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Numerical simulation of CO_2 transport through hollow fiber membrane: Effect of chemical solvent

N. Belkhiri*, O. Saouli and K. Djerafi
Process Engineering Laboratory for Sustainable –Development and Health Products. Polytechnic School of Constantine. Algeria.
*Corresponding author, email: Naziha.Belkhiri@enp-constantine.dz

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Abstract
In this study , a two-dimensional mathematical model is proposed to describe the transport of CO2through HFMC with chemical reaction in the liquid phase .Numerical method of finite volume was used to solve the equation obtained for the three sections of the membrane contactor with the appropriate boundary conditions , The liquid solvents considered for this study include aqueous solution of Monoethanolamine (MEA) and water with a thin layer of the enzyme carbonic anhydrase (CA) .The modeling predictions indicated removal of CO2 using enzyme (CA) is more efficient than using MEA.

Key words: *Carbone dioxide absorption, Membrane Gas Absorber, 2D Mathematical Modeling, Monoethanolamine , Carbone Anhydrase .*

1. Introduction

Carbone dioxide represents about 80% of greenhouse gases. Among these greenhouse gases, CO2 has the greatest adverse impact and contributes to the global warming. Therefore, it is important to find techniques to capture the CO2 produced by industry and power plants using fossil fuels [1]. Carbone dioxide can be removed by a wide variety of technologies such as absorption and membrane separation. Conventional amine absorption has some drawbacks such as flooding, expensive solvents, entraining, low efficiency, consumption of energy for solvent generation, and high capital cost. Therefore, there is a need to find an alternative technology to reduce energy consumption and cost such as membrane contactors. This type of contactor offers many practical Advantages including flow without flooding, loading, weeping; high surface area; low corrosion problems and low operation cost [2]. In these contactors, the membrane acts as a physical barrier between two phases (gas and liquid). Mathematical modeling of membrane contactors Using solvents such as MEA has been studied in the literature [3-4]. Since a few years, researchers are Interested by the enzymatic method or the use of the carbonic anhydrase for the capture of CO2 [5]. The Canadian CO2 project gives a process for the manufacturing of the synthetic carbonic anhydrase, by means of bacteria. Obtained product is a fine brown powder which can be easily transported [6].

The objective of this paper is to develop and solve a 2D mathematical model in hollow fiber membrane contactor. In addition to the investigation of influence of various parameters on CO2 removal, comparison between MEA and CA for selecting the most effective one was presented.

2. Transport Model

In the present work, a steady-state two-dimensional mathematical model has been considered. The model is developed for a segment of a hollow fiber, as shown in Figure 1. This study is based on the searches which were made by (Ion .I and al) [7].The membrane with hollow fiber contains three sections: shell - membrane – tube.

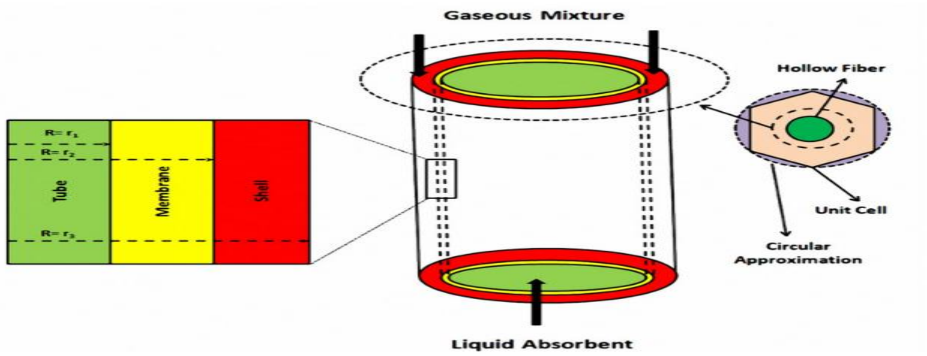

Figure 1. Schematic ofhollow fiber membrane scheme.

2.1. Transport equations in the gas phase

The convective-diffusion equation for the CO2using Fick's law of diffusion can be expressed as follows:

$$D_{CO2-S}\left[\frac{d^2C_{CO2-S}}{dr^2}+\frac{1}{r}\frac{dC_{CO2-S}}{dr}+\frac{d^2C_{CO2-S}}{dz^2}\right] = V_{Z-shell}\frac{dC_{CO2-S}}{dz} \quad (1)$$

The boundary conditions used for the shell are as follows:

At r=r_2,$C_{co2-shell} = C_{co2-membrane}$ (2)

At r=r_3, $\frac{C_{CO2-shell}}{dr} = 0(symmetry)$ (3)

At z=L,$C_{co2-shell} = C_0(inlet)$ (4)

For the transfer of the momentum, we used the equation of Happel which gives the axial velocity [8]:

$$V_{Z-shell} = \left[1-\left(\frac{r_2}{r_3}\right)^2\right] * \left[\frac{\left({r}/{r_3}\right)^2-\left({r_2}/{r_3}\right)^2+2ln\left({r_2}/{r}\right)}{3+\left({r_2}/{r_3}\right)^4-4\left({r_2}/{r_3}\right)^2+4ln\left(\frac{r_2}{r_3}\right)}\right]$$

