

Optimization of the electrochemically mediated amine regeneration (EMAR) for CO₂ capture through computational modeling

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ABSTRACT

The electrochemically mediated amine regeneration (EMAR) for CO₂ capture presents a promising CO₂ capture approach. The EMAR process relies on the competitive binding between Cu²⁺ and CO₂ to solvent, and employs an externally powered electrochemical cell to the desorption of the absorbed CO₂. This study focuses on the simulation of the EMAR process in the EDA-Cu system. Firstly, a chemical reaction equilibrium model for the Cu(II)-EDA-CO₂-H₂O system is established, and the concentration changes of each component in the electrolyte under different copper loads are obtained, providing a basis for simplifying the loaded EMAR process. Next, a multiphysics model is constructed using COMSOL software to simulate the EMAR process in a simple flat-plate reactor, employing the three-dimensional Nernst-Planck model and bubble flow model. The results show that the distribution of reactive ions in the electrolyte during operation conforms to ion liquid-phase mass transfer theory. The presence of CO₂ bubbles during the electrolysis process enhances the electrode reactions to some extent. The co-current flow in the anode and cathode chambers exhibits better system stability and desorption performance compared to counter-current flow. The findings of this study provide valuable guidance for the design and application of EMAR system reactors.

Keywords: CO₂ capture, EMAR, Simulation, Optimization

1. INTRODUCTION

CO₂, as the primary greenhouse gas, contributes to climate change with a share exceeding 60% [2]. The annual CO₂ emissions reached 36.4 billion tons, with a significant proportion originating from human

activities[3, 4], mainly from the continuous consumption of fossil fuels. However, fossil fuels will remain the primary energy source in the foreseeable future, making carbon capture, utilization, and storage (CCUS) technology indispensable for achieving the temperature control goals outlined in the Paris Agreement.

In response to the growing demand, electrochemical separation technology has gained considerable attention in renewable energy-driven CO₂ capture methods[5,6]. Electrochemically-mediated amine regeneration (EMAR) CO₂ capture technology emerges as a promising alternative, effectively combining the high desorption efficiency of amine absorption methods with the efficiency of electrochemical systems. The EMAR process relies on the competitive binding between CO₂ and Cu²⁺ to a solvent molecule (e.g., ethylenediamine (EDA)). Similar to the amine-based thermal scrubbing CO₂ capture process, the EMAR process also consists of absorption and desorption stages, but the high-temperature desorption stage is replaced with an electrochemical cell for electrochemical desorption, as shown in Figure 1.

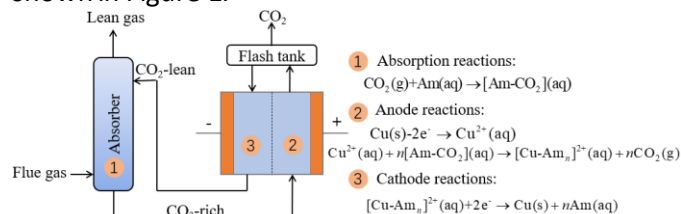


Fig. 1. The EMAR for CO₂ capture process

In the EMAR for CO₂ capture process, the absorption stage is the same as that of the traditional amine(Am)-based CO₂ capture process, and the regenerated solvent, Am-rich (CO₂-lean) solution, enters the absorption column, where amine (Am) solvent bond with CO₂ in the flue gas to form CO₂-rich solvent

($\text{CO}_2(\text{g})+\text{Am}(\text{aq})\rightarrow[\text{Am}-\text{CO}_2](\text{aq})$). Then the CO_2 -rich solvent is introduced to the anode chamber, in which the anode copper electrode is dissolved under the effect of positive potential to form cupric ions (Cu^{2+}) into the solution ($\text{Cu}(\text{s})-2\text{e}^- \rightarrow \text{Cu}^{2+}(\text{aq})$). These dissolved cupric ions are more competitive to binding with solvent molecules, preempting the binding site with CO_2 , and leading to the absorbed CO_2 desorption ($\text{Cu}^{2+}(\text{aq})+n[\text{Am}-\text{CO}_2](\text{aq})\rightarrow[\text{Cu}-\text{Am}_n]^{2+}(\text{aq})+n\text{CO}_2(\text{g})$). Then, the solution is delivered to a flash tank, where the desorbed CO_2 is completely separated. Next, the CO_2 -lean (Cu -rich) solution is introduced to the cathode chamber, where the cupric ions are reduced and precipitated on the cathode electrode under negative cathode potential ($[\text{Cu}-\text{Am}_n]^{2+}(\text{aq})+2\text{e}^- \rightarrow \text{Cu}(\text{s})+n\text{Am}(\text{aq})$). Then the regenerated amine (Am) solvent solution is sent to the absorber for the next absorption cycle.

