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Experimental measurement and modeling study on CO_2 equilibrium solubility, density and viscosity for 1-dimethylamino-2-propanol (1DMA2P) solution

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ABSTRACT

In this study, new experimental data of CO_2 equilibrium solubility for an aqueous solution of 1DMA2P, a novel ternary amine, are presented over a CO_2 partial pressure range of 3–168 kPa, at different concentrations of 1DMA2P (2, 3 and 4 M), and in a temperature range of 298.15–333.15 K. Besides, new experimental data of viscosity and density are reported in a concentration range from 20 wt% up to pure 1DMA2P, in a temperature range of 298.15–333.15 K, and in atmospheric pressure. CO_2 equilibrium solubility data were predicted by Deshmukh–Mather (D-M) thermodynamic model. From the experimental data of density and viscosity, thermodynamic properties including the thermal expansion coefficient (α_p), excess molar volume (V^E), viscosity deviation ($\Delta\eta$), activation molar enthalpy (ΔH), activation molar entropy (ΔS), and activation molar Gibbs free energy (ΔG) were obtained. We have modeled and predicted the experimental data of viscosity based on Eyring's theory and nonrandom two-liquid (NRTL) and Wilson models. The results showed that the Eyring-Wilson model predicts the experimental viscosity data better than Eyring-NRTL. For CO_2 equilibrium solubility, D-M model gave a good prediction with an absolute average relative deviation of 2.64%.

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1. Introduction

The CO_2 solubility, density, and viscosity of amine solutions are important properties for the designing and simulation of absorption-desorption units, for example, in the field of CO_2 capture or gas sweetening processes [1,2]. Well-known amine solutions such as monoethanolamine (MEA), diethanolamine (DEA), and methyldiethanolamine (MDEA) have been widely used in amine plant units [3]. However, these amines have some drawbacks; for example, MEA and DEA consume high energy for their regeneration (about 70% of plant cost), increase corrosion rate, and increase thermal and oxidation degradation [4]. MDEA as a ternary amine has a low reaction rate with CO_2 in comparison with MEA and DEA, but it consumes lower energy than MEA and DEA for its regeneration. Therefore, research activities are ongoing to find the ideal amine solution to overcome the mentioned problems [5]. In general, a ternary amine requires low energy for its regeneration, which can reduce the cost of the amine plant. Recently, Chowdhury, et al. [6] have evaluated 24 kinds of novel tertiary amines, and they found that 7 amines have good potential for application in CO_2 removal processes. Among these amines, 1-dimethylamino-2-propanol (1DMA2P), compared to MDEA, showed good potential for absorption of CO_2 because of its high absorption rate and high equilibrium loading [7,8]. There are many studies about CO_2 solubility, density, and viscosity of amine solutions in literature, and the studies are associated with experimental and theoretical subjects [9–12]. We have only reviewed some recently studies related to 1DMA2P solution as follows: Chowdhury et al. [13] have measured the densities of 1DMA2P at different mole fractions and temperature ranges from 303.15 K to 323.15 K. They correlated the V^E by applying the Redlich–Kister equation; Idris et al. [14] have measured and correlated the new experimental data of density of unloaded and loaded with CO_2 for 1DMA2P solution at different weight fractions from 10 wt % to pure 1DMA2P and at temperature ranging from 298.15 K to 353.15 K. They correlated the experimental data by using the Redlich–Kister equation. In associated with CO_2 equilibrium solubility, Liu, et al. [8] have presented the equilibrium CO_2 solubility data for 1DMA2P concentrations of 1, 2 and 5 M within the temperature range of 298.15–333.15 K and the

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CO_2 partial pressure range from 3-to 101 kPa. They predicted the solubility data based on the stoichiometric approach called modified Kent-Eisenberg model. In associated with viscosity, there is no experimental data for the 1DMA2P solution published in the literature.

Therefore, our objective of this study was to present new experimental data for equilibrium solubility of CO_2 into 1DMA2P solution in concentrations of 2, 3 and 4 M within the temperature range of 298–333 K and the CO_2 partial pressure range from 3-to 168 kPa. In addition, we have measured the density and viscosity of the 1DMA2P solution at different weight fractions from 20 wt % to pure 1DMA2P and a temperature ranging from 298.15 K to 333.15 K. We have modeled the V^E by applying the Redlich–Kister equation, and ΔH, ΔS, and ΔG were obtained by using the Eyring equation. For the prediction of the experimental data of the viscosity of the 1DMA2P solution, we have applied the models based on Eyring's theory and the functional forms of the Wilson model and NRTL model. To predict the CO_2 solubility data, Deshmukh–Mather (D-M) model was applied by considering non-ideality in liquid phase. In D-M model, the interaction parameters of short range between ion–molecule and ion–ion species in the activity model were evaluated as a function of temperature. The adjustable parameters of applied models for the equilibrium CO_2 solubility, density, and viscosity were determined to fit our experimental data, presented in this study by using the Simplex optimization algorithm in MATLAB software.