(

2.2. **Transport equations in the liquid phase**

The equation of continuity of the CO_2 in the liquid phase is given by:

$$D_{CO2-T}\left[\frac{d^2C_{CO2-T}}{dr^2}+\frac{1}{r}\frac{dC_{CO2-T}}{dr}+\frac{d^2C_{CO2-T}}{dz^2}\right] = V_{Z-shell}\frac{dC_{CO2-T}}{dz} - R_{CO2} \quad (6)$$

The boundary conditions are given by:

At r=0 ,$\frac{dC_{CO2-tube}}{dr} = 0(symmetry)$ (7)

At r=r_1 , $C_{CO2-tube} = m * C_{CO2-membrane}$ (8)

At z=0,$C_{CO2tube} = 0\ (inlet\ boundary)$ (9)

The distribution of the velocity is given by[10]:

$$V_{Z-shell} = \left[1-\left(\frac{r}{r_1}\right)^2\right] \quad (10)$$

2-2-1-Reacion rate for CO_2 absorption into aqueous solution (MEA)

The reaction mechanism of CO2 with MEA is given below:

$$H2O + ZnHCO3 \leftrightarrow HCO3 + ZnH2O \quad (Ew)$$

$$B + ZnH2O \leftrightarrow BH + Zn \ \ (E)$$

$$HCO3 + ZnH2O \leftrightarrow CO2 + H2O + Zn(E)$$

The reaction rate is approximated by the following equation [5].

$$R_{co2} = \{(k_1+k_6)+k_2[OH^-]\}[CO2] - \left\{(k_1+k_6)[H^+] + \frac{k_2}{k_w}\right\}\frac{[HCO_3^-]}{K_{HCO3}} \quad (11)$$

2.3. Transport Equation in the membrane

The membrane (non-wetting condition) can be considered to be diffusion controlled and may be written as:

$$D_{CO2-S}\left[\frac{d^2C_{CO2-S}}{dr^2}+\frac{1}{r}\frac{dC_{CO2-S}}{dr}+\frac{d^2C_{CO2-S}}{dz^2}\right] = 0 \quad (12)$$

In which boundary conditions can be written as follow:

At r=r_1,$C_{CO2-membrane} = \frac{C_{CO2-tube}}{m}$ (13)

At r=r_2, $C_{CO2-membrane}$ =$C_{CO2-shell}$ (14)

Table1: the dimensions of the (HFMC) [9].

Characteristics	Module
Fiber material	Polypropylene
Fiber inner diameter (μm)	222
Fiber outer diameter (μm)	300
Thickness d (μm)	15
Porosity ε	0.25
Active module length (mm)	225
m	0.814

3. Results

The governing equations in membrane, tube and shell side were solved using finite volume method with Rectangular mesh elements. The chemical system connected to the chemical reactivity is solved by Newton's method to estimate the concentration of every species in the tube at equilibrium. A Matlab code was developed to visualize the concentration distribution in the contactor. This code requires data used as input parameters in the model which are given in table (1).

3.1 Concentration distribution of CO2 in the shell side

Distribution of dimensionless concentration (C/C_0) for CO_2 is illustrated in Figure (1). Represents the variation of the report of concentration of the CO_2in the radiator grill according to the report r/R for various values of the beam of the radiator grill (Rs). She indicates that the concentration decreases as we approach the membrane or we shall have a fall of in the effect of the condition in limit.For the effect of the thickness of the radiator grill, we see clearly that the distribution decreases with the increase of the thickness what is physically justified.

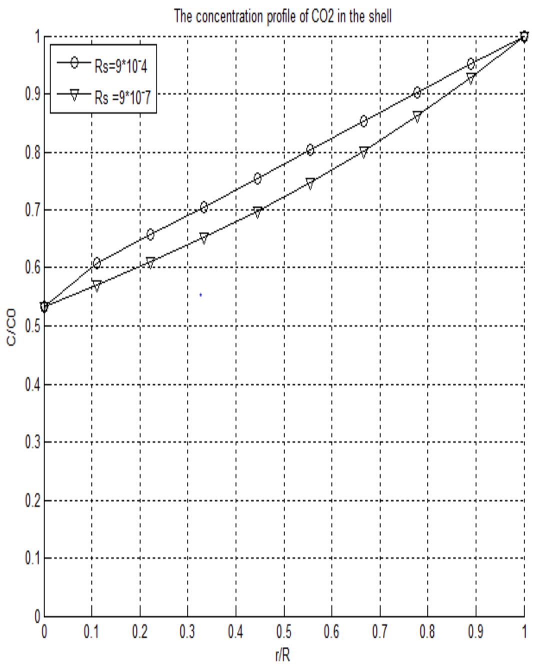

Figure 2. Concentration distribution of CO_2 in the shell side.

