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# Numerical Investigation on the Effect of Flow Parameters in $CO_2$ Capturing Using Aqueous MEA Absorbent in HFMC Systems

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**ABSTRACT**

Nowadays, $CO_2$ as the product of fossil fuel combustions, is polluting the air and the human environment, and it causes global warming. To reduce the negative effect of $CO_2$ presence, it should be removed from the air by capturing methods. Hollow fiber membrane contactor (HFMC) system is one of the most efficient method for $CO_2$ capturing than the other feasible capturing methods. In the present paper an HFMC absorbing system has been simulated using COMSOL Multiphysics software and the effect of flow rates of gas and liquid on the amount of $CO_2$ removal has been studied. Aqueous solution of Mono-ethanolamine (MEA) is entered as the absorbent liquid in the tubes, and $CO_2$ is removed from the shell side by the diffusion phenomena by participating in the chemical reaction with MEA. The results show that the higher liquid flow rate the higher %$CO_2$ removal from the inserted gas. Against this result, the percentage of $CO_2$ removal decreases with increasing the gas flow rate as expected. Higher gas flow rate leads the gas velocity to higher values and less possibility of absorbing by the diffusion method. The rate of the $CO_2$ removal variation with liquid flow rate is higher than the $CO_2$ removal variation whit the gas flow rate.

***Keywords:*** $CO_2$ capturing, HFMC system, MEA, Flow parameters

## Introduction

Due to population growth, nowadays the use of fossil fuels to supply primary energy of power plants and industrial centers has increased significantly. The gases of fuels combustion, pollute the air. This kind of energy supply, has harmful results on the health of alive creatures on Earth, also it affects climatic and environmental conditions. So that the phenomenon of global warming has now become one of the major environmental problems. Among the pollutants from the fossil fuels combustion, the $CO_2$ pollutant approximately whit a share of two-thirds in greenhousing affect, is responsible for 55% of global warming. As respects that the use of fossil fuels for supplying energy is the most accessible option, it is expected that fossil fuels will continue to be used as the main source of energy production for the next few decades, so it to paying attention to $CO_2$ controlling is necessary and it needs to remove the $CO_2$ from air [1].

There are different ways for removing $CO_2$ like as, cyclonic separators, wet collectors, fabric filter, electrostatic precipitators, condensate, burning, and absorption [2]. Membrane separation is an absorption method for removing $CO_2$ which is utilized in present research. Chemical adsorption is one of the most common methods of $CO_2$ removal, which is based on the reaction of $CO_2$ with a solvent, this reaction improves the mass transfer. In chemical adsorption, less flow is required to separate from the solvent than in physical adsorption, but the need for energy to reduce the solvent or separation process increases due to chemical reactions. In this method, different chemical solvents are used to react with $CO_2$, in 2017 Saidi [3] investigated the influence of different solvents like as MEA, DEA, TEA, and MDEA on the separation performance of HFMC.

In recent years, the separation of pollutants using the membrane contact system has been considered. The



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operation of this system is based on the transfer of mass (pollution) between the two phases. Obviously, the efficiency of the system mainly depends on the amount of mass transfer (pollution) between the two phases. Membrane adsorbents have many advantages over other adsorbents. Their most important advantage is that they provide a high level of contact without mixing the two phases [4]. In addition, the speed of the two phases of the system can be independent of each other. The system investigated in this dissertation, as shown in Figure 1, is called the membrane contactor, which consists of two main parts, the shell and the tube. In 2011, Kazemi [5] had a study on the simultaneous transport of $CO_2$ through a HFMC using methyl-di-ethanolamine (MDEA) as chemical absorbent, in which the effect of absorbent (MDEA) concentration, was studied on $CO_2$ removal. In 2016, Azari [6] studied the effect of gas flow rate and liquid flow rate with different chemical absorbents on the function of HFMC system.

