

## Supplementary information for

### Tuning CO<sub>2</sub> reaction enthalpy *via* metal complexes for advanced amine technology

Kangkang Li<sup>1,\*</sup>, Jian Chen<sup>2</sup>, Simeng Li<sup>2</sup>, Yang Liu<sup>2</sup>, Paul Feron<sup>3</sup>, Hai Yu<sup>3</sup>, Hanming Liu<sup>4</sup>, Yong Cai<sup>5</sup>, Kaiqi Jiang<sup>6,\*</sup>

<sup>1</sup> Department of Energy and Resources Engineering, College of Engineering, Peking University, Beijing, China

<sup>2</sup> State Key Laboratory of Chemical Engineering, Tsinghua University, Beijing 100084, PR China

<sup>3</sup> CSIRO Energy, 10 Murray Dwyer Circuit, Mayfield West, NSW 2304, Australia

<sup>4</sup> Beijing Key Laboratory of CO<sub>2</sub> Capture and Process, Huaneng Clean Energy Research Institute, Beijing, China

<sup>5</sup> China National Petroleum Corporation, Yard 7 Kunlun Road, Changping District, Beijing

<sup>6</sup> Key Laboratory of Resources and Environmental Systems Optimization, College of Environmental Science and Engineering, North China Electric Power University, Beijing, 102206, P. R. China

**\*Corresponding author:**

Email address: [kangkang.li@pku.edu.cn](mailto:kangkang.li@pku.edu.cn) & [kaiqi.jiang@ncepu.edu.cn](mailto:kaiqi.jiang@ncepu.edu.cn)

The SI contains 2 tables and 2 Figures:

**Table S1.** Chemical reactions and their equilibrium constants in Ni(II)-MEA-CO<sub>2</sub>-H<sub>2</sub>O system

**Table S2.** CO<sub>2</sub> loading performance in CO<sub>2</sub> absorption-desorption experiments in 2M MEA solution

**Figure S1.** Desorption system boundary to analyze the three components of regeneration duty including sensible heat, latent heat and reaction heat.

**Figure S2.** Rich split configuration of CO<sub>2</sub> desorption process to recover the latent heat.

Table S1. Chemical reactions and their equilibrium constants in Ni(II)-MEA-CO<sub>2</sub>-H<sub>2</sub>O system.

MEA-CO <sub>2</sub> -H <sub>2</sub> O reaction <sup>a</sup>					
No.	Reactions	Equilibrium Constant $\ln K = A + \frac{B}{T} + C \ln T + DT$			
		A	B	C	D
R1		170.7	-8477.7	21.9	0.005781
R2	$\leftrightarrow H^+ + HCO_3^-$	231.46	-12092.1	-36.8	0
R3	$HCO_3^- \leftrightarrow H^+ + CO_3^{2-}$	216.0	-12431.7	-35.5	0
R4	$MEA + H^+ \leftrightarrow MEAH^+$	1974.4	-7.5	56.0	0
R5	$MEACOO^- + H_2O \leftrightarrow MEA + HCO_3^-$	47.7	-1.67	-13.07	0.0651
Ni-MEA complexation <sup>b</sup>					
	Reactions	Equilibrium Constant $lgK$		$\Delta H$ , kJ/mol	
R6	$Ni^{2+} + MEA \leftrightarrow Ni(MEA)^{2+}$	3.12		-14	
R7	$Ni^{2+} + 2MEA \leftrightarrow Ni(MEA)_2^{2+}$	5.60		-30	
R8	$Ni^{2+} + 3MEA \leftrightarrow Ni(MEA)_3^{2+}$	7.30		-41	

Note: <sup>a</sup> Equilibrium constants are from Kim et al<sup>22</sup>; <sup>b</sup> stability constants and enthalpies are from NIST Data Gateway<sup>23</sup>.