3.2 Concentration distribution of CO2 in the membrane

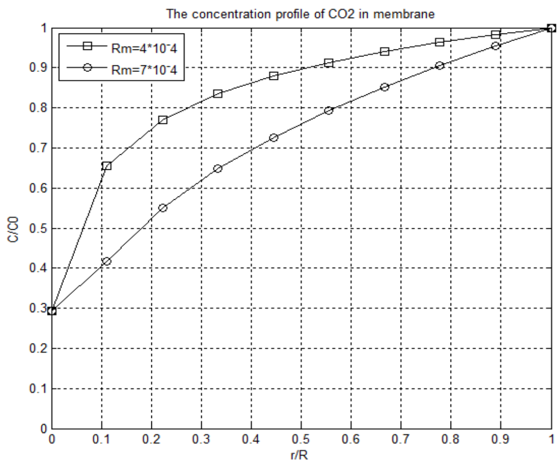

Figure 3. Concentration distribution of CO2 in the membrane with MEA

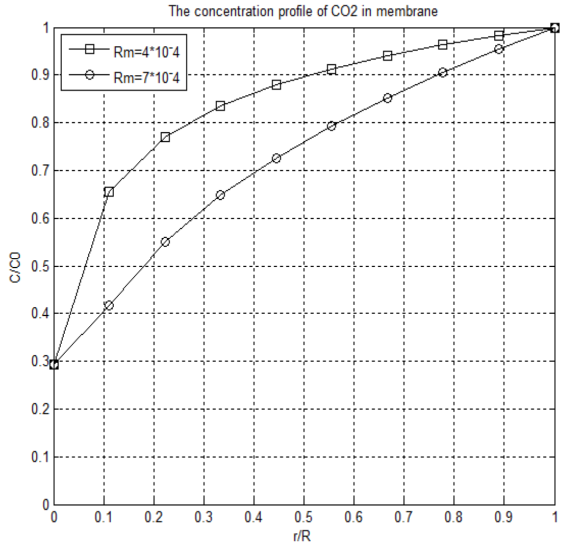

Figure 4. Concentration distribution of CO_2 in the membrane with CA.

Figure (3) and (4) indicates that the concentration of the CO_2 decreases in the membrane of in the phenomenon of distribution only.

3.3. The profile of the concentration in the tube:

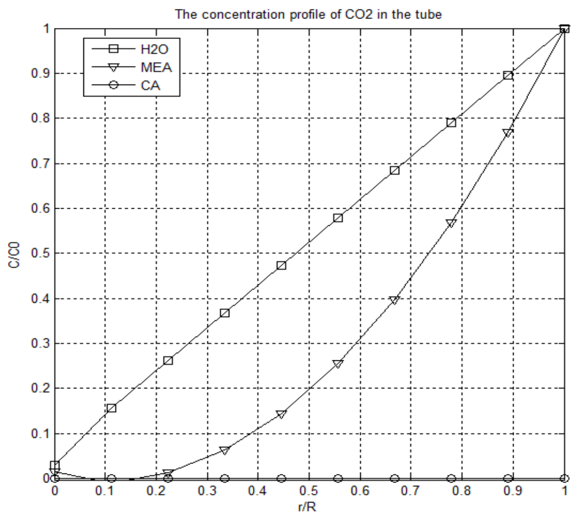

Figure 5. Concentration distribution of CO_2 in the tube side.

It's found that varies with the variation of the absorbent used, as it's observed that the CO_2 in the case of CA is completely absorbed, in contrast in the case of MEA and the water elimination is gradually depending on (r/R).

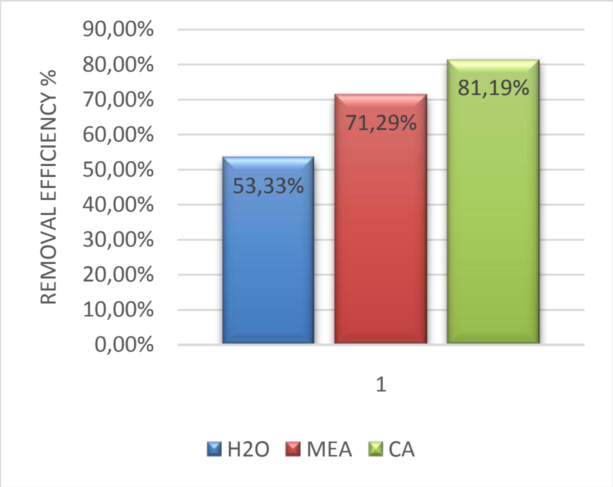

Figure 6. Effect of solvent on the removal efficiency of CO_2.

4. Conclusion

Chemical absorption of CO_2 was studied in this work. A two dimensional mathematical model was proposed to describe the transport of CO_2 in hollow fiber membrane using MEA and CA. The finite volume method was applied to solve the system of equations obtained. The chemical system obtained in the liquid phase was solved using Newton's method.The results show that the yield in the case of the CA is better than that of the MEA and water.

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