Data Article

Data in brief on CO₂ absorption-desorption of aqueous-based amino acid solvents with phase change behaviour

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The data presented in this paper are related to the published research article "Development of aqueous-based phase change amino acid solvents for energy-efficient CO₂ capture: The role of antisolvent" [1]. The raw and analyzed data include the equilibrium and kinetics of CO₂ absorption, the density and concentration of different CO₂-containing species at upper and lower liquid phases, and particle size distribution of solid particles precipitated during CO₂ absorption of aqueous and aqueous-based amino acid solvents. In addition, the SEM images of solid precipitates at the end of CO₂ absorption are presented. The detailed values of this phase change amino acid solvent are crucial for large-scale implementation of CO₂ capture systems with phase change behavior.

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The data presented in this article are associated with the research article (M.S. Alivand et al., 2019 [1]) which were acquired using CO2 absorption-desorption rigs of the University of Melbourne. Fig. 1 shows the CO2 absorption-desorption rig for measuring dynamic CO2 absorption capacity, monitoring solid particle precipitation and highly-accurate heat transfer calorimetry analysis. Fig. 2a and b shows the effect of potassium hydroxide (KOH)/potassium glycinate (GlyK) ratio on the pH value and dynamic CO2 absorption capacity of aqueous 3 M potassium glycinate solvent at 40°C, respectively. Figs. 3 and 4 demonstrate the number of precipitated solid particles and particle size distribution for different initial GlyK and anti-solvent concentrations during dynamic CO2 absorption. The density, CO2 absorption capacity, carbamate and carbonate/bicarbonate concentration of prepared aqueous and aqueous-based GlyK solvents are presented in Tables 1 and 2. The spontaneous liquid-liquid phase separation of aqueous-based GlyK-70 and GlyK-80 solvents before CO2 absorption is illustrated in Fig. 5. Fig. 6 shows the SEM images of solid precipitated particles at the end of CO2 absorption for aqueous-based GlyK-55, GlyK-60 and GlyK-65 solvents.

1. Data

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2. Experimental design, materials, and methods

2.1. Dynamic CO$_2$ absorption/desorption experiments

The rate of dynamic CO$_2$ absorption in the loaded solution can be computed by the total mass balance of CO$_2$:

$$Q_{CO_2} = n_{in}^{CO_2} - n_{out}^{CO_2}$$

(1)

where $Q_{CO_2}$ is the rate of CO$_2$ absorption; $n_{in}^{CO_2}$ is the CO$_2$ molar flowrate at inlet stream; $n_{out}^{CO_2}$ is the CO$_2$ molar flowrate at outlet stream.

The recorded CO$_2$ concentration at outlet streams can be defined as:

$$x_{out}^{CO_2} = \frac{n_{out}^{CO_2}}{n_{out}^{CO_2} + n_{out}^{N_2}}$$

(2)

where $x_{out}^{CO_2}$ is the volume fraction of CO$_2$ at outlet stream; $n_{out}^{N_2}$ is the N$_2$ flowrate at outlet stream. Equation (2) can be represented by:

![Fig. 1](image1.png)

Fig. 1. Dynamic CO$_2$ absorption-desorption rig equipped with Focused Beam Reflectance Measurement (FBRM) probe for online monitoring solid precipitation and HFCal probe for quantitative heat flow calorimetry analysis.

![Fig. 2](image2.png)

Fig. 2. (a) pH value of potassium glycinate solution at different KOH/Gly molar ratios and (b) dynamic CO$_2$ absorption capacity of aqueous 3 M GlyK-0 solvent at 40 °C.
Fig. 3. Total number of precipitated solid particles and the amount of added DMF to the aqueous solution during CO₂ absorption time.
Using both Equation (1) and Equation (3), the rate of CO₂ absorption is calculated by:

\[ Q_{CO₂} = \frac{n_{CO₂}^{in} - \frac{x_{CO₂}^{out}}{1-x_{CO₂}^{out}} n_{CO₂}^{out}}{N_2} \]  

(4)

The amount of absorbed CO₂ over a given time, \( t \), is computed by:

\[ N_{CO₂} = \int_{0}^{t} Q_{CO₂} \, dt \]  

(5)
Similarly, for regeneration, the amount of desorbed CO$_2$ over a given time, $t$, can be obtained by:

$$N_{CO_2} = \int_0^t \frac{x_{CO_2}^{out}}{1 - x_{CO_2}^{out}} n_{CO_2}^{out} \, dt$$  \hspace{1cm} (6)$$

| Solvent | Density (mg/L) | Upper liquid phase | Lower liquid phase |
|---------|----------------|--------------------|--------------------|
| GlyK-0  | 1.2867         | –                  | –                  |
| GlyK-10 | 1.2868         | –                  | –                  |
| GlyK-25 | 1.2930         | –                  | –                  |
| GlyK-40 | 1.1326         | 1.3216             |                    |
| GlyK-50 | 1.1281         | 1.3604             |                    |
| GlyK-55 | 1.0894         | 1.4236             |                    |
| GlyK-60 | 1.0815         | 1.4475             |                    |
| GlyK-65 | 1.0798         | 1.4719             |                    |

