New Approach with Universal Applicability of Evaluating the Heat Requirements in Solvent Regeneration Process for Post-Combustion CO_2 Capture

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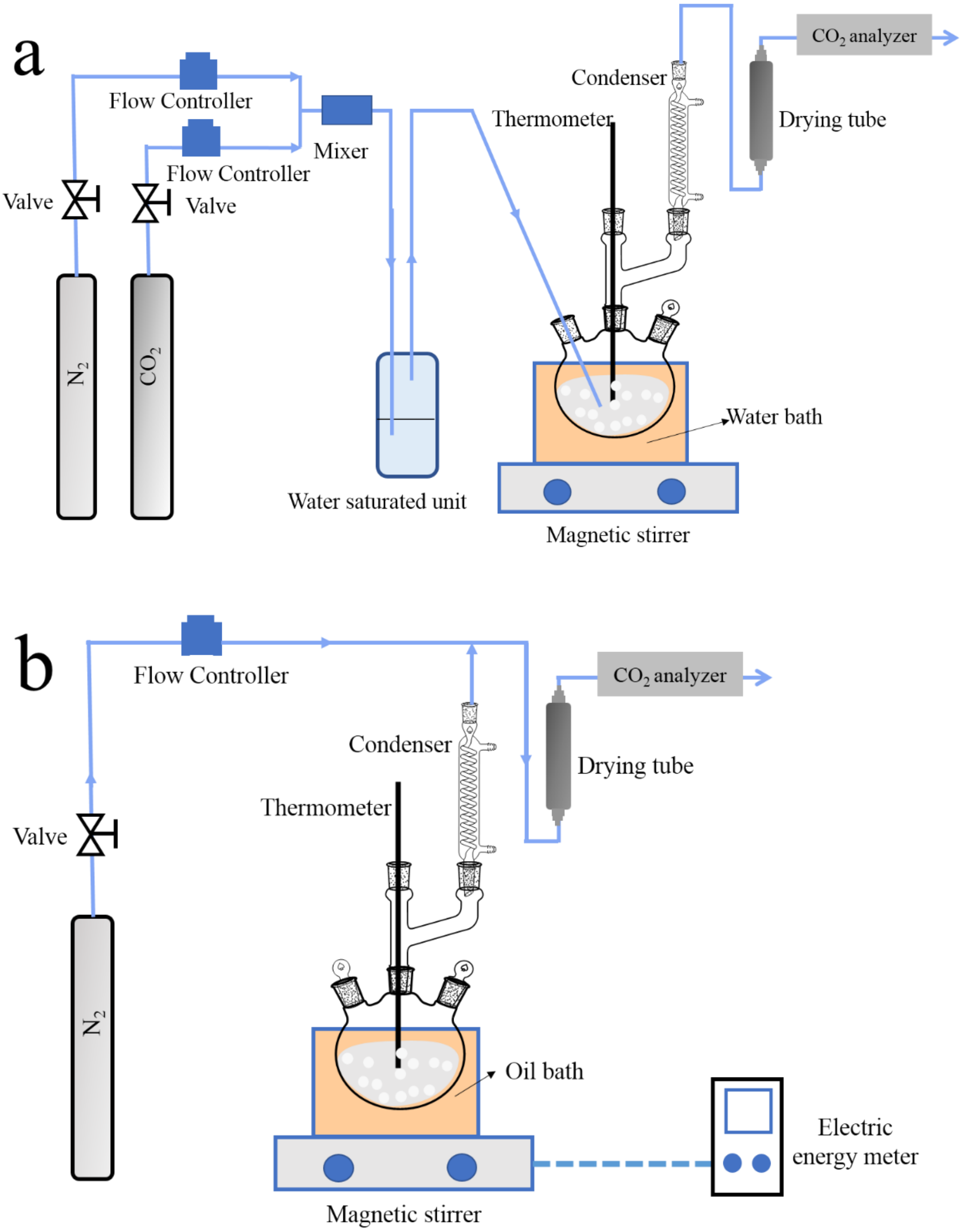
Figure S1.

The schematic diagrams for CO_2 absorption experiment, CO_2 desorption experiment and measurement of CO_2 equilibrium solubility are present in the figure S1.