No extra heating and steam are needed in the EMAR process, potentially reducing the energy consumption of the CO_2 desorption process and the degradation of amine solvents. Preliminary research results suggest that energy consumption can be lowered to 40-80 kJ/mol CO_2 [7], while thermodynamic calculations indicate

desorption energy below 30 kJ/mol CO_2 [8], with CO_2 removal rates exceeding 90%. However, the current status of EMAR CO_2 capture technology remains in its initial research stage, and several challenges need to be addressed before its practical application in carbon capture. Notably, the design and implementation of efficient reactors represent a pressing concern.

This research focuses on investigating the EMAR CO_2 capture process using ethylenediamine (EDA) as the absorbent and copper (Cu) as the mediating substance. Initially, a chemical reaction equilibrium model was constructed for the $\text{Cu}(\text{II})$ -EDA- CO_2 - H_2O system to obtain concentration variations of different components in the electrolyte under varying copper loads. Based on the obtained results, a rational simplification of the EMAR system reaction process was performed. Subsequently, simulations were conducted on a simple planar reactor using COMSOL software to create a multi-physics model, employing the Nernst-Planck model and bubble flow model for EMAR process simulation. The distribution of reactive ions and the influence of the flow direction of the electrolyte were investigated. The outcomes of this study can provide valuable guidance for the design and application of EMAR system reactors.

Table 1 Chemical reactions and equilibrium constants of the $\text{Cu}(\text{II})$ -EDA- CO_2 - H_2O system at 25 °C

Reaction types	No.	Reactions	Equilibrium constant, K	log K
CO_2 - H_2O interaction	R1	$\text{H}^+ + \text{OH}^- \xrightleftharpoons{K_1} \text{H}_2\text{O}$	$K_1 = \frac{1}{C_{\text{H}^+} C_{\text{OH}^-}}$	14 [1]
	R2	$\text{HCO}_3^- + \text{H}^+ \xrightleftharpoons{K_2} \text{CO}_2 + \text{H}_2\text{O}$	$K_2 = \frac{C_{\text{CO}_2}}{C_{\text{H}^+} C_{\text{HCO}_3^-}}$	6.35 [1]
	R3	$\text{CO}_3^{2-} + \text{H}^+ \xrightleftharpoons{K_3} \text{HCO}_3^-$	$K_3 = \frac{C_{\text{HCO}_3^-}}{C_{\text{H}^+} C_{\text{CO}_3^{2-}}}$	10.33 [1]
Amine protonation	R4	$\text{EDA} + \text{H}^+ \xrightleftharpoons{K_4} \text{EDA}\text{H}^+$	$K_4 = \frac{C_{\text{EDA}\text{H}^+}}{C_{\text{H}^+} C_{\text{EDA}}}$	9.94 [5, 6]
	R5	$\text{EDA}\text{H}^+ + \text{H}^+ \xrightleftharpoons{K_5} \text{EDA}\text{H}_2^{2+}$	$K_5 = \frac{C_{\text{EDA}\text{H}_2^{2+}}}{C_{\text{H}^+} C_{\text{EDA}\text{H}^+}}$	6.86 [5, 6]
Carbamate formation	R6	$\text{EDA} + \text{CO}_2 \xrightleftharpoons{K_6} \text{EDACO}_2$	$K_6 = \frac{C_{\text{EDACO}_2}}{C_{\text{EDA}} C_{\text{CO}_2}}$	3.69 [5, 6]
Cu-EDA complexation	R7	$\text{Cu}^{2+} + \text{EDA} \xrightleftharpoons{K_7} [\text{Cu}(\text{EDA})]^{2+}$	$K_7 = \frac{C_{[\text{Cu}(\text{EDA})]^{2+}}}{C_{\text{EDA}} C_{\text{Cu}^{2+}}}$	10.64 [5, 6]
	R8	$\text{Cu}^{2+} + 2\text{EDA} \xrightleftharpoons{K_8} [\text{Cu}(\text{EDA})_2]^{2+}$	$K_8 = \frac{C_{[\text{Cu}(\text{EDA})_2]^{2+}}}{C_{\text{Cu}^{2+}} (C_{\text{EDA}})^2}$	19.90 [5, 6]

