Optimized structural parameters and heat extraction capacity of a mixing device for constant pressure CO₂ mineralization using alkaline waste

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Abstract
Alkaline waste such as calcium carbide slack is an ideal material for mineralizing CO₂ and promoting atmospheric carbon reduction. In this study, the structural parameters of a mixing device and a thermal extraction method for the high-efficiency mineralization of CO₂ using alkaline waste were optimized. First, the influence of structural parameters was studied by means of numerical simulation, and it was found that when the length–diameter ratio, blade angle, spacing, and diameter of the mixing device were 3, 15, 6 cm, and 14 cm respectively, 2.14 t CO₂ can be mineralized within 1 h. The amount of heat extracted from mineralization of 1 t CO₂ reached 189.60 MJ. In addition, the winding configuration of the heat pipe, which is beneficial for extracting more reaction heat, was optimal, and a model of the relationship between the heat pipe outlet water temperature and flow velocity at the outlet of the heat pipe was established. This study provides theoretical guidance for the field application of alkaline waste for high-efficiency mineralization of CO₂, which can accelerate the realization of peak CO₂ emissions and carbon neutrality.

Keywords Alkaline waste · CO₂ mineralization · Mixing device · Structural parameters · Reaction heat extraction

Introduction
Mixing technology is widely used in the desalination of seawater, chemical and metallurgical processing, and other industrial processes (Mauro et al. 2010; Li and Xu 2017). With the increasing industrial demand for ethylene production and coal and iron resource mining, a large amount of alkaline waste is produced, such as calcium carbide slack and fly ash (Miao et al. 2022; Wu et al. 2021a). At the same time, many of the alkaline components in these wastes can mineralize and sequester large amounts of CO₂ (Mayoral et al. 2013; Yang et al. 2019; Wang et al. 2021). A mixing device that can ensure that the alkaline waste mineralizes and absorbs a large amount of CO₂ and that can efficiently extract a large amount of reaction heat can accelerate the realization of peak CO₂ emissions and carbon neutrality (Nazari et al. 2018a; Pan et al. 2020).

Improving the efficiency of the mixing device is imperative for the efficient mineralization of CO₂ using alkaline waste, where the structural parameters of the mixing device are known to affect its efficiency (Geng et al. 2021). Methods of achieving efficient mass and heat transfer in mixing devices have been widely studied in scholastic settings. For example, Moradkhani et al. (2017) studied the influence of five impeller structures and three different aeration flow rates on the mass transfer coefficient based on the “k-ε” Reynolds-averaged Navier-Stokes (RANS) model. They found that a stirring speed of 300–800 rpm provided the most effective rate of oxygen mass transfer in a two-phase distribution bioreactor. Tatterson and Morrison (1987) studied the length–diameter ratio of the agitator in a mixing device and found that when the length–diameter ratio was greater than 4, the hydrodynamics of the fluid near the blade was close to solid rotation. Ranade and Joshi (1989) studied the influence of the blade inclination on the flow pattern in a mixing device and determined that the blade inclination has a
significant effect on the flow characteristics. Ameer (2016) found that the stirring power increases with an increase in the blade inclination angle. Wu et al. (2021b) studied the heat transfer performance of a rotating fluidized bed using the Euler-Lagrangian hybrid method. It was found that the heat transfer coefficient of the bed wall increased by 20% when the blade inclination angle was changed from 45 to 12°.

Kumaresan and Joshi (2016) obtained a higher average shear rate, average normal stress, and turbulent kinetic energy of a downflow impeller by studying the influence of the blade inclination angle on the power. Zuo et al. (2020) studied the effect of different blade numbers on the mixing efficiency of an agitator using the discrete element method and found that increasing the blade number can promote the mixing efficiency. Bao et al. (2020) used the discrete element method to study the effect of the impeller structure on particle flow and mixing. The results showed that the mixing efficiency and axial diffusion coefficient increased with an increase in the blade diameter.

