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A Mathematical Model for CO2 Capture via Mineral Carbonation Using Hydrated Lime

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A Mathematical Model for CO_2 Capture via Mineral Carbonation Using Hydrated Lime

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Abstract. The construction sector contributes to approximately 37% of global GHG emissions. To mitigate this impact, this study develops a mathematical model to analyze CO_2 capture via hydrated lime carbonation. The model integrates reaction kinetics, diffusion and heat balance, considering the effects of liquid water saturation, the influence of porosity on diffusion and the heat generated by both the reaction and water evaporation. For a specific case, the carbonation front and temperature gradient along the reactor are analyzed. Then, the model is validated, demonstrating promising results for optimizing future carbonation processes.

Keywords: mineral carbonation, hydrated lime, CO_2 capture

1 Introduction

In the current era, the construction sector contributes around 37% of global emissions [1]. To reduce this contribution, this study proposes a mathematical model for CO_2 capture through mineral carbonation using hydrated lime (CH). The research is part of the Mineral Loop project, funded by the Walloon Region (Belgium), which aims to develop a pilot unit for transforming mineral waste into high-value materials.

The modeled reaction involves the ex-situ and direct carbonation of hydrated lime in solid state [2]. The simplified carbonation reaction considers CH and CO_2 as reactants, forming calcium carbonate and water as products. Although water does not directly participate as a reactant, its initial addition is critical for dissolving carbon dioxide and calcium ions to initiate the carbonation process [3]. The water-to-solid ratio (w/s), defined as the mass of water added relative to the solid material, plays a pivotal role. Insufficient water hinders the dissolution steps, while larger amounts slow down the CO_2 diffusion towards the source of calcium ions.

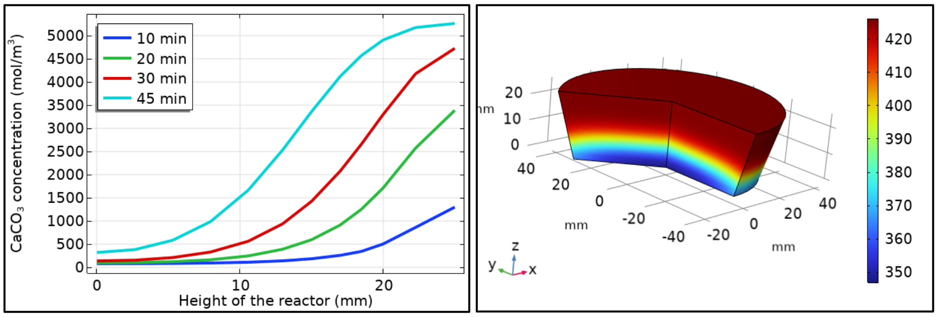
1.1 Methodology

The liquid water saturation parameter (S) is used to describe water behavior within the model, influencing three key phenomena: reaction kinetics, CO_2 diffusion, and water evaporation. The reaction kinetics are modeled as a piecewise linear function of liquid water saturation. A minimum saturation of S=0.03 is required to initiate the reaction, and the reaction achieves its maximum velocity (k= 0.0025 $m^3 \cdot (mol \cdot s)^{-1}$) at a saturation value of 0.8, beyond which the material is fully saturated. Between these two values, the kinetics of the reaction assume a constant reaction rate equal to k*S $m^3 \cdot (mol \cdot s)^{-1}$ [4]. On the other hand, the model incorporates the influence of porosity. Porosity increases during carbonation, which could be validated through mercury intrusion porosimetry. Porosity enhances the diffusion of CO_2 while liquid water saturation negatively affects it [3]. Moreover, carbonation is an exothermic reaction, releasing 109 $kJ.mol^{-}$

^{1} at standard conditions and 25°C. The reaction heat drives water evaporation leaving a thin film of water adhered to CH particles, preventing complete evaporation at short carbonation times. A heat balance integrated into the model predicts a temperature gradient along the carbonation reactor. The model, implemented in COMSOL Multiphysics 6.2, simulates the carbonation of a semi-conical granular bed with an initial CH concentration of 5356.8 mol.m^{3}. The initial bed porosity, w_s, and CO_2 flow rate are set to 0.65, 0.10, and 200 ml.min^{-1}.

2 Results and Conclusion

Figure 1(a) illustrates the calcium carbonate concentration gradient along the reactor at four carbonation times (x=0 represents the bottom of the reactor and x=25 represents the top). The carbonation front progresses through the reactor in alignment with CO_2 diffusion, resulting in layers with varying degrees of carbonation. Figure 1(b) depicts the temperature gradient after 45 minutes of carbonation. The completed carbonation layers exhibit a higher temperature of 420 K.



(a) (b)

Figure 1. (a) Calcium carbonate concentration along the reactor at different carbonation times. (b) Temperature gradient along the reactor after 45 minutes of carbonation.

The proposed model has been validated through experiments conducted with varying water-to-solid ratios, carbonation periods, and CO_2 flow rates. The Fisher test was performed to validate the total carbon results of the model against the total carbon results of the experiments, with the calculated F-value ($F_{calculated}$=1.087) compared to the critical F-value ($F_{critical}$=2.03) at a 95% confidence level. This result indicates a low variance difference, confirming that the model accurately predicts the experimental results and effectively explains the carbonation behavior of hydrated lime.

In conclusion, this work proposes a mathematical modeling approach to enhance CO_2 capture using hydrated lime. This approach effectively integrates reaction kinetics, CO_2 diffusion, and water evaporation phenomena. It predicts critical parameters, including carbonation progress and temperature distribution, which are essential for optimizing the carbonation process in industrial applications.

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