Experimental and an electrolyte non-random two-liquid model to predict the vapor–liquid equilibrium of CO₂ in aqueous solutions of diethylenetriamine

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Abstract
The absorption and desorption data of CO₂ in aqueous solutions with a mass fraction of 10% and 20% of diethylenetriamine are measured at 313.15, 343.15, 373.15, and 393.15 K. The electrolyte non-random two-liquid theory is developed using Aspen V9.0 to correlate and predict the vapor–liquid equilibrium of CO₂ in aqueous diethylenetriamine solutions. The model predicted the heat capacity and saturated vapor pressure data of diethylenetriamine, the mixed heat of a diethylenetriamine–H₂O binary system, and the vapor–liquid equilibrium data of a diethylenetriamine–H₂O–CO₂ ternary system. The physical parameters and the interaction parameters of the model system are calculated. The model predicted CO₂ solubility showing a 10% average absolute deviation from experimental data. The calculated values of the model are basically consistent with the experimental values.

Keywords
Aspen Plus, CO₂ capture, diethylenetriamine, non-random-two-liquid-electrolyte thermodynamic model, polyamine

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Introduction
With the development of economies and society, the demand for fossil fuels is increasing rapidly, which makes the emission of CO₂ and global warming increasingly serious. A recent study by Rosenfeld¹ shows that global warming problem is more serious than previously estimated. As a greenhouse gas, carbon dioxide is a major factor contributing to the growth of global warming.²,³ While coal’s coal-based energy structure demands that any potential approach toward large-scale and effective CO₂ emission reduction is CO₂ capture and storage.⁴ As for CO₂ capture, the solvent absorption method is mainly adopted in industry to realize large-scale CO₂ treatment, which has advantages of fast absorption, a simple process, and large processing capacity, but also has disadvantages of high consumption and significant corrosion of equipment.⁵ In order to develop CO₂ capture and storage technology with low energy consumption and low cost, it is necessary to model, expand simulations, and utilize thermodynamic properties such as phase equilibrium and chemical equilibrium, and optimize CO₂ capture processes. There are three kinds of commonly used thermodynamic models for evaluating the thermodynamic properties of acidic gas absorption processes: the first is the KE model with simple and non-strict form.⁶ This model has poor universality, but the fitting effect is a good in the specific load range. It cannot be extended to the absorption process of a mixed gas, and it cannot be used to predict the reaction heat of each component. The second category is the more rigorous activity coefficient model and equation of state. For the activity coefficient model, more variables are required and the model is more complex. As the most widely used model in this class, Deshmukh and Mather⁷ model has been successfully used to calculate the phase equilibrium of the monoethanolamine–H₂O–CO₂ (MEA–H₂O–CO₂) system. The third category encompasses more complex and more rigorous models, including non-random dual fluid electrolyte (e-NRTL) and extended UNIQUAC.
models, which have been widely used in aqueous amine systems,\(^8\) while extended UNIQUAC models are rarely used. In the CO\(_2\) capture based on amines, the reaction between CO\(_2\) and the aqueous solution of amine will form numerous ions. Due to interactions between ions, the non-ideal nature of the electrolyte system is relatively strong. How to accurately describe the non-ideal nature of the solution is the key to simulate the electrolyte solution system. The e-NRTL model proposed by Mock et al.\(^9\) can correct the non-ideal nature of the multi-component electrolyte system and can be used to simulate the capture process of CO\(_2\). Therefore, this paper selects the e-NRTL model for the relevant thermodynamic simulation.

Diethylenetriamine (DETA) is a polyamine containing three amine functionalities (two primary and one secondary amine), which is expected to have high CO\(_2\) loading capacity.\(^10,11\) Compared to typical alkanolamines, DETA has a high capacity for binding CO\(_2\), a high absorption rate and a high boiling point.\(^12,13\) Therefore, aqueous solutions of DETA can be potential solvents for CO\(_2\) capture. Due to the advantages mentioned above, a series of studies have been carried out on DETA recently, including impregnating of plaza-acti-

In this work, new experimental CO\(_2\) solubility data in aqueous DETA solutions (mass fraction of 10\% and 20\% of DETA) are generated over a wide pressure range (up to 480 kPa) and temperature (313.15–393.15 K) to extend the limited experimental data found in the literature.\(^20,21\)

Results and discussion

Chemical equilibrium

The chemical reaction of DETA is complex because DETA is a tertiary amine consisting of primary and secondary amine groups in its structure. So a wide range of chemical reactions is possible with a large number of species formed. The following possible parallel reversible chemical reactions in liquid phase for the (DETA–H\(_2\)O–CO\(_2\)) system are presented below. The constant-volume method, combined with gas chromatography analysis was used to measure the equilibrium solubility at different concentrations. The schematic diagram of the CO\(_2\) absorption measurement device is presented in Figure 1.