2. METHOD

2.1 Chemical model for the Cu(II)–EDA–CO₂–H₂O system

A chemical model for the Cu(II)–EDA–CO₂–H₂O system is established with the assistance of ReactLab–Equilibria software written in MATLAB [9] to obtain the changes of ion concentrations in the electrolyte with the copper load under the equilibrium state. The chemical model is governed by several chemical reactions, which can be divided into CO₂ hydration, carbamate formation, amine protonation, and metal-amine complexation. The chemical reactions and equilibrium constants in the system were shown in Table 1. It is assumed that there is no precipitation occurs at different solution compositions, and just consider the equilibrium reactions that take place in the liquid phase. By specifying the total concentration of EDA-related species ($C_{\text{EDA,tot}}$), Cu-related species ($C_{\text{Cu,tot}}$), and CO₂-related species ($C_{\text{CO}_2,\text{tot}}$), expressed as Eqs. (1)–(3), and combining with the mass balance in the system, the concentrations of chemical species involved in the solution can be calculated.

$$C_{\text{EDA,tot}} = C_{\text{EDA}} + C_{\text{EDAH}^+} + C_{\text{EDAH}_2^{2+}} + C_{\text{EDACO}_2} + C_{[\text{Cu}(\text{EDA})]^{2+}} + 2C_{[\text{Cu}(\text{EDA})_2]^{2+}} \quad (1)$$

$$C_{\text{Cu,tot}} = C_{\text{Cu}^{2+}} + C_{[\text{Cu}(\text{EDA})]^{2+}} + C_{[\text{Cu}(\text{EDA})_2]^{2+}} \quad (2)$$

$$C_{\text{CO}_2,\text{tot}} = C_{\text{CO}_2} + C_{\text{HCO}_3^-} + C_{\text{CO}_3^{2-}} + C_{\text{EDACO}_2} \quad (3)$$

2.2 Multi-physics field modeling

In this study, a simple plate reactor is simulated, which is divided into anode region, interlayer and cathode region. The copper metal electrode has a strong electrical conductivity, so it can be simplified to the electrode boundary. The simplified results of the calculation model are shown in Figure 2, and the parameters for geometry are shown in Table 2.

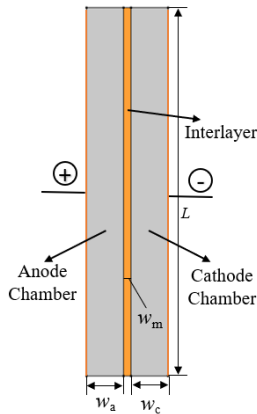


Fig. 2. Simulation model

Table 2 Parameters for Geometry.

Geometry Parameter	Name	Value /mm
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Anode chamber width	w_a	5
Cathode chamber width	w_c	5
Interlayer width	w_m	1
Anode/Cathode length	L	50

To model the EMAR process in this study, the Tertiary Nernst-Planck interface was used to solve for the electrolyte potential, the current density distribution, and the concentrations of various species.