We found by reviewing the literature that heat pipes are widely used in the field of heat exchange. Many scholars have studied the effect of heat pipe structure parameters on the efficiency of heat exchange. For example, Jouhara et al. (2017) manufactured and tested a flat heat pipe heat exchanger with a heat recovery rate of about 5 kW and verified through experiments that the heat recovery rate was basically consistent with the theoretical value. Deng et al. (2020) used heat pipe to recycle underground heat resources, and the heat extracted is used to heat water for regional heating. Nazari et al. (2018b) added surfactant into pure water to improve the thermal performance of pulsating heat pipe. Ramezanizadeh et al. (2019) carried out a lot of research on the heat transfer performance of pulsating heat pipe by adding different materials to water. The results show that pulsating heat pipe has superior heat transfer performance when applied to cooling equipment and heat exchanger, and the maximum heat transfer performance can reach 100%.

Different from previous studies (Yuan et al. 2022), this paper mainly studies the effect of mixing devices with different structural parameters on thermal extraction efficiency. In addition, heat extraction by the heat pipe using different winding configurations is studied. The heat extraction ability of the heat pipe at different fluid velocities is analyzed. Despite numerous studies on the structural parameters of mixing devices, there are few studies of the influence of the length–diameter ratio, blade inclination angle, blade diameter, and blade spacing on the reaction heat transfer and heat transfer efficiency. In order to realize high efficiency and maximize the mineralization and storage of CO2 using waste, it is urgent to develop a device for the rapid mineralization of CO2. Therefore, in this study, the influence of various factors, including the length–diameter ratio of the mixing device, inclination angle, spacing, and diameter of the blades, on the degree of CO2 mineralization using carbide slag (where the mineralization degree refers to the ratio of the mass of carbide slag participating in the CO2 mineralization reaction to the total mass of carbide slag filled into the mixing device) and reaction heat extraction during the mineralization process is investigated through experiments and numerical simulations. The relationship between the heat pipe outlet water temperature and fluid velocity at the outlet of the heat pipe is analyzed by numerical simulation.

This research is of great significance for the early realization of peak CO2 emissions and carbon neutrality and enhances the extraction and utilization of reaction heat during the mineralization process. In the “Mechanism of CO2 mineralization and mathematical model” section, the mechanism of CO2 mineralization with carbide slag is analyzed, and a mathematical model of CO2 mineralization with carbide slag slurry under constant pressure is established and verified. In the “Numerical simulation of CO2 mineralization in mixing devices” section, a mixing device model with different structural parameters is established and the effects of different structural parameters on the degree of mineralization and reaction heat extraction under constant-pressure and continuous-feed conditions are studied by numerical simulation. A model of the relationship between the heat pipe outlet water temperature and flow velocity at the outlet of the heat pipe is established.

Mechanism of CO2 mineralization and mathematical model

The total reaction during CO2 absorption by the carbide slag slurry can be expressed as Eq. (1) (Meng et al. 2022; Liu et al. 2021):

\[ Ca(OH)_2(s) + CO_2(g) = Ca(CO)_3(s) + H_2O(l) \]  (1)

Figure 1 shows a schematic of the instantaneous mass transfer near the gas-slurry interface of the carbide slag slurry.

When the pH is greater than 11, reactions (1) are expected to occur at a high rate (Gupta and Fan, 2002). Therefore, the process of CO2 absorption by calcium carbide slag slurry can be replaced by reaction (1) (Rigopoulos and Jones, 2003).

The validity of the mathematical model used in this paper has been verified in the previously published articles (Yuan et al. 2022). In this mathematical model, turbulence, component transport and other models are used to realize the chemical reaction and the source phase is established to ensure that the CO2 inside the mixing device is in a constant pressure state. This mathematical model is independent of
the structural parameters of the mixing device (Heydarifard et al. 2020; Liu et al. 2020; Malakhov et al. 2020, and it is feasible to apply the mathematical model to the study of the structural parameters of the mixing device on the mineralization degree and the extraction temperature of the heat pipe (Wu et al. 2018; Xuan et al. 2016). The maximum error between the numerical simulation results and the experimental results is less than 10%, which shows that the mathematical model is effective in simulating the CO2 mineralization process of carbide slag. Therefore, next, the CO2 mineralization process of mixing devices with different structural parameters is studied.

