

1 **A Novel Diamine Non-Aqueous Absorbent Based on N-methyl diethanolamine**
2 **Regulation for Energy-efficient CO₂ Capture**

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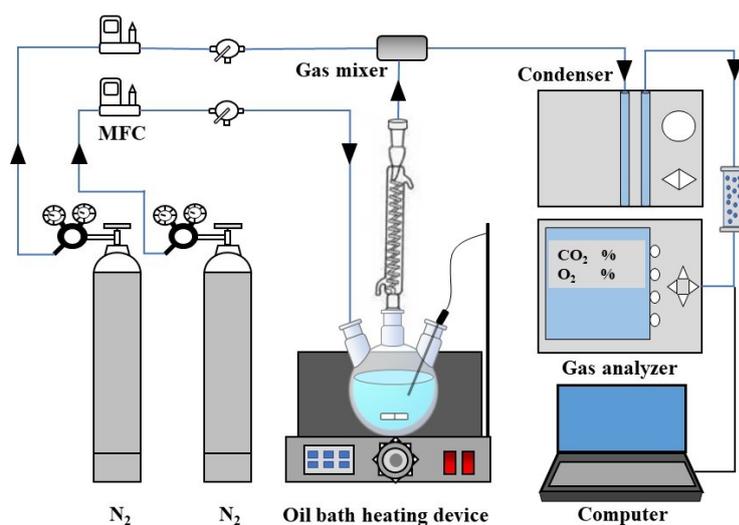
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10 **1. Schematic diagram of CO₂ desorption setup**



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Fig. S1. Schematic diagram of CO₂ desorption setup.

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1 2. Different non-aqueous absorbent systems.

2 Table. S1. Different MEA/MDEA/PEG200 non-aqueous absorbent systems.

No.	Solvent	Abbreviation
1	30 wt.% MEA, 70 wt.% PEG200	30M/P
2	25 wt.% MEA, 5 wt.% MDEA, 70 wt.% PEG200	25M5M/P
3	22.5 wt.% MEA, 7.5 wt.% TEA, 70 wt.% PEG200	22.5M7.5M/P
4	20 wt.% MEA, 10 wt.% TEA, 70 wt.% PEG200	20M10M/P
5	17.5 wt.% MEA, 12.5 wt.% TEA, 70 wt.% PEG200	17.5M12.5M/P
5	15 wt.% MEA, 15 wt.% TEA, 70 wt.% PEG200	15M15M/P

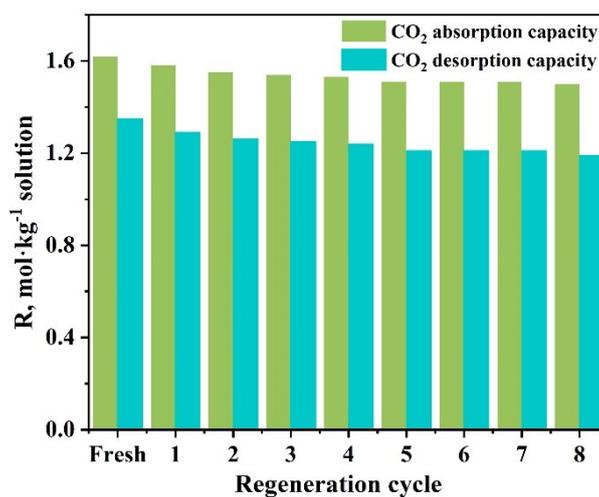
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4 3. Cyclic CO₂ absorption-desorption capacity of MEA/MDEA/PEG200 system

5 It could be seen from Fig. S2. that 20 MEA/10 MDEA/70 PEG200 showed good CO₂

6 capture capacity in 8 cycles absorption and desorption experiments.

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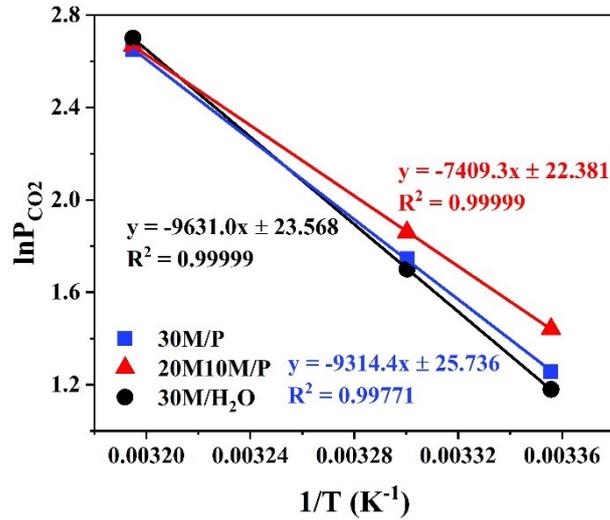
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9 Fig. S2. Cyclic CO₂ absorption-desorption capacity of MEA/MDEA/PEG200

10 system.