In electrolyte, the material balance (Eq. 4), the charge conservation equation (Eq. 5), and the local electroneutral equation (Eq. 6) are satisfied.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i - z_i u_i F c_i \nabla \phi + c_i \mathbf{u}) = R_i \quad (4)$$

$$\nabla \cdot [F \sum z_i (-D_i \nabla c_i - z_i u_i F c_i \nabla \phi + c_i \mathbf{u})] = 0 \quad (5)$$

$$\sum_i z_i c_i = 0 \quad (6)$$

where D_i , c_i , z_i , u_i is the diffusivity, concentration, charge, and mobility of species i ; F is Faraday's constant; ∇c_i is concentration gradient;

$\nabla \phi$ is the electrolyte potential gradient; and \mathbf{u} is the velocity vector. By synthesizing equations (4), (5), and (6), we can obtain variables in the electrolyte such as substance concentration, electric potential, and current.

The current density in the electrolyte adjacent to the electrode has the following relationship with the local current density term in a modified form of the Butler-Volmer Equation.

$$i_{\text{loc}} = i_0 \left[\frac{c_{\text{R,S}}}{c_{\text{R,B}}} \exp\left(\frac{\alpha_a z F}{RT} \eta\right) - \frac{c_{\text{O,S}}}{c_{\text{O,B}}} \exp\left(\frac{\alpha_c z F}{RT} \eta\right) \right] \quad (7)$$

where i_{loc} is the charge transfer current density at the interface, i_0 is equilibrium exchange current density,

$c_{\text{R,S}}$ is the surface concentration reduced species, $c_{\text{R,B}}$ is the bulk concentration of the reduced species, $c_{\text{O,S}}$ is the surface concentration of the oxidized species, $c_{\text{O,B}}$ is the bulk oxidant concentration of the oxidized species,

α_a is the anodic symmetry factor, α_c is the cathodic symmetry factor, z is the number of electrons transferred in the rate limiting step (typically 1), R is the gas constant (8.31 J/(mol·K)), T is the absolute temperature.

To determine cell voltages, the equilibrium potential of the anodic and cathodic reactions was calculated by the Nernst Equation:

$$E = E_{\text{eq}} = E_{\text{eq}}^0 + \frac{RT}{nF} \ln \left(\frac{a_{\text{products}}}{a_{\text{reactants}}} \right) \quad (8)$$

where a_{products} and $a_{\text{reactants}}$ are the product and reactant activities; E_{eq}^0 is standard equilibrium potential.

The reaction in the electrolyte is characterized by the Equilibrium Reaction Theory, supposing the kinetics is so fast that the equilibrium condition is fulfilled at all times. The equilibrium condition is based on the defined equilibrium constant.

$$K_{\text{eq}} = \frac{\prod_{m \in \text{products}} a_m^{v_m}}{\prod_{m \in \text{reactants}} a_m^{-v_m}} \quad (9)$$

where a_m is the species activities of the reacting species; v_m is the stoichiometric coefficients.

In the process of EMAR system, there are CO_2 gas was generated in the electrolyte for the working process of the EMAR system, and the Bubbly Flow model was adopted to solve the two-phase flow for CO_2 gas bubbles in a liquid electrolyte. With the assumption that the fluid is noncompressible, the gas phase density is insignificant compared to the liquid phase density, and the motion between the phases is determined by a balance of viscous and pressure forces, the form of the bubbly flow (BF) equations is derived.

$$\phi_1 \rho_1 \frac{\partial \mathbf{u}_1}{\partial t} + \phi_1 \rho_1 \mathbf{u}_1 \cdot \nabla \mathbf{u}_1 = -\nabla p + \nabla \cdot \left[\phi_1 (\mu_1 + \mu_T) \left(\nabla \mathbf{u}_1 + \nabla \mathbf{u}_1^T - \frac{2}{3} (\nabla \cdot \mathbf{u}_1) \mathbf{I} \right) \right] + \phi_1 \rho_1 \mathbf{g} + \mathbf{F} \quad (10)$$

where ϕ is the phase volume fraction; μ_1 is the dynamic viscosity of the liquid; μ_T is the turbulent viscosity.

For laminar flow the gas velocity \mathbf{u}_g is calculated from:

$$\mathbf{u}_g = \mathbf{u}_1 + \mathbf{u}_{\text{slip}} \quad (11)$$

where \mathbf{u}_1 stands for the liquid-phase velocity, and \mathbf{u}_{slip} stands for the relative velocity between gas and liquid, the so-called slip velocity.