Dissociation of water

\[
2\text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{OH}^- \quad \text{(1)}
\]

Formation of bicarbonate

\[
2\text{H}_2\text{O} + \text{CO}_2 \leftrightarrow \text{H}_3\text{O}^+ + \text{HCO}_3^- \quad \text{(2)}
\]

Formation of carbonate

\[
\text{HCO}_3^- + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{CO}_3^{2-} \quad \text{(3)}
\]

Amine deprotonation

\[
\text{DETAH}^+ + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{DETA} \quad \text{(4)}
\]

\[
\text{DETAH}_2^{2+} + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{DETAH}^+ \quad \text{(5)}
\]

\[
\text{DETAH}_3^{3+} + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{DETAH}_2^{2+} \quad \text{(6)}
\]

Dissociation of carbamate

\[
\text{DETAHCOO}^- + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{HCO}_3^- + \text{DETA} \quad \text{(7)}
\]

\[
\text{DETA(COO)}_2^{2-} + \text{H}_2\text{O} \leftrightarrow \text{H}_3\text{O}^+ + \text{CO}_3^{2-} + \text{DETA} \quad \text{(8)}
\]

Due to the complex species of the system, there are many isomers. The main reaction equations are outlined. The chemical equilibrium constants of equations (1)–(8) are a function of temperature, which can be expressed by the following formula

\[
\ln K = A + \frac{B}{T} + C \ln T + D \times T \quad \text{(9)}
\]

where \(K\) is the reaction equilibrium constant; \(T\) is the reaction temperature; \(A, B, C,\) and \(D\) are the parameters of each reaction equilibrium constant, the values of which are taken from the literature\(^22,23\) and are listed in Table 1.

Phase equilibrium

The vapor–liquid equilibrium is defined by the equality of the fugacity at a given temperature and pressure. In the process of thermodynamic calculations, different reference states correspond to different phase equilibrium relations, so the appropriate reference state must be selected for our case study. In the model, CO\(_2\) was set as the Henry component, so the reference states of the ions and CO\(_2\) in the solution were in a state of infinite dilution, and the reference states of water and DETA were pure liquid. Therefore, DETA and H\(_2\)O have the following phase equilibrium relationship

\[
y_i \varphi_i P = x_i \gamma_i^{*} P^0_i \quad \text{(10)}
\]

The phase equilibrium relationship between CO\(_2\) and ions is as follows

\[
y_i \varphi_i P = x_i \gamma_i^{*} H_i \quad \text{(11)}
\]

where \(y_i\) and \(x_i\) are the molar composition of the gas phase and the liquid phase, respectively, \(\varphi_i\) is the fugacity coefficient for the gas phase, \(\gamma_i\) and \(\gamma_i^{*}\) are the activity coefficients of the species \(i\) when the reference states are pure and a state of infinite dilution, \(P^0_i\) and \(H_i\) are the saturated vapor pressure and Henry coefficient of the pure component \(i\). The e-NRTL model is used to calculate the activity coefficient of each component in the liquid phase and the gas phase fugacity coefficient is obtained from the
Redlich–Kwong state equation. The specific equations are as follows
\[ P = RT V_m - b - \frac{a}{T^{0.5} V_m (V_m + b)} \]  
\[ \ln H_i = A_i + B_i \ln T + C_i \ln T + D_i \times T \]  

The model results

DETA systems

By fitting the data of the liquid heat capacity and saturated vapor pressure for DETA, the coefficients of the Antoine equation and specific heat capacity equations (14) and (15) were obtained. The results are shown in Tables 2 and 3. The experimental values and the calculated values from the model for the specific heat capacity are shown in Figure 2. The average relative deviation of DETA is 0.41%. Figure 3 compares the experimental values of the saturated vapor pressure with the model fitting values, and the average relative deviation of saturated vapor pressure is 1.3%. It can be seen from the figures that the experimental values are in good agreement with the model fitting values, and the parameters obtained can accurately describe the properties of the pure absorbent.

\[ \ln p_i = C_i + \frac{C_{i2}}{T + C_3} + C_4 T + C_5 \ln(T) + C_6 T^{C_7} \]  
for \( C_8 \leq T \leq C_9 \)

\[ C_i^{\text{eq}} = C_i + C_{i2} T + C_3 T^2 + C_4 T^3 + C_5 T^4 + C_6 T^5 \]  
for \( C_8 \leq T \leq C_9 \)

\[ C_i^{\text{eq}} = C_i + C_{i2} T^{C_3} \]  for \( T \leq C_7 \)

Binary systems: DETA–H₂O

The binary interaction coefficients of the e-NRTL model were obtained by fitting the mixed heat data of the DETA–H₂O system. Figure 4 compares the experimental values and the model calculation values of the mixed heat data of the DETA–H₂O system. The average relative deviation of the mixed heat data of \{DETA–H₂O\} is about 5%. It can be seen from the figure that the thermodynamic model can accurately predict the vapor–liquid equilibrium and mixed heat data of the system.