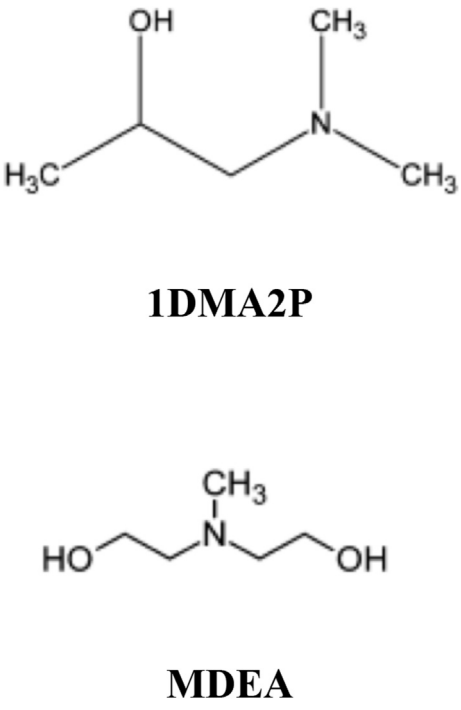

Fig. 1. Molecular structures of MDEA and 1DMA2P.

2. Experimental section

2.1. Material

1DMA2P and MDEA, each with mass purity of 99.0%, were purchased from Merck Chemical Company. The mentioned amine solutions were prepared by using deionized water to the required concentrations without further purification and with uncertainty within 0.01%. CO_2 with a purity of 99.99% was obtained from LIAN OXYGEN ARIA Co. Properties, sources, purities of the chemicals used and their molecular structures are presented in Table 1 and Fig. 1, respectively.

2.2. Experimental setup for measuring CO_2 solubility

In this study, a static-synthetic apparatus was used for measuring the equilibrium solubility data of CO_2 + 1DMA2P + H_2O system (Fig. 2). The static-synthetic apparatus has been widely used by researchers in the literature [15–18]. We have also used this apparatus to calculate the amount of absorbed CO_2 by amine solution based on the material balance and measuring of data for pressure, volume, and temperature of vapor-liquid equilibrium (VLE) cell and buffer cell. The main parts of our apparatus consist of buffer cell, VLE cell, isolation valves, vacuum pump, magnetic stirrer, water bath, data recorder and temperature and pressure indicators. Both VLE cell and buffer cell were made of stainless steel. The volume of VLE cell plus its connection tube (from top of VLE cell up to v4) is 360 ml and the volume of buffer cell plus their connection tubes is 1470 ml. The buffer cell was used to keep the CO_2 gas under pressure before absorption the CO_2 by amine solution. The equilibrium temperature for both cells was adjusted with stability of ±0.05 K by using a water bath (LAUDA Alpha, Model: RA 8). The temperature and pressure in each cell were measured by using the K-type thermocouple with an accuracy of ±0.01 K and a pressure indicator (Sensys, model; PSCH0025BCIJ), respectively. In our setup, the data recorder (ATRON, Model: SL-45) was used to record the temperature and pressure data for both cells as a function of time. In the VLE cell, magnetic stirrer (MTOPS, Model: HS180) was placed for stirring the amine solution and achieving the equilibrium faster, and its speed set at a 360 rpm during all the experiments performed.

2.2.1. Experimental procedure

To perform each test, 20 ml of an aqueous solution of the

Table 1
Properties, purities and sources of MDEA and 1DMA2P.

Chemical Name	Formula Weight	Freezing point °C	Boling point °C	Vapor pressure (mm Hg) at 20 °C	Water solubility	Mass fraction purity	Source	CAS number	purification method
MDEA[a]	119.16	−21.0	247.1	0.01	Miscible	99.0	E.Merck, Germany	105-59-9	none
1DMA2P[b]	103.16	−85.0	127.0	8.0	Miscible	99.0	E.Merck, Germany	108-16-7	none
CO_2[c]	44.01	−56.55[d]	78.46[d]	42939.99[d]	88[d] (mL CO_2/100 mL H_2O) at 760 mm Hg and 20 °C	99.99	LIAN OXYGEN ARIA Co	–	none

[a] Methyldiethanolamine (C5H13NO2).
[b] 1-dimethylamino-2-propanol (C5H13NO).
[c] Carbon dioxide.
[d] [37].

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