**Numerical simulation of CO2 mineralization process in a mixing device**

**Numerical simulation of CO2 mineralization using calcium carbide slag and optimum process parameters**

The mass transfer and heat pipe outlet water temperature for CO2 mineralization with calcium carbide slag were studied by controlling the length-to-diameter ratio (A), blade inclination angle (B), blade spacing (C), and blade diameter (D) in the device. The numerical simulation was carried out by designing orthogonal experiments, and the gradient was divided, as shown in Table 1. The 3D physical model of the mixing device centered on (0,0,0) was established using Solidworks software (Fig. 2). The model includes a slurry inlet and outlet, a CO2 source phase, and a heat pipe (screw thread spacing of 10 cm); the function of the middle heat pipe in the mixing device is to extract the reaction heat released by the mineralization reaction, so as to reduce the heat loss and the mineralization cost. The data from domestic and foreign studies on the degree of mineralization promoted by different factors were summarized, from which the rotational speed, pressure, solid–liquid ratio, and slurry

**Table 1** Gradients in the orthogonal simulation

| Group | Factor |
|-------|--------|
| A     | B      | C     | D     |
| 1     | 1.5    | 15°   | 3 cm  | 11 cm |
| 2     | 2      | 25°   | 4 cm  | 12 cm |
| 3     | 2.5    | 35°   | 5 cm  | 13 cm |
| 4     | 3      | 45°   | 6 cm  | 14 cm |

Note: The inlet speed of the heat pipe (water temperature 300 K) was 2 m/s.
entry speed were set to 2000 rpm, 5 Mpa, 0.25, and 0.8 m/s, respectively.

The length–diameter ratio, blade angle, spacing, and diameter of the mixing device are 1.5–3, 15–45°, 3–6 cm, and 11–14 cm, respectively, and were equally divided into four gradients for orthogonal numerical simulation. The gradient was divided as shown in Table 1.

The degree of mineralization and the heat pipe outlet water temperature were calculated when the mass of the CaCO₃ outlet was stable. Sixteen groups of mineralization degree data and heat pipe outlet water temperature were obtained by orthogonal simulation, as shown in Table 2.

The range of $R_j$ reflects the influence of this factor on the degree of mineralization or temperature rise. The greater the $R_j$ value, the greater the influence of this factor on the results. As can be seen from Table 2, for the degree of mineralization, $R_j$ follows the order $A > D > B > C$. For the heat pipe outlet water temperature, $R_j$ follows the order $A > D > C > B$. Therefore, factor $A$ has the greatest influence on both the degree of mineralization and the heat pipe outlet water temperature.

Combined with the data in Tables 3 and 4, the analysis of variance shows that when the mineralization degree is an objective function (Wu et al. 2020), the $F_{ratio}$ for factors $A$, $B$, and $D$ (3.54, 0.08, and 0.37, respectively) is greater.

Table 2: Mineralization degree and water temperature after orthogonal simulation

| Group | Factor | Result A (%) | Result T (K) |
|-------|--------|--------------|--------------|
| 1     | 1.5    | 15           | 3            | 11            | 41.79 | 307.66 |
| 2     | 2      | 15           | 4            | 12            | 54.59 | 304.65 |
| 3     | 2.5    | 15           | 5            | 13            | 68.76 | 315.42 |
| 4     | 3      | 15           | 6            | 14            | 78.19 | 319.21 |
| 5     | 2      | 25           | 3            | 13            | 61.32 | 311.62 |
| 6     | 1.5    | 25           | 4            | 14            | 44.89 | 308.02 |
| 7     | 3      | 25           | 5            | 11            | 64.40 | 316.57 |
| 8     | 2.5    | 25           | 6            | 12            | 61.12 | 315.82 |
| 9     | 2.5    | 35           | 3            | 14            | 66.89 | 316.23 |
| 10    | 3      | 35           | 4            | 13            | 74.37 | 317.49 |
| 11    | 1.5    | 35           | 5            | 12            | 42.01 | 307.66 |
| 12    | 2      | 35           | 6            | 11            | 48.32 | 309.31 |
| 13    | 3      | 45           | 3            | 12            | 67.19 | 315.91 |
| 14    | 2.5    | 45           | 4            | 11            | 60.24 | 313.53 |
| 15    | 2      | 45           | 5            | 14            | 57.39 | 311.63 |
| 16    | 1.5    | 45           | 6            | 0.8           | 41.04 | 308.35 |

Note: $A$ is the mineralization degree, and $T$ is the water temperature. $K_{ij}$ represents the average mineralization degree and outlet temperature rise corresponding to level $i$ in column $j$. $R_j$ stands for $k_{max} - k_{min}$ in column $j$.