3. RESULTS AND DISCUSSION

3.1 The results of chemical model

Figure 3(a) shows the change in the concentration of ions involved in the EMAR system with the total concentration of copper. It can be found that the concentration of H^+ , OH^- , CO_3^{2-} , EDA, Cu^{2+} and $[\text{Cu}(\text{EDA})_2]^{2+}$ are relatively small, and they are treated as a minority of ions. The concentrations of HCO_3^- , CO_2 , EDACO_2 , EDAH^+ , EDAH_2^{2+} , and $[\text{Cu}(\text{EDA})_2]^{2+}$ are relatively large. Figure 3(b) shows the changes in Cu-related species with the total concentration of copper. We can see that the main form of the complex formed by EDA and Cu^{2+} is $[\text{Cu}(\text{EDA})_2]^{2+}$. Figure 6 (c) and (d) show the changes of CO_2 -related species and EDA-related species with the total concentration of copper. We can see that the change in the concentration of EDACO_2 plays a leading role in the changes in CO_2 -related species.

Therefore, the EMAR process can be reasonably simplified. Firstly, the reaction of $\text{Cu}(\text{s}) - 2\text{e}^- \rightarrow \text{Cu}^{2+}(\text{aq})$ occurs on the anode. The resulting Cu^{2+} enters the electrolyte and reacts with EDACO_2 in the electrolyte as follows, $\text{Cu}^{2+}(\text{aq}) + 2[\text{EDACO}_2](\text{aq}) \leftrightarrow [\text{Cu}(\text{EDA})_2]^{2+}(\text{aq}) + 2\text{CO}_2(\text{g})$, and then the CO_2 produced in the reaction is released as a gas, the resulting $[\text{Cu}(\text{EDA})_2]^{2+}$ is reduced on the cathode through the reaction of $[\text{Cu}(\text{EDA})_2]^{2+}(\text{aq}) + 2\text{e}^- \rightarrow \text{Cu}(\text{s}) + 2\text{EDA}(\text{aq})$.

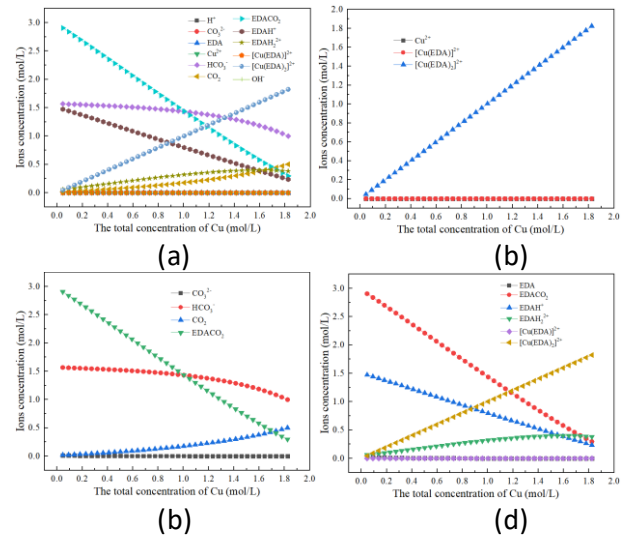


Fig. 3. (a) the change in the concentration of ions involved in the EMAR system; (b) the change of Cu-related species; (c) the change of CO_2 -related species; (d) the change of EDA-related species.

3.2 The results of multi-physics field modeling

The current density of electrode reactions is directly related to the concentration of reaction ions (Cu^{2+} and $[\text{Cu}(\text{EDA})_2]^{2+}$) on the electrode surface. Figure 4(a) shows the distribution of $[\text{Cu}(\text{EDA})_2]^{2+}$ concentration. The concentration of $[\text{Cu}(\text{EDA})_2]^{2+}$ ions gradually decreases from the diffusion zone to the cathode surface. The