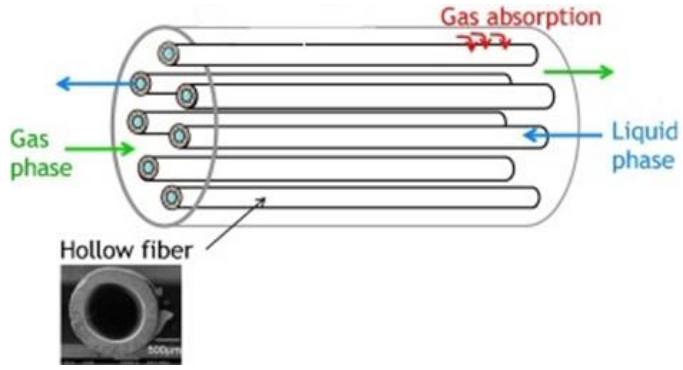


**Figure 1.** Schematic diagram of the hollow fiber membrane contactors [7].

In the proposed system, the gas phase containing $CO_2$ in the membrane contactor and the liquid phase containing the mono ethanol amine as a suitable chemical adsorbent flow in the opposite direction. Due to the contact of the two phases, $CO_2$ gas moves to the liquid phase through the micro-sized pores of the membrane and is absorbed into the liquid by a chemical reaction, and the solution is purified. In general, the performance of the system is influenced by the operating parameters related to the three main components of the gas phase (feed stream), the liquid phase (chemical adsorbent) and the porous membrane that separates the two phases.

**Problem Definition**

**Material**

In the gas absorption membrane contact system, gas and liquid flow on both sides of the membrane. The pollute gas is outside of the membrane (shell side) and the adsorbent fluid of $CO_2$ flows inside the tube. The adsorption process will be a physical adsorption, a chemical reaction, or a combination of both. Membrane adsorption is shown schematically in Figure 2. The mass transfer process consists of three main stages, which are: penetration from the gas mass to the outer surface of the membrane, penetration through the membrane cavities, dissolution and penetration into the liquid phase.

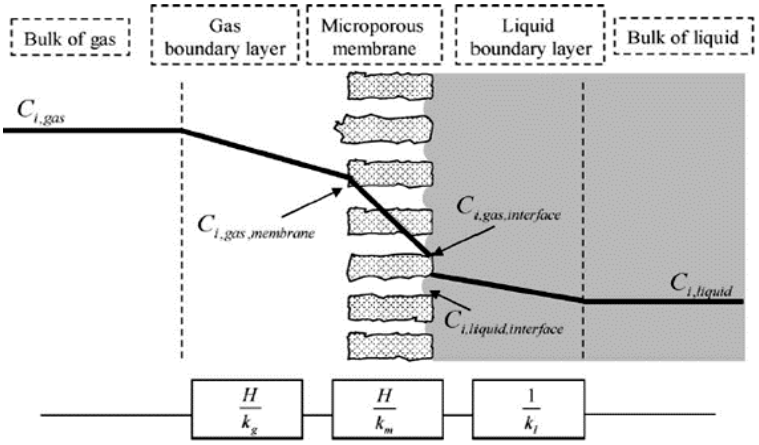


**Figure 2.** Mass transfer mechanism in the porous membrane media [7].





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As stated before, instead of using water as a physical adsorption fluid, the aqueous mono-ethanolamine (MEA) solution is utilized in tube side. Unlike many membrane processes, in contactors, the membrane does not play a significant role in separating of components. What is important is to choose a membrane that does not have a negative effect on the mass transfer and separation process. Therefore, the efficiency of membrane contactors is highly dependent on minimizing the resistance of the membrane against mass transfer.

At all, parameters which are listed in Table 1, affect system's efficiency. By changing these properties, we can control the performance of the system and achieve the desired result expected from the system.

**Table 1**
Classification of factors affecting system performance [8].

| Liquid phase (Tube) | Perouse membrane separator | Gas phase |
|---|---|---|
| - Fluid temperature | - Gender | - Speed |
| - Fluid velocity | - Diameter | - Temperature |
| - Type of (MEA) | - Thickness | - Initial concentration |
| - Concentration of (MEA) | | |

**Governing equations**

In the mass transfer model of hollow fiber, which is shown in Figure 2, some assumptions considered [9]:
1. Steady state and isothermal conditions
2. Fully developed parabolic gas velocity profile
3. Ideal gas behavior
4. Henry's law is applicable for gas–liquid interface
5. Laminar flow for gas and liquid phases in the HFMC
6. Cross sectional area of the HFMC is based on Happel's free surface model