Table 3: Numerical simulation—analysis of variance for mineralization degree

| Sum of squared deviation | Degree of freedom | Fratio $F_{ratio}$ | $F_{critical (0.05)}$ | Significant |
|--------------------------|------------------|--------------------|-----------------------|-------------|
| 1831.33                  | 3.00             | 3.54               | 3.49                  | Significant |
| 40.31                    | 3.00             | 0.08               | 3.49                  | Significant |
| 9.41                     | 3.00             | 0.25               | 3.49                  | Significant |
| 190.16                   | 3.00             | 0.37               | 3.49                  | Significant |

Note: $F_{ratio}$ represents $F$ value; $F_{critical (0.05)}$ represents significance level 0.05.
than that when the heat pipe outlet water temperature is the objective function (0.02). Therefore, C₄ was selected as the objective function for the heat pipe outlet water temperature. The optimal combination is A₄B₁C₄D₄, that is, the length-to-diameter ratio of the mixing device is 3, and the angle, spacing, and diameter of the blade are 15°, 6 cm, and 14 cm, respectively, which is the fourth group of sixteen orthogonal simulations.

**Numerical simulation of CO₂ mineralization and quantification of heat extraction for mixing device**

The length-to-diameter ratio of the mixing device has the greatest influence on the mineralization capacity and the heat pipe outlet water temperature. To a certain extent, increasing the length of the mixing device can increase the contact time between the calcium carbide slag and CO₂, leading to greater reaction, a longer heat exchange time between the heat pipe, and the high-temperature slurry in the mixing device, and improve heat exchange efficiency. Group 4 of the numerical simulation data was imported into TECPLOT post-processing software, and the nephograms of the CaCO₃ concentration and temperature distribution (after the mass of CaCO₃ at the outlet stabilized) were obtained (Fig. 3).

The nephograms of the CaCO₃ concentration and temperature distribution show that the CaCO₃ concentration and temperature were high near the entrance and low near the exit. This is because a large amount of heat is released after the reaction of Ca(OH)₂ and CO₂ to form CaCO₃, which increases the temperature of the slurry containing CaCO₃, resulting in a similar CaCO₃ concentration distribution and temperature distribution. Table 2 shows that after the mass of CaCO₃ at the outlet stabilized, the degree of mineralization and the temperature of the outlet reached 78% and 319.21 K, respectively. The calculation indicates that the mixing device with the A₄B₁C₄D₄ structure parameters can mineralize about 2.14 t of CO₂ and consume 4.53 t carbide slag within 1 h, which is equivalent to the CO₂ released by complete combustion of 0.957 t coal. In addition, 2.35 m³ of water can be heated from 300 to 319.21 K for the mineralization of 1 t CO₂, where the amount of heat extracted reached 189.60 MJ.

**Effect of heat pipe configuration on heat extraction capacity**

As shown in Table 2, the simulated mineralization capacity and the heat pipe outlet water temperature were the highest in the fourth group. Therefore, the structural parameters from the fourth group simulation were used; that is, the length–diameter ratio, blade angle, spacing, and diameter of the mixing device were 3, 15, 6, and 14 cm, respectively. The influence of the winding density of the heat pipe on the heat extraction capacity was investigated. The distance between the outlet and the inlet of the heat pipe in the mixing device was 120 cm, which was divided into a, b, and c regions on average, and the pitch of the three areas was changed from 10 to 5 cm to encrypt the heat pipe in the corresponding area, after which the calculation was carried out. The heat pipe outlet water temperatures with different winding densities are shown in Fig. 4.