Table 1
The density values of aqueous and aqueous-based GlyK-X solvents after CO$_2$ absorption.

| Solvent | CO$_2$ loading | Carbamate | Carbonate/bicarbonate |
|---------|----------------|-----------|-----------------------|
| GlyK-0  | 0.433          | 94.60     | 55.81                 |
| GlyK-10 | 0.435          | 97.33     | 53.75                 |
| GlyK-25 | 0.448          | 123.80    | 36.16                 |
| GlyK-40 | 0.483          | 152.72    | 162.26                |
| GlyK-50 | 0.513          | 237.44    | 167.66                |
| GlyK-55 | 0.539          | 340.41    | 208.81                |
| GlyK-60 | 0.546          | 413.25    | 230.15                |
| GlyK-65 | 0.551          | 426.06    | 223.49                |

Table 2
The CO$_2$ absorption capacity and CO$_2$-containing species distribution of different aqueous and aqueous-based GlyK-X solvents.

Fig. 5. The picture of aqueous-based (a) GlyK-70 and (b) GlyK-80 solvents before CO$_2$ absorption.
2.2. CO$_2$ vapor-liquid equilibrium (VLE) experiments

The solubility of CO$_2$ in aqueous/aqueous-based solutions was measured by an in-house rig. Initially, inlet valve opened and the CO$_2$ container was pressurized by pure CO$_2$ to a desired pressure. Then, the inlet valve closed and the pressure of container was recorded ($P_1$). Afterward, the outlet valve was opened for 2–3 sec, while inlet valves were still closed, and pure CO$_2$ was injected into the equilibrium reactor. As a result, the pressure of CO$_2$ container decreased and reached a new pressure ($P_2$). Total moles of CO$_2$ molecules injected into the equilibrium reactor was calculated by:

$$n_{CO_2} = \frac{V_c}{RT_a} \left( \frac{P_1}{Z_1} - \frac{P_2}{Z_2} \right)$$

(7)
where $V_c$ is the total volume of CO$_2$ container; $P_1$ and $P_2$ are the initial and final pressure of CO$_2$ container, respectively; $Z_1$ and $Z_2$ are gas compressibility factors associated to the initial ($P_1$) and final pressure ($P_2$) of CO$_2$ container; $R$ is the universal gas constant; $T_a$ is ambient temperature.

To calculate the compressibility factors Soave-Redlich-Kwong (SRK) was employed:

$$Z = \frac{a b P^2}{R^2 T^3}$$

(8)

All $a$, $b$ and $m$ coefficients can be calculated by:

$$a = 0.4274 \frac{R^2 T_c}{P_c} \left( 1 + m \left( 1 - \sqrt{T_r} \right) \right)^2$$

(9)

$$b = 0.0866 \frac{R T_c}{P_c}$$

(10)

$$m = 0.48 + 1.574 \omega - 0.176 \omega^2$$

(11)

where $T_c$ is the critical temperature; $T_r$ is the reduced temperature; $\omega$ is the acentric factor.

The equilibrium pressure of CO$_2$ in reactor is represented as:

$$P_{CO_2} = P_R - P_V$$

(12)

where $P_R$ is the reactor pressure recorded by pressure transmitter and $P_V$ is the vapor pressure of solution.

The total number of CO$_2$ moles in the gaseous part of equilibrium reactor was calculated by:

$$n_{CO_2}^g = \frac{V_g P_{CO_2}}{Z_{CO_2} R T_R}$$

(13)

where $V_g$ is the volume of gaseous part in the equilibrium reactor (total volume of equilibrium reactor minus the volume of loaded solution); $T_R$ is the reactor temperature; $Z_{CO_2}$ is the CO$_2$ compressibility factor at $T_R$ and $P_{CO_2}$. Thus, the amount of absorbed CO$_2$ in liquid phase was obtained by:
\[ n_{CO_2}^l = n_{CO_2} - n_{CO_2}^g \]  

The final amount of absorbed CO2 into the loaded solution was computed by:

\[ m_{CO_2} = \frac{n_{CO_2}^l}{w_{sol}} \]  

where \( w_{sol} \) is the weight of loaded solvent.

2.3. Validation and measurement accuracy

In order to validate the accuracy of VLE rig and calculation procedure (Equations (7)–(15)), the equilibrium CO2 absorption capacity of 5 mol/L (M) MEA solution at 40 °C was compared with the previously reported data [2] and the results are illustrated in Fig. 7. As it can be seen, there is an excellent agreement between experimental data and the reported values which represent the good reliability of CO2 VLE rig.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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