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# Modelling of Accelerated CO<sub>2</sub> Absorption Using an Enzyme in a Hollow Fiber Membrane Contactor

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#### ABSTRACT

Carbon dioxide (CO<sub>2</sub>) is widely recognized as the main cause of climate change affecting our planet. In recent years, the concentration of CO<sub>2</sub> in the atmosphere has increased significantly due to the intensive combustion of fossil fuels. This study is devoted to the simulation of the 1D case of the CO<sub>2</sub> capture process by aqueous Potassium carbonate  $K_2CO_3$  as chemical solvent promoted with BCa (Bovine carbonic anhydrase), using a membrane contactor in the counter current case. The system of partial differential equations resulting from the modelling were solved using MATLAB's PDEPE function. We also carried out a parametric analysis to see the impact of various parameters on the CO<sub>2</sub> capture process. Among these parameters, we studied the influence of solvent concentration, gas velocity and liquid velocity. The results show that 13% increase (74% to 87%) on CO<sub>2</sub> capture while the increase of solvent concentration from 20 to 50 (mol/m3), also for gas and liquid velocity from 0.001 to 0.05 and 0.006 to 0.05 (m/s) we have 52% and 3 % increase of CO<sub>2</sub> capture respectively.at final the Enzyme had an effect of average 7% of absorption of CO<sub>2</sub>.

**Keywords:** Absorption, BCa, CO<sub>2</sub>, Potassium carbonate (K<sub>2</sub>CO<sub>3</sub>), Hollow fibre membrane contactor (HFMC), Modeling

## 1 Introduction

Carbon dioxide (CO<sub>2</sub>) is widely recognized as a major contributor to global climate change. In recent years, the concentration of CO<sub>2</sub> in the atmosphere has increased significantly due to the intensive combustion of fossil fuels. Rising CO<sub>2</sub> emissions are a major cause of catastrophic environmental change that has led to growing interest in successful CO<sub>2</sub> capture [1]. Over the past decades, various technologies have been used for CO<sub>2</sub> capture. Chemical absorption by absorbents in trays and packed columns is the traditional method [2]. However, this method has economic and operational problems. Membrane contactor absorption is a new technology with many advantages, including: Prevention of interphase dispersion, high specific surface area, and compact size of the contactor [3]. In porous membrane contactors, absorption typically occurs when CO<sub>2</sub> diffuses from the shell side through the membrane pores and contacts the liquid phase within the fibers. One of the intensification processes using to increase the absorption of CO<sub>2</sub> is using Bovine Carbonic anhydrase (BCa) is an excellent candidate for novel biocatalytic processes based on the capture and utilization of CO<sub>2</sub> [4].

# 2 Methods

In this work, the study was made by taking a volume element of the  $\rm CO_2$  absorption model using a membrane. The equation of balances was:

#### Gas phase:

$$\frac{\partial c_{CO2,g}}{\partial t} = D_{CO2,g} \frac{\partial^2 c_{CO2,g}}{\partial z^2} - V_g \frac{\partial c_{CO2,g}}{\partial z} - K_G a \left( H \times C_{CO2,g} - C_{CO2,l} \right)$$



(1)



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## Liquid phase: (For CO<sub>2</sub> and K<sub>2</sub>CO<sub>3</sub>)

$$\frac{\partial C_{CO2,l}}{\partial t} = D_{CO2,l} \frac{\partial^2 C_{CO2,l}}{\partial z^2} - V_l \frac{\partial C_{CO2,l}}{\partial z} + K_G a \left( H \times C_{CO2,g} - C_{CO2,l} \right) - K_{K2CO3} \times C_{CO2,l} \times C_{K2CO3} \qquad (2)$$

$$\frac{\partial C_{K2CO3}}{\partial t} = D_{K2CO3,l} \frac{\partial^2 C_{K2CO3}}{\partial z^2} - V_l \frac{\partial C_{K2CO3}}{\partial z} - K_{OH} \times C_{CO2,l} \times C_{K2CO3} \qquad (3)$$

#### **3** Results and Discussion









Figure4 : Effect of loading concentration of K2CO3 on CO2 removal

# 4 Conclusions

In a nutshell, robust and reliable mechanistic model and simulation methodology was validated and implemented to study the effects of concentration, gas velocity and liquid velocity on  $CO_2$  capture by  $K_2CO_3$  accelerate by BCa using membrane process to study the performance of the hollow fibre membrane contactor in terms of  $CO_2$  removal. The  $CO_2$  removal was increased by 52% in the range of 20–50 (mol/m3) of Concentration of flow rate, also the results show that 13% increase (74% to 87%) on  $CO_2$  capture while the increase of solvent concentration from 20 to 50 (mol/m3), also for gas and liquid velocity from 0.001 to 0.05 and 0.006 to 0.05 (m/s) we have 52% and 3% increase of  $CO_2$  capture respectively. The Enzyme had an effect of average 7% of absorption of  $CO_2$ .

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