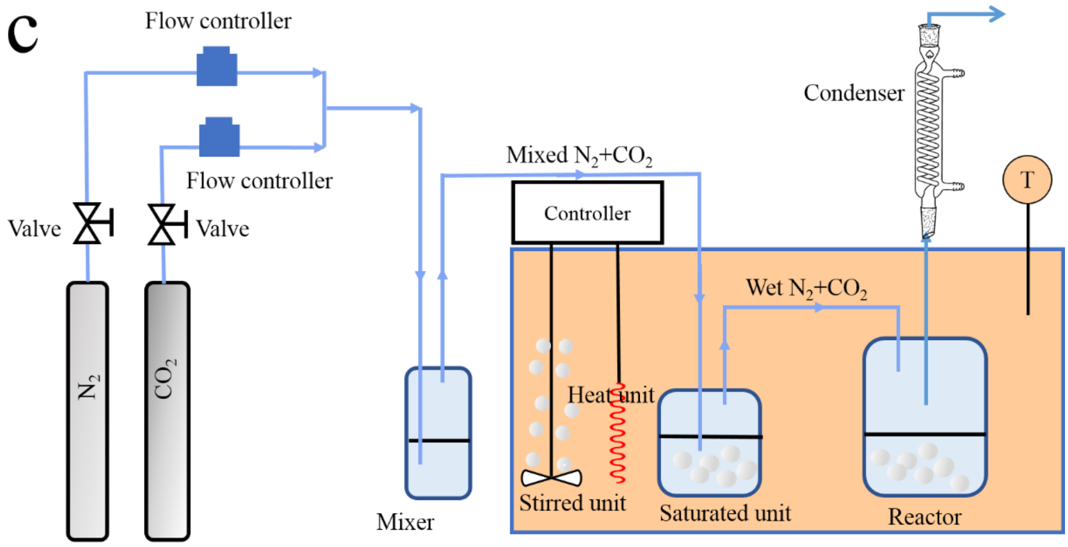


Figure S1. The schematic diagram for CO_2 absorption experiment (a), CO_2 desorption experiment (b) and measurement of CO_2 equilibrium solubility (c).

Text S1.

In CO_2 absorption process, 200 mL fresh amine solution is added into a 500 mL flask with three necks, and then a gas mixture (15% CO_2 + 85% N_2) is bubbled into the reactor with the temperature remains at 313.15 K. The gas is bubbled through a quartz distributor of 100 μm to ensure the gas can be evenly distributed into the solution, under stirring at 900 rpm. The CO_2 concentration in the outlet is recorded by a CO_2 analyzer at the intervals of 10 seconds. A saturated unit and a condenser are used to keep the absorption equilibrium inside the reactor.

The CO_2 desorption process is similar to the absorption process, except that only N_2 is bubbled into the reactor for increasing the sensitivity of CO_2 analyzer and the desorption temperature is initiated from 338.15 K. The flask containing 200 mL CO_2 saturated amine solution is immersed into an oil bath with the temperature constant at 338.15 K. At the same time, the stirring system and condenser keep running. The temperature of the oil bath is set up to 363.15 K at the beginning of desorption. The temperature inside the amine solution is recorded in the intervals of 1 minute, the CO_2 concentration of the outlet is measured by the CO_2 analyzer with a10-second interval. A plug-in power meter (Zhejiang Tepsung Electric Co., Ltd. China) is used to monitor the energy consumption during the CO_2 desorption process. Absorption or desorption process will be considered to be completed or reach equilibrium when the CO_2 concentration in the gas phase remains unchanging.

In the measurement of the CO_2 solubility at equilibrium, the gases are mixed through a gas-mixer and the saturated unit before bubbling into the reactor. 60 mL fresh amine solution was added into the reactor and then start the measurement. The equilibrium solubilities of tested blends were measured between 313 – 333 K under different CO_2 partial pressures. Each run continues for at least 9 hours to ensure the reaction system reach the equilibrium. The CO_2 equilibrium solubility was measured by titration using 1M aqueous HCl solution[1]. For the final CO_2 loading determination, at least three times titrations were performed with the interval of 30 minutes after reacting for 9 hours. If the last two measurements show the same value of CO_2 loaded, the process is considered to have reached its equilibrium at the corresponding experimental conditions. The last CO_2 loading amount will be regarded as the CO_2 equilibrium solubility at this situation.