Table S2 CO<sub>2</sub> loading performance in CO<sub>2</sub> absorption-desorption experiments in 2M MEA solution

Ni(II) concentration	CO <sub>2</sub> loading			
	Ni/MEA=0	Ni/MEA=0.05	Ni/MEA=0.10	Ni/MEA=0.15
CO <sub>2</sub> absorption at 25 °C	0.53	0.51	0.46	0.41
CO <sub>2</sub> desorption at 40 °C	0.47	0.47	0.36	0.30
CO <sub>2</sub> desorption at 60 °C	0.33	0.32	0.25	0.21
CO <sub>2</sub> desorption at 80 °C	0.26	0.22	0.20	0.15
Cyclic loading between 25°C and 40 °C	0.06	0.04	0.15	0.16
Cyclic loading between 25°C and 60 °C	0.20	0.19	0.21	0.20
Cyclic loading between 25°C and 80 °C	0.27	0.29	0.26	0.26

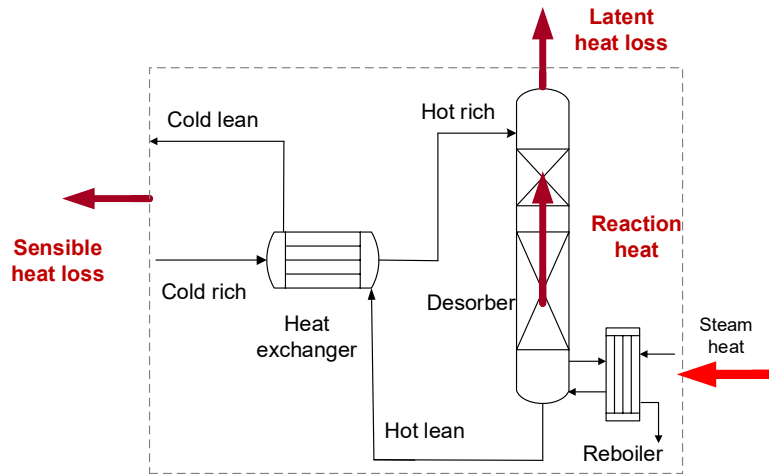


Figure S1. Desorption system boundary to analyze the three components of regeneration duty including sensible heat, latent heat and reaction heat.

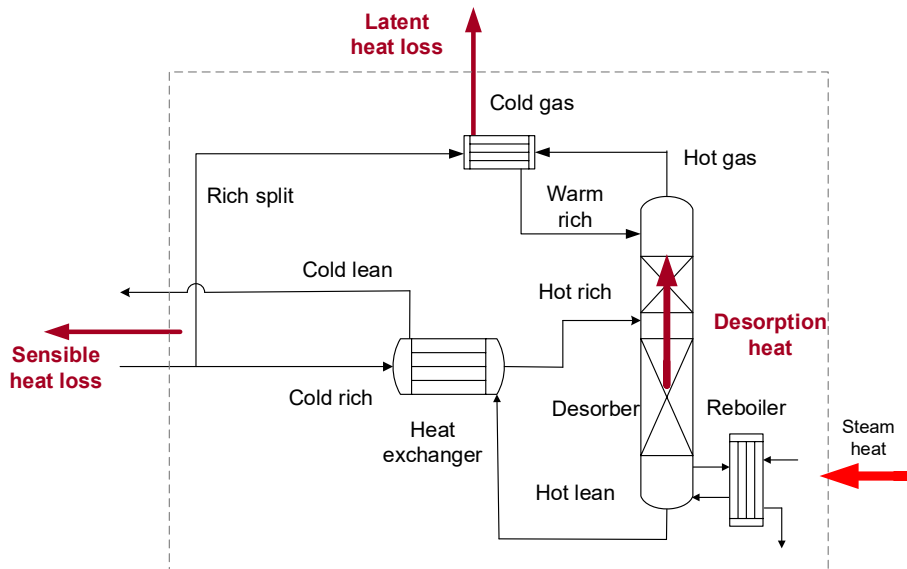


Figure S2. Rich split configuration of CO<sub>2</sub> desorption process to recover the latent heat.