Ternary systems: DETA–H₂O–CO₂

As the system of polyamines is relatively complex compared with that of monoamines, the thermodynamic reactions between substances in the system should be clarified before setting up the thermodynamic model. Hartono determined the species distribution of the DETA–H₂O–CO₂ system by nuclear magnetic resonance (NMR) spectrometry, and found that there were 24 species in the system. The main species are DETA(COO)⁺, DETA(COO)₂⁺ A⁺, HCO₃⁻ and CO₃²⁻. No clear evidence was found of any tricarbamate species and free CO₂ in the system.

For the amine + H₂O + CO₂ system, there is not only the interaction between the amine and the CO₂ and H₂O...
molecules, but also the interaction between ion pairs and molecules. The values of the action parameters can be obtained by fitting the solubility data of CO₂ in amine aqueous solutions of different concentrations at different temperatures by applying the short-range term of e-NRTL. DETA has two symmetric primary amines (p) and a tertiary amine (s), so the species in aqueous solution is complex and there are many isomers. For the DETA⁺H₂O⁺CO₂ system, regression parameters are required as follows: a binary interaction parameter of H₂O–DETA, an interaction parameter between the molecule {H₂O, DETA, CO₂} and the ion pair {DETAH⁺(s), DETAH⁺(p), DETAH₂⁺(pp), DETAH³⁺, HCO₃⁻, DETACOO⁻(s), DETACOO⁻(p), DETACOO⁻(pp), and DETA(COO)₂⁻ (pp)}. The parameters obtained are shown in Tables S1 and S2 of the supporting information.

Figures 5 and 6 describe the CO₂ solubility in DETA solutions with mass fractions of 10% and 20%, respectively, and compare the calculated results with the experimental values. The measured temperatures of solubility were 313.15, 343.15, 373.15, and 393.15 K, respectively, and the CO₂ loading ranged from 0.0 to 1.9. The deviation of experimental data and fitting data is shown in the Table 4. As DETA is a tertiary amine, the species of the system is relatively complex. In the model calculation, some isomers were approximated, and the calculation error at low temperature was slightly larger. Under the conditions of low pressure, the partial pressure of CO₂ in the gas phase is relatively low, the amount of CO₂ in the vapor

### Table 2. Values of the specific heat capacity equation parameter (kJ/kmol/K).

| C₁  | C₂   | C₃   | C₄    | C₅ | C₆   | C₇   | C₈  | C₉ | C₁₀ | C₁₁ |
|-----|------|------|-------|----|------|------|-----|----|-----|-----|
| DETA| -2039.19 | 20.016 | -0.058193 | 5.63E-05 | 0   | 0    | 1.26E-08 | 1000 | 0   | 0   | 0   |

DETA: diethylenetriamine.

### Table 3. Values of the Antoine equation parameter (atm).

| C₁    | C₂   | C₃   | C₄      | C₅    | C₆   | C₇   | C₈      | C₉   | C₁₀    |
|-------|------|------|---------|-------|------|------|---------|------|--------|
| DETA  | 58.72324 | -9047.33 | -9.94509381 | -3.65E-03 | -6.1241 | 7.82E-18 | 234.15 | 676    |

DETA: diethylenetriamine.

Figure 2. Comparison of the e-NRTL model predictions with experimental data for the specific heat capacity of DETA from 300 to 400 K.
The points ■ are from the experimental result of study by Peng and Robinson.²⁴ The solid line is the fitting values of the model. e-NRTL: electrolyte non-random two-liquid; DETA: diethylenetriamine.

Figure 3. Comparison of the e-NRTL model predictions with experimental data for the saturated vapor pressure of DETA from 350 to 550 K.
The points ■ are from the experimental result of study by Lee et al.²⁵ The solid line is the fitting values of the model. e-NRTL: electrolyte non-random two-liquid; DETA: diethylenetriamine.