The steady-state continuity equation for mass transport of $CO_2$ in each three parts of the model (Tube – Membrane - Shell) respectively is written in equation (1), (2), and (3) [5]:

$$D_{i-tube}\left[\frac{\partial^2 C_{i-tube}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{i-tube}}{\partial r}+\frac{\partial^2 C_{i-tube}}{\partial z^2}\right]=V_{z-tube}\frac{\partial C_{i-tube}}{\partial z}-R_i \quad (1)$$

$$D_{CO_2-shell}\left[\frac{\partial^2 C_{CO_2-shell}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{CO_2-shell}}{\partial r}+\frac{\partial^2 C_{CO_2-shell}}{\partial z^2}\right]=V_{z-shell}\frac{\partial C_{CO_2-shell}}{\partial z} \quad (2)$$

$$D_{i-membrane}\left[\frac{\partial^2 C_{i-membrane}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{i-membrane}}{\partial r}+\frac{\partial^2 C_{i-membrane}}{\partial z^2}\right]=0 \quad (3)$$

where $C_i$ (mol/m$^3$), $R_i$ (mol/m$^3$ s), and V (m/s) are concentration, reaction rate of species *i*, and the velocity respectively, where r and z also refer to radial and axial coordinates.

The reaction system of $CO_2$-MEA-H2O involves a scheme of reversible and consecutive reactions in the liquid phase the main reactions of $CO_2$ absorption in liquid phase are.

What we are looking for is the concentration of $CO_2$ on the tube side, as written in equations (1), (2), and (3), the velocity of the fluid is unknown too, firstly we need to determine the velocity distribution. Velocity distribution in the tube side is obtained from momentum and the continuity equations, which are coupled and solved simultaneously. By obtaining velocity distribution, the concentration distribution of the solutes will also be determined.

**Simulation**

In order to simulate the $CO_2$ absorption phenomena in the HFMC system, the COMSOL Multiphysics software is utilized. The modeling is based on 2D axisymmetric formulation, contains three domains. As shown in Figure 3, the inlet of liquid and gas is determined as counter-current flow. In a meshed model of this work the parameters of system is shown and the amounts of parameters is categorized in Table 2.



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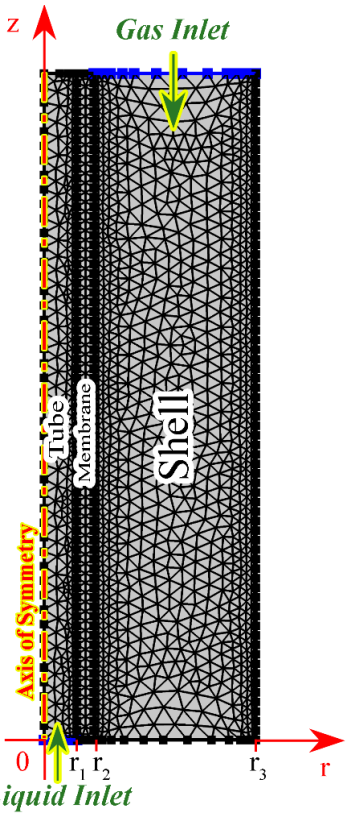


**Figure 3.** The meshed geometry that is used in the HFMC system simulation in COMSOL Multiphysics software.

**Table 2**
Specifications of hollow fiber membrane contactor.

| Parameters | Symbol | Value(s) |
|---|---|---|
| Fiber material | pp | *Polypropylene* |
| Number of fibers | n | *3000* |
| Fiber length (cm) | L | *20* |
| Fiber inner radius ($\mu m$) | $r_1$ | *100* |
| Fiber outer radius ($\mu m$) | $r_2$ | *150* |
| Module inner diameter (cm) | R | *3.5* |
| Gas flow rate (ml/min) | $Q_g$ | *400-800* |
| Liquid flow rate (ml/min) | $Q_l$ | *400-800* |
| Henry coefficient | H | *0.67* |
| Absorbent density (kg/$m^3$ ) | $\rho$ | *999.22* |
| Absorbent viscosity (Pa.s) | $\mu$ | *994.74* |
| Reaction rate coefficient ($m^3$/s.mol) | K | *6.2* |

The liquid absorbent flows in the tube side, whereas the pollute gas ($CO_2$) flows in shell side of the HFMC. Velocity distribution is used for the gas and liquid flow was determined from Navier–Stokes equations. To obtain the concentration profile, an axial and radial diffusions were considered in model equations. The boundary conditions for solving the governing equations are mentioned above are given in Table 3.