Figure 4 shows that the heat pipe outlet water temperature was highest when the winding density corresponded to a. Combined with Fig. 4b, it can be seen that the reaction heat produced by the reaction of Ca(OH)₂ and CO₂ was mainly concentrated in the area of the mixing device. When the winding number of the heat pipe was increased, the heat exchange area increased, and the outlet water temperature decreased. The mass of CaCO₃ at the outlet stabilized is shown in Table 2.
pipe in this area is increased, the heat exchange time between the water inside the heat pipe and the high-temperature slurry outside the heat pipe can be increased, allowing the water inside the heat pipe to absorb more heat, thus increasing the heat pipe outlet water temperature and improving the heat exchange efficiency. Therefore, the winding configuration of the heat pipe (Fig. 4a) was employed in studying the effect of the flow velocity of the internal liquid on the heat extraction capacity.

**Effect of flow rate on thermal extraction ability**

In this section, the variation of the heat pipe outlet water temperature at flow velocities of 0.2–4 m/s in the heat pipe (where the flow velocity refers to the flow velocity in the heat pipe) was studied. After locally encrypting the density of the heat pipe, there were 16 turns of the heat tube in the mixing device. To monitor the real-time change in the heat pipe outlet water temperature, four points a (5.24, −60, 30.69), b (0, 50, 21), c (0, −22.5, −21), and d (0, −55, 21) were set up at lap 2, lap 8.5, lap 15, and at the outlet of the heat pipe when the water enters the mixing device. The temperature change at each point was determined after the mass of CaCO$_3$ at the outlet stabilized. The curve $t$ represents the temporal evolution of water flow from the inlet of the heat pipe to the outlet, and the data in curve $b$ corresponds to $T_b = 12$ K.

As shown in Fig. 5, the slope of curve $t$ decreased gradually overall. As the flow velocity increased, the time for water to flow from the heat pipe inlet to the outlet decreased. The time required for heat exchange between water in the heat pipe and high-temperature calcium carbide slag slurry decreased with an increase in the flow velocity, leading to a less pronounced decrease in the heat exchange capacity. Therefore, the temperature of points a, b, c, and d decreased slowly with an increase in the flow velocity, and the extent of the decrease gradually became smaller.

The values $A = 6.77$, $t = 2.67$, and $y_0 = 315.91$ were obtained for the exponential decay by using the Expdecl model ($y = A\exp(x/t) + y_0$) in Origin software to analyze the data in curve $a$. The functional relationship between the heat pipe outlet water temperature and flow velocity at the outlet of the heat pipe is represented by Eq. (2).

$$T = 6.77 \times \exp \left(-\frac{V_H}{2.67}\right) + 315.91$$  \hspace{1cm} (2)

The amount of heat extracted from the water in the heat pipe in 1 h is related to the increase in the heat pipe outlet water temperature. Therefore, the function $Q$ describing the relationship between the amount of heat extracted and the flow velocity can be obtained from Eq. (3).

$$Q = \left[T(v_H) - 300\right] \times \pi r^2 \times v_H \times c$$  \hspace{1cm} (3)

Here, $r$ is the radius of the heat pipe, $t$ is time, and $c$ is the specific heat capacity of water ($4.2 \times 10^3$ J/(kg·K)).

From Fig. 6, when the flow velocity is 1 m/s, the heat pipe outlet water temperature is 320.56 K, the heat extraction is
Conclusions

The effects of the length–diameter ratio, blade inclination angle, spacing, and diameter on the CO₂ mineralization degree and extraction of the reaction heat using alkaline waste were studied in constant-pressure and continuous-feed systems through experiments and numerical simulations.

(1) Orthogonal numerical simulation showed that when mineralizing CO₂ in the constant-pressure and continuous-feed systems, the influence of the length–diameter ratio, blade inclination angle, spacing, and diameter on the mineralization degree follows the order: length–diameter ratio of mixing device > blade diameter > blade inclination angle > blade spacing. The influence on the heat pipe outlet water temperature follows the order: length–diameter ratio > blade diameter > blade spacing > blade inclination angle.

(2) When the length–diameter ratio, blade inclination angle, spacing, and diameter of the mixing device are 3, 15°, 6 cm, and 14 cm, respectively, the amount of heat extracted from CO₂ mineralization using alkaline waste calcium carbide slag and a heat pipe is optimal; that is, 2.14 t CO₂ can be mineralized at most in 1 h, and 4.53 t carbide slag is consumed at the same time.