Figure 4. Excess molar enthalpy for the binary mixtures {DETA (2) + H₂O (1)}.
■ Experimental values at 303.15 K; ▲ experimental values at 323.15 K. The solid lines are the fitting values of the model. DETA: diethylenetriamine.
phase is relatively small, and the average relative deviation will be large. At low temperature, the error in the fitting results is relatively large. The reason may be that at low temperature, the solution has a strong CO₂ absorption capacity and a low gas pressure, resulting in a large measurement error, which will affect the final simulation results.

**Conclusion**

In this work, new experimental CO₂ solubility in aqueous DETA solutions (mass fraction of 10% and 20% of DETA) have been measured over a wide range of pressure (up to 480 kPa) and temperature (313.15–393.15 K) to extend the limited experimental database. A thermodynamic model based on e-NRTL was established and used to correlate VLE data to predict CO₂ partial pressure for the DETA–CO₂–H₂O system. The model predicted results are in good agreement with experimental VLE data with an average relative deviation of 10%. The parameters of the thermodynamic model can be used to simulate and optimize CO₂ absorption process.

**Experimental section**

**Materials**

The molecular formula, CAS number, purity, and source are reported in Table 5. The aqueous solutions are prepared using ultrapure water, which was prepared using a Center 120 FV-S ultrapure water generator. All reagents were used as supplied without any further purification.

**Apparatus and procedure**

The constant-volume method, combined with gas chromatography analysis was used to measure the solubility at different concentrations. The schematic diagram of the CO₂ absorption measurement device is presented in Figure 1. A detailed description of the vapor–liquid equilibrium apparatus can be found in the literature.²⁹ It is comprised of two stainless steel tanks for the buffer and reaction. Both tanks are equipped with temperature probes and pressure transducers. The principle of this method is to absorb a known volume of gas known volume of polyamine solution. The amount of CO₂ gas introduced into the reaction tank was determined by the change in the buffer tank, before and after injection. After equilibrium was achieved at a constant temperature, the amount of CO₂ gas absorbed in the solution was equal to the amount of CO₂ in the vapor phase subtracted by the amount of CO₂ in the liquid phase. The CO₂ solubility, α₁₂, in the liquid phase is defined as divided by the number of moles.

**Figure 5.** Solubility of CO₂ in a DETA solution with a mass fraction of 10%.

The points are the experimental values and the line is the fitting values of Aspen. ■ 313.15 K; ● 343.15 K; ▲ 373.15 K; ▼ 393.15 K. DETA: diethylenetriamine.

**Figure 6.** Solubility of CO₂ in a DETA solution with a mass fraction of 20%.

The points are the experimental values and the line is the fitting values of Aspen. ■ 313.15 K; ● 343.15 K; ▲ 373.15 K; ▼ 393.15 K. DETA: diethylenetriamine.

**Table 4.** The average relative deviations.

| Temperature   | 10 mass% DETA | 10 mass% DETA | 20 mass% DETA | 20 mass% DETA |
|---------------|---------------|---------------|---------------|---------------|
| 313.15 K      | 0.0960        | 0.0718        | 0.0956        | 0.0982        |
| 343.15 K      | 0.0766        | 0.0808        | 0.0974        | 0.1065        |
| 373.15 K      |               |               |               |               |
| 393.15 K      |               |               |               |               |

**Table 5.** Specifications and sources of the chemicals used in this work.

| Chemical         | CAS number | Molecular formula | Purity*       | Supplier                        |
|------------------|------------|-------------------|---------------|---------------------------------|
| Diethylenetriamine | 111-40-0  | C₆H₁₃N₃         | 0.99 (mass fraction) | J&K Scientific                 |
| Carbon dioxide   | 124-38-9   | CO₂              | 0.99999 (mole fraction) | Beijing Millennium Capital Gas Co. Ltd |
| Nitrogen         | 7727-37-9  | N₂              | 0.99999 (mole fraction) | Beijing Millennium Capital Gas Co. Ltd |