**Table 3**
Boundary conditions in the simulation of HFMC system.

| | r = 0 | r = $r_1$ | r = $r_2$ | r = $r_3$ | Z = 0 | Z =L |
|---|---|---|---|---|---|---|
| Tube | Axial symmetry | $C_t$=$H * C_m$ | - | - | $C_g$=0 | Convective flux |
| Membrane | - | $C_m$= $C_t$/H | $C_m$=$C_g$ | - | Isolated | Isolated |
| Shell | - | - | $C_g$=$C_m$ | Isolated | P=$p_{atm}$ | $C_{in-shell}$= 9 molar |





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To estimate the shell radius ($r_3$), Happel's free surface model can be used. Free surface radius ($r_3$) can be calculated by equation (4) [6]:

$$r_3 = \left(\frac{1}{1-\phi}\right)^{1/2} r_2 \quad (4)$$

Where $\phi$ is volume fraction of the void section. It can be calculated by equation (5):

$$1 - \phi = \frac{nr^2}{R^2} \quad (5)$$

Where n and R represent the number of fibers and the inner radius of the modules, respectively. They are defined in Table 2. To calculate Henry coefficient (H), absorbent density ($\rho$), and absorbent viscosity ($\mu$), we need the molar concentration of the inlet MEA ($0.001(mol/m^3)$). By using the molar of inlet MEA and the tables that are available from recent researches, the amount of H, $\rho$, and $\mu$ is calculated.

As mentioned before, the aqueous MEA solution is reacting with $CO_2$ and absorbs it from the gas of the membrane side. This chemical reaction follows equation (6) and (7) [10] and the rate of this reaction can be calculated using equation (8). In the reaction term that is defined in the tube side of HFMC, K is the reaction rate coefficient and its value is given in Table 2.

$$CO_2 + OH^- \leftrightarrow HCO_3^- \quad (6)$$

$$CO_2 + MEA + H_2O \leftrightarrow MEACOO^- + H_3O^+ \quad (7)$$

$$R = K \times C_{CO_2} \times C_{MEA} \quad (8)$$

## Results and Discussion

### Velocity plots

The velocity profile of gas that are obtained from Navier-Stokes equations is shown in Figure 4 (a) for 500 ml/min gas flow rate in the shell side. These velocities are used in the diffusion equations as the convection terms. As stated before, the gas flow is considered fully developed from the inlet to the outlet. Thus, the profile doesn't vary with the variation of z coordinate. But as seen in Figure 4 (b) the velocity changes along the r axis and the profile is approximately parabolic as expected for the fully developed flow regimes. This figure shows the velocity profile for the minimum and the maximum considered gas flow rates [11].

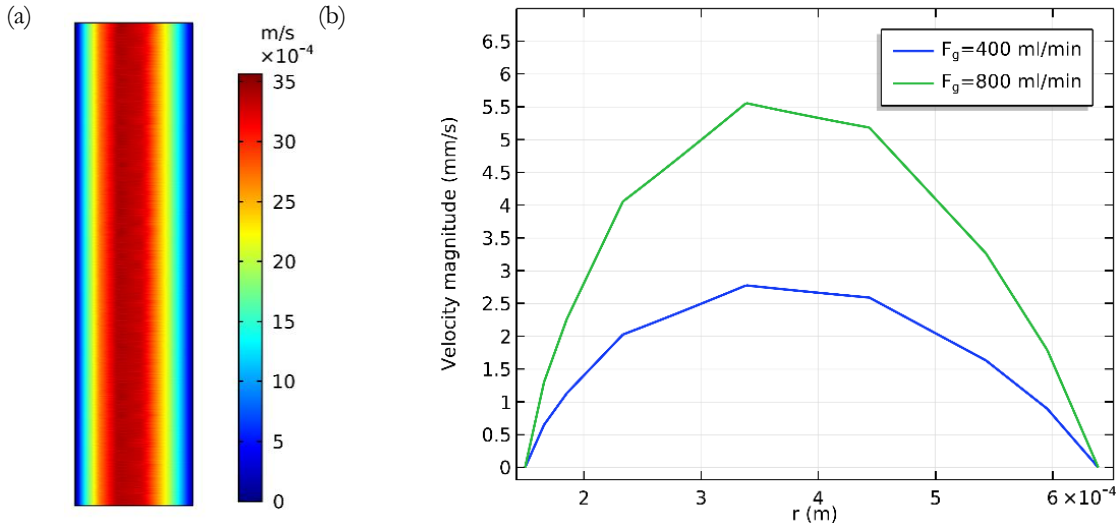


**Figure 4.** (a) The velocity profile in the shell side for $F_g$=500 ml/min and (b) The parabolic velocity profile of the gas at z = 0 for the minimum (400 ml/min) and the maximum (800 ml/min) gas flow rates.