1 $(V_L = 0.05 \text{ kg}, C_{MEA} = 20 \text{ wt.}\%, C_{MDEA} = 10 \text{ wt.}\%, C_{PEG200} = 70 \text{ wt.}\%, T_{absorption} =$
 2 $313 \text{ K}, T_{desorption} = 393 \text{ K}).$

3 4. Vapor-liquid equilibrium (VLE) data of different absorbents



4

5 Fig. S3. Vapor-liquid equilibrium (VLE) data of different absorbents.

6 5. Comparison of the viscosity of different non-aqueous absorbents

7 Table. S2. Comparison of the viscosity of different non-aqueous absorbents

Regulator	Absorbent	Viscosity, mPa·s	
		Fresh solution	CO ₂ -rich solution
/	30M/P	25.6	456.60
DEA	25M5D/P	30.6	535.70
TEA	25M5T/P	42.5	483.50
MDEA	25M5M/P	27.2	303.20
MDEA	22.5M7.5M/P	30.5	242.60
MDEA	20M10M/P	32.6	182.50
MDEA	17.5M12.5M/P	35.7	145.60
MDEA	15M15M/P	38.2	113.70

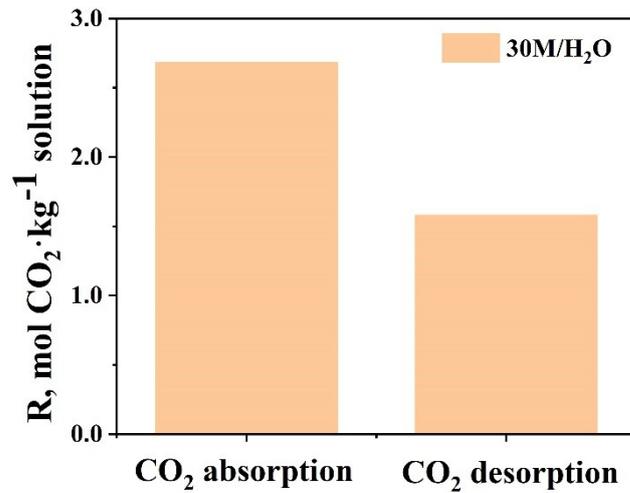
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9 In non-aqueous absorbent viscosity tests, it was found that the viscosity of
 10 MEA/MDEA/PEG200 absorbent after CO₂ absorption decreased with increased

1 MDEA mass fraction. It might be attributed to two factors. On the one hand, it is due
2 to the fact that all non-aqueous absorbents keep at a constant total amine concentration,
3 and an increase in the mass fraction of MDEA will result in a decrease in MEA
4 concentration. Since MEA played a major CO₂ absorption role in diamine non-aqueous
5 absorbents. Thus, a decrease in MEA concentration results in a decrease in CO₂
6 absorption products, which reduces the viscosity of diamine non-aqueous absorbents.
7 On the other hand, the viscosity of absorbent is related to the hydrogen bonding
8 generated between carbamate and protonated amine. While MDEA is not introduced in
9 MEA, CO₂ absorption products of MEA/PEG200 absorbent are primary amine
10 carbamate and protonated MEA. The primary amine carbamate and protonated MEA
11 have a relatively high stability and can result in a large number of stable hydrogen
12 bonds, which keeps the viscosity of CO₂-rich absorbent at a high level. It can be noticed
13 by ¹³C NMR that the addition of MDEA can change the type of protonated amine in
14 non-aqueous absorbent, and generate more protonated MDEA rather than protonated
15 MEA. Compared with protonated MEA, protonated MDEA has a relatively weaker
16 stability. Therefore, the hydrogen bonds formed between it and carbamate have a
17 weaker stability, which results in a lower viscosity of CO₂-rich absorbents.

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1 **6. CO₂ absorption and desorption performance of 30M/H₂O system.**



2

3 Fig. S4. CO₂ absorption and desorption performance of 30M/P system.

4 ($V_L = 0.05$ kg, $C_{total} = 30$ wt.%, $T_{absorption} = 313$ K, $T_{desorption} = 373$ K).

5 The results showed that CO₂ absorption capacity of 30 wt.% MEA aqueous solution

6 reached 2.62 mol/kg, CO₂ desorption capacity reached 1.52 mol/kg, and CO₂

7 desorption efficiency was only 58 %. In addition to these, the regeneration energy

8 consumption of 30 wt.% MEA aqueous solution was as high as 3.66 GJ/ton CO₂ by

9 thermodynamic analysis.

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1 **7. Physicochemical properties of various components.**

2 Table. S3. Physicochemical properties of various components.

Component	$C_p, \text{kJ}\cdot\text{K}^{-1}\cdot\text{kg}^{-1}$	$\Delta H_{\text{sol}}^{\text{vap}}(T_R), \text{kJ}\cdot\text{kg}^{-1}, 393 \text{ K}$
Water	4.179	2194.8
PEG200	2.37	/
MEA	3.01	/
MDEA	3.59	/
DEA	/	/
TEA	/	/
CO ₂	0.84	/

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4 **8. The mass of CO₂ absorbent, desorbed CO₂ and absorbent loss during**
 5 **regeneration**

6 Table. S4. The mass of CO₂ absorbent, desorbed CO₂ and absorbent loss during

7 regeneration

	$m_{\text{sol}}, \text{kg}$	$m_{\text{CO}_2}, 10^{-3} \text{ kg}$	$m_{\text{sol}}^{\text{vap}}, 10^{-3} \text{ kg}$	$Q_{\text{lat}}, \text{GJ/ton CO}_2$
20M10M/P	0.103	7.342	0.192	0.06
30M/P	0.107	11.205	0.306	0.06
30M/H ₂ O	0.104	12.264	7.264	1.30

8

9 In order to calculate the latent heat of evaporation, it is necessary to determine the mass
 10 loss of different adsorbents during regeneration. Thus, the mass loss of adsorbent after
 11 regeneration was completed was derived by weighing the mass change of adsorbents
 12 before and after desorption. It was found that under the same regeneration conditions,
 13 30 wt.% MEA aqueous solution showed the highest mass loss of 7.264 g. In contrast,

1 MEA/PEG and MEAMDEA/PEG systems showed very low solvent losses of 0.306 g
2 and 0.192 g, respectively. Therefore, the addition of PEG200 can significantly reduce
3 the latent heat of evaporation of non-aqueous absorbents compared to MEA aqueous
4 solutions.