*Used without any further purification.
| T (K) | α_{CO_2} | P_{CO_2} | α_{am} | P_{CO_2} | α_{am} | P_{CO_2} | α_{am} | P_{CO_2} |
|-------|---------|---------|--------|---------|--------|---------|--------|---------|
| 313.15 | 0.8744 ± 0.0699 | 0.098 ± 0.0010 | 0.0662 ± 0.0531 | 0.3558 ± 0.0036 | 0.3168 ± 0.0253 | 0.092 ± 0.0092 | 0.2547 ± 0.0203 | 3.1 ± 0.0310 |
| 343.15 | 1.0231 ± 0.0818 | 0.3 ± 0.0030 | 0.8045 ± 0.0643 | 0.776 ± 0.0078 | 0.6157 ± 0.0493 | 4.48 ± 0.0448 | 0.459 ± 0.0367 | 8.75 ± 0.0875 |
| 373.15 | 1.2112 ± 0.0977 | 1.48 ± 0.0148 | 0.9516 ± 0.0761 | 1.81 ± 0.0181 | 0.9128 ± 0.0730 | 19.11 ± 0.1911 | 0.6358 ± 0.0523 | 21.52 ± 0.2152 |
| 393.15 | 1.3019 ± 0.1042 | 2.98 ± 0.0298 | 1.0429 ± 0.0834 | 3.45 ± 0.0345 | 1.1326 ± 0.0906 | 61.96 ± 0.6196 | 0.8318 ± 0.0665 | 47.21 ± 0.4721 |
| DETA 10% | 1.409 ± 0.1127 | 9.67 ± 0.0967 | 1.1521 ± 0.0922 | 7.87 ± 0.0787 | 1.2891 ± 0.1031 | 139.12 ± 1.3912 | 0.9567 ± 0.0765 | 87.6 ± 0.8760 |
| 1.4906 ± 0.1192 | 23.58 ± 0.2358 | 1.2586 ± 0.1007 | 18.23 ± 0.1823 | 1.3936 ± 0.1115 | 241.76 ± 2.4176 | 1.0426 ± 0.0834 | 135.56 ± 1.3556 |
| 1.5593 ± 0.1247 | 46.88 ± 0.4688 | 1.3448 ± 0.1076 | 42.96 ± 0.4296 | 1.4434 ± 0.1155 | 308.76 ± 3.0876 | 1.1156 ± 0.0892 | 198.13 ± 1.9813 |
| 1.6254 ± 0.1300 | 85.48 ± 0.8548 | 1.4307 ± 0.1145 | 81.76 ± 0.8176 | 1.4923 ± 0.1194 | 380.1 ± 3.8010 | 1.2690 ± 0.1269 | 241.76 ± 2.4176 |
| 1.6827 ± 0.1346 | 131.48 ± 1.3148 | 1.5017 ± 0.1201 | 138.26 ± 1.3826 | 1.5274 ± 0.1222 | 444.91 ± 4.4491 | 1.3659 ± 0.1366 | 308.76 ± 3.0876 |
| 1.7298 ± 0.1384 | 193.28 ± 1.9328 | 1.5511 ± 0.1241 | 193.31 ± 1.9321 | 1.5468 ± 0.1237 | 483.8 ± 4.8380 | 1.4781 ± 0.1478 | 365.56 ± 3.6556 |
| 1.7826 ± 0.1426 | 278.08 ± 2.7808 | 1.5932 ± 0.1275 | 255.96 ± 2.5596 | 1.6279 ± 0.1307 | 429.67 ± 4.2967 | 1.5970 ± 0.1497 | 432.56 ± 4.3256 |
| 1.8255 ± 0.1460 | 357.68 ± 3.5768 | 1.6339 ± 0.1307 | 321.56 ± 3.2156 | 1.6751 ± 0.1340 | 460.46 ± 4.6046 | 1.7109 ± 0.1510 | 508.36 ± 5.0836 |

**Table 6.** CO₂ solubility (α_{CO_2}) in 10 wt% and 20 wt% amine aqueous solution at different temperatures: α_{am} (mol CO₂/mol amine), P_{CO_2} (kPa). *Standard uncertainties u(c) = ±0.01 mol/L, u(T) = ±0.1 K, u(p) = ±0.5%, u(α_{am}) = ±8%
of mole of amine. In accordance with the Peng–Robinson (PR) equation, the precise amount of CO₂ in the gas phase was determined using the volume, pressure, and temperature.²⁴ The accuracy of the volume, pressure, and temperature is ±0.1 mL, ±0.1 K, and ±0.5%, respectively. According to the above description, the experimental error of CO₂ solubility can be calculated, and is about ±8%.

At low partial pressure (<10 kPa), the pressure transducer error may have a greater impact on the results. Therefore, the CO₂ partial pressure was obtained using gas chromatography (Agilent 7890). The apparatus was verified by determining the solution of CO₂ in 30 mass% MEA solution at T = 313.15 and 393.15 K. The results are compared with reported data.²⁵,³⁰,³¹ Our results are in agreement with reported data.²⁵,³⁰,³¹ The solubility of DETA aqueous solutions with mass fractions of 10% and 20% at 313.15, 343.15, 373.15, and 393.15 K are measured using the above-mentioned CO₂ absorption device. The values are shown in Table 6.

Declaration of conflicting interests
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Supplemental material
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