### $CO_2$ concentration distribution in the HFMC

The dimensionless $CO_2$ concentration profile of three domains (Tube - Membrane - Shell) is shown in the Figure 5. When the gas mixture enters in the shell side of the HFMC, with highest concentration of $CO_2$ at z=L, the absorbent liquid enters on the counter side at z = 0 of the tube, where the concentrations of $CO_2$ is assumed to be zero. As the gas and liquid move in opposite directions, due to the concentration difference, $CO_2$ moves to the membrane by diffusion mechanisms so the $CO_2$ concentration of the gas decreases because of the physical and chemical reaction of the absorbent liquid.

At all there are two mass transfer mechanism, convection and diffusion. There is fluid flow in the z-





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direction so the predominant mass transfer mechanism is convection in z-direction, while in the r-direction, because of large concentration differences, diffusion occurs.

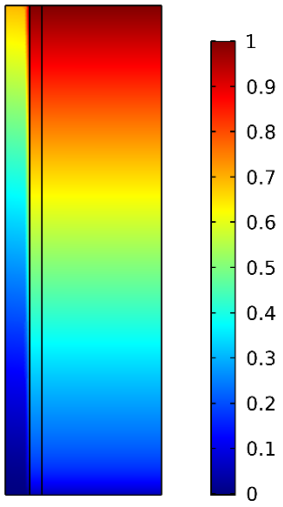


**Figure 5.** Concentration profile of $CO_2$ in the HFMC simulation for $F_g$=500 ml/min and $F_L$=600 ml/min.

**Effects of liquid flow rate and gas flow rates on $CO_2$ absorption**

As is shown in Figure 6 (a), increasing the liquid flow rate increases the $CO_2$ removal percentage. Generally, increasing the liquid flow rate, enhances the concentration variation of $CO_2$ and absorbent in the liquid phase so the mass transfer increases and in the result the $CO_2$ removal percentage increases [12], on the other hand by increasing the liquid flow rate, fresh MEA replaces in tube and the probable of the absorption increases, so the $CO_2$ removal percentage improves again. On the contrary, in the case of chemical absorption gas phase is the controlling phase, because the mass transfer resistance of gas phase is more significant with respect to mass transfer resistance of liquid phase, so increasing the gas flow rate decreases the residence time of gas phase in the HFMC, and reduces the percentage of $CO_2$ removal [5]. It's observable in the Figure 6 (b).

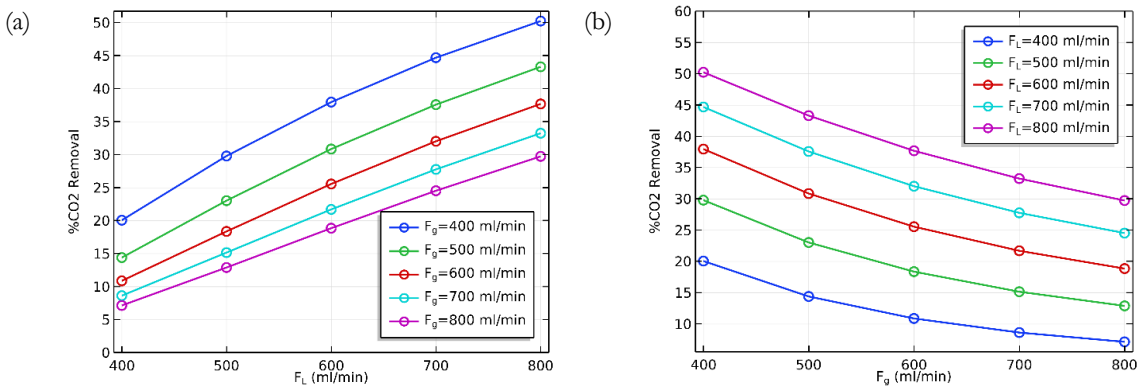


**Figure 6.** Variation of the percentage of $CO_2$ removal versus (a) liquid flow rate $F_L$ and (b) gas flow rate $F_g$.

**Conclusion**

Chemical absorption of $CO_2$ in a HFMC system is presented in this work. For simulating a chemical absorption of $CO_2$, a 2D mathematical model was proposed. The MEA aqueous solution was considered as absorbent liquid. The steady-state continuity equation of mass transport and momentum and the continuity equations are coupled in all domains to find the $CO_2$ concentration on different positions. The