Text S2.

1. Dissolved CO_2 concentration determination in the liquid phase

The dissolved CO_2 concentration, α (mol CO_2/mol amine), in gas phase is calculated as shown in equations (1) – (4). n_{CO_2} (mol/min) is the instantaneous absorbed CO_2 amount inside amine solution. N_{in} and N_{out} (mol/min) present the instantaneous CO_2 amounts of inlet and outlet, respectively. F_{CO_2} and F_{N_2} (mL/min) present the flow rates of CO_2 and N_2, respectively. x refers to the CO_2 fraction in the gas outlet. V (mL) is the volume of tested amine solution (200 mL). R_{abs} (absorption rate, mol CO_2/ (L·min)) was calculated by equation (5).

$$\mathrm{n}_{CO_2} = N_{in} - N_{out} \quad (1)$$

$$N_{in} = \frac{F_{CO_2}}{22.4} \times \frac{273.15}{273.15+T} \quad (2)$$

$$N_{out} = \frac{\mathrm{F}_{N_2} * x}{(1-x) * 22.4} \times \frac{273.15}{273.15+\mathrm{T}} \quad (3)$$

$$\alpha = \int_{t0}^{t} \mathrm{n}_{CO_2} dt \quad (4)$$

$$R_{abs} = \frac{n_{CO_2}}{V*t} \tag{5}$$

In the desorption process, CO_2 loading amount is calculated with equations (6-7).

$$\alpha = \alpha_{rich} - \int_{t0}^{t} n_{CO_2} dt \tag{6}$$

$$n_{CO_2} = N_{out} \tag{7}$$

2. Cyclic capacity

Cyclic capacity (CC, mol) is the amount of the desorbed CO_2 which was calculated with equation (8).

$$CC = (\alpha_{rich} - \alpha_{lean}) \times C_{amine} \times V \tag{8}$$

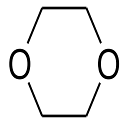
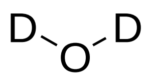
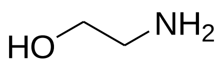
3. Relative heat duty

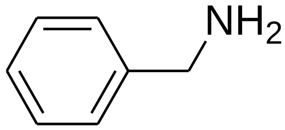
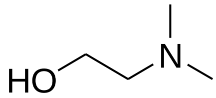
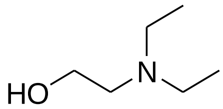
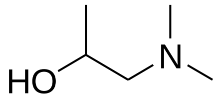
The heat duty (H, kJ/mol) is an important parameter to evaluate the amine solvent regeneration performance, which is calculated by equation (9). Q_{CO2} (kJ) refers to the required energy for releasing CO_2, which is measured by the pug-in power meter. Relative heat duty (RH) is defined as the ratio of tested solvent's heat duty relative to MEA's heat duty as shown in equation (10), which indicates the reduction degree of tested amine system's regeneration performance compared to MEA. 6M MEA is set as the reference in this work.

$$H = \frac{Q_{CO2}}{CC} \tag{9}$$

$$RH = \frac{H_i}{H_{MEA}} \tag{10}$$

Table S1. The materials of the chemicals used in this work.

Chemicals	Abbreviation	Mol Wt	Purity (%)	Molecular structure
1,4-dioxane	-	88.1	99.8	
Deuterium oxide	D_2O	20.03	99.9	
Monoethanolamine	MEA	61.08	99%	

Benzylamine	BZA	107.15	99%	
2-Dimethylaminoethanol	DMEA	89.14	99%	
2-(Diethylamino)ethanol	DEEA	117.19	99%	
1-Dimethylamino-2-propanol	1DMA2P	103.16	99%	

1. Official Methods of Analysis of the Association of Official Analytical Chemists. *Journal of Pharmaceutical Sciences* **1971,** *60*, (2), 334.