$[\text{Cu}(\text{EDA})_2]^{2+}$ in the convective zone are replenished to the diffusion zone through the convective mass transfer of the electrolyte. Under the combined effect of mass transfer and electrolysis, the concentration of $[\text{Cu}(\text{EDA})_2]^{2+}$ on the cathode plate surface and its adjacent region will reach a dynamic equilibrium. Therefore, the distribution of $[\text{Cu}(\text{EDA})_2]^{2+}$ concentration shows an increasing trend in the anode region due to the reaction of anodic copper dissolution and the EDACO₂ reaction to generate $[\text{Cu}(\text{EDA})_2]^{2+}$, which gradually stabilizes along the electrode direction. In the vertical direction of the electrode, the concentration first decreases rapidly and then stabilizes. In the cathode region, as $[\text{Cu}(\text{EDA})_2]^{2+}$ is continuously reduced on the electrode, the concentration decreases gradually along the electrode direction and then stabilizes. In the vertical direction of the electrode, the concentration first increases rapidly and then stabilizes.

Similarly, for the distribution of Cu^{2+} concentration in the anode region, as shown in Figure 4(b), under the combined effect of anodic copper dissolution, reaction consumption, and flow field, it shows an increasing trend along the electrode direction and then stabilizes. At the same horizontal plane, with an increasing distance from the anode plate, the Cu^{2+} concentration first decreases and then stabilizes, which is consistent with the conclusions derived from the liquid-phase mass transfer theory.

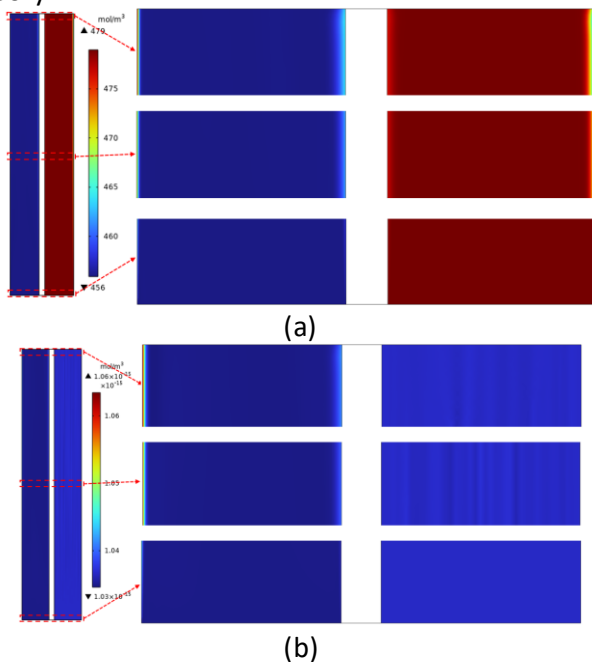


Fig. 4. (a) the distribution of $[\text{Cu}(\text{EDA})_2]^{2+}$ concentration; (b) the distribution of Cu^{2+} concentration

In the working process of the EMAR system, according to the electrolyte inlet method, there are two ways: co-current flow and counter-current flow, as

shown in Figure 5. Figure 6(a) shows the CO₂ generation rate under different inlet conditions, indicating that the CO₂ generation rate is higher in the co-current flow state than in the counter-current flow state. This is because in the co-current flow state, there is a relatively large concentration difference between the anode and cathode reaction ions, which favors the progress of the reactions. Figure 6(b) illustrates the specific desorption energy consumption under different inlet conditions, revealing that the specific desorption energy consumption is slightly lower in the co-current flow state compared to the counter-current flow state. Figure 6(c) presents the variation of anode and cathode electrode thickness along the electrode direction under different inlet conditions. It is observed that for the anode, the corrosion rate is higher in the co-current flow condition than in the counter-current flow condition, with a trend of first decreasing and then increasing along the electrode direction. For the cathode, the deposition thickness shows an increasing trend along the electrode direction in the co-current flow condition, while it shows the opposite trend in the counter-current flow condition. Additionally, the difference between the deposition and corrosion rates of the anode and cathode in the same flow direction is greater than that in the counter-current flow state.

In conclusion, considering system stability and desorption performance, the co-current flow state is superior to the counter-current flow state.