The amount of heat extracted from mineralization of 1 t CO₂ reached 189.60 MJ. The study shows that increasing the length-to-diameter ratio of the blade in the mixing device can further improve the degree of mineralization and the thermal extraction ability.

(3) The relationship between the winding mode, flow velocity, and water temperature at the heat pipe outlet was evaluated through numerical simulations, showing that when the left area of the heat pipe was encrypted, more reaction heat could be extracted for utilization. On this basis, a model of the relationship between the water temperature and flow velocity was established. When the flow velocity was 1–2 m/s, the heat extraction reached 97.66–181.50 MJ, which provides a theoretical basis for the application of the reaction heat extraction in the field.

Nomenclature $t$: time, s; $\alpha_j$: volume fraction of $j$th phase; $j$: $j$th phase; $\rho$: density, kg/m³; $\tau$: velocity vector, m/s; $m_j$: mass transfer rate from phase $j$ to phase $l$; $G$: gravitational constant, (m·s⁻²); $\sigma$: stress tensor, N/m²; $M_j$: the interphase momentum exchange between phase $j$ and other Phase; $h$: total energy per unit mass, (Nm/kg); $p$: pressure, MPa; $\rho$: interphase heat exchange, (J/(s·m³)); $S$: source term in the species balance equation, (kg/s·m³); $\mu$: viscosity, kg/(m·s); $I$: ionic concentration, (kmol·m⁻³); $f$: mass fraction; $i$: substance $i$ in the phase $j$; $D$: mass diffusion coefficient of matter; $D$: net production rate of chemical reaction, (kg/(s·m³)); $R$: the rate constant; $A$: Pre-exponential factor, (unit time⁻¹); $T$: temperature, K; $\beta$: temperature index; $c$: natural logarithm; $E_a$: activation energy, (j/(kg·mol)); $R$: gas constant, J/(mol·K); $v_{in}$: inlet velocity of heat pipe water, m/s; $r$: heat pipe radius, m; $c$: specific heat capacity, 4.2 × 10³ J/(kg·K)

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Author’s specific contributions

| Author’s name | Term | Definition |
|---------------|------|------------|
| Wei Lu        | 1. Investigation | 1. Conducting a research and investigation process, specifically performing the experiments, or data/evidence collection |
|               | 2. Writing—original draft | 2. Verification, whether as a part of the activity or separate, of the overall replication/reproducibility of results/experiments and other research outputs |
|               | 3. Writing—review&editing | 3. Writing—review& editing |
| Yang Yuan     | 1. Investigation | 1. Conducting a research and investigation process, specifically performing the experiments, or data/evidence collection |
|               | 2. Visualization | 2. Preparation, creation and/or presentation of the published work, specifically writing the initial draft |
|               | 3. Writing—review&editing | 3. Writing—review& editing |
Author’s name | Term | Definition
--- | --- | ---
Xiangming Hu | 1. Investigation | 1. Provision of study materials, reagents, materials, laboratory samples, animals, instrumentation, computing resources, or other analysis tools
Guansheng Qi | 1. Resources | 1. Acquisition of the financial support for the project leading to this publication
 | 2. Funding acquisition | 2. Provision of study materials, reagents, materials, laboratory samples, animals, instrumentation, computing resources, or other analysis tools
 | 3. Project administration | 3. Management and coordination responsibility for the research activity planning and execution
Lulu Sun | 1. Investigation | 1. Conducting a research and investigation process, specifically performing the experiments, or data/evidence collection
Maoyuan Zhang | 1. Investigation | 1. Conducting a research and investigation process, specifically performing the experiments, or data/evidence collection
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Availability of data and materials We guarantee the authenticity and reliability of the data.

Author contribution All authors contributed to the study conception and design. Material preparation, data collection, and analysis were performed by Wei Lu, Xiangming Hu, Guansheng Qi, Lulu Sun, Maoyuan Zhang, MingJun Wang, and Min He. The first draft of the manuscript was written by Yang Yuan, and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript. The following are the author’s specific contributions.

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Declarations

Ethical approval We guarantee that our work is original and has not been submitted to other journals.

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