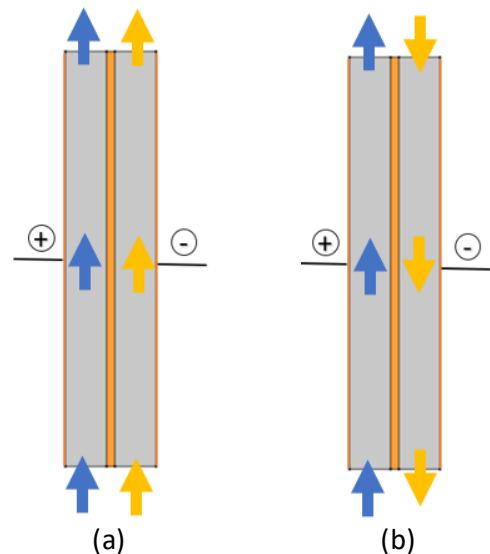


Fig. 5. Flow diagram (a) co-current flow; (b) counter-current flow

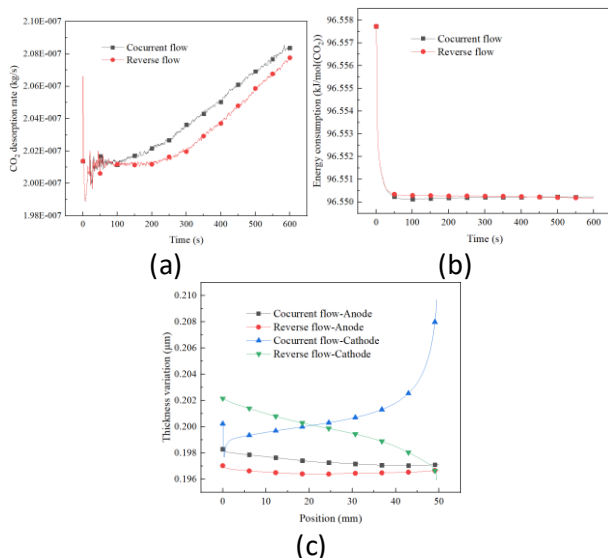


Fig. 6. Desorption performance under different feeding modes. (a) CO₂ desorption rate; (b) energy consumption per unit of desorption; (c) changes in electrode thickness

4. CONCLUSIONS

This work investigates the Electrochemical Mediated Amine Regeneration (EMAR) process for CO₂ capture, using ethylenediamine (EDA) as the absorbent and copper (Cu) as the mediator.

Firstly, a chemical reaction equilibrium model was constructed for the Cu(II)-EDA-CO₂-H₂O system, obtaining the concentration variations of different components in the electrolyte under various copper loads. The results indicate that the main form of the copper amine complex formed by EDA and Cu²⁺ is [Cu(EDA)₂]²⁺, and the variation in EDACO₂ concentration plays a dominant role among CO₂-related species. Based on this, the EMAR process can be simplified, considering the reactions $\text{Cu(s)} - 2\text{e}^- \rightarrow \text{Cu}^{2+}(\text{aq})$, $[\text{Cu(EDA)}_2]^{2+}(\text{aq}) + 2\text{e}^- \rightarrow \text{Cu(s)} + 2\text{EDA}(\text{aq})$ and $\text{Cu}^{2+}(\text{aq}) + 2[\text{EDACO}_2](\text{aq}) \leftrightarrow [\text{Cu(EDA)}_2]^{2+}(\text{aq}) + 2\text{CO}_2(\text{g})$ occurring at the anode, cathode, and in the electrolyte respectively.

Subsequently, a multi-physics field model was built using COMSOL software, and the Nernst-Planck model and bubble flow model were employed to simulate the EMAR process in a simple plate-type reactor. The results demonstrate that the distribution of reaction ions in the electrolyte follows the ion-liquid phase mass transfer theory during the operational process. The presence of CO₂ bubbles in the electrolyte has a certain promoting effect on the electrode processes. Comparing co-current flow with counter-current flow in the anode-cathode

chamber, co-current flow exhibits better system stability and desorption performance.

These research findings provide effective guidance for the design and application of EMAR system reactors.

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DECLARATION OF INTEREST STATEMENT

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. All authors read and approved the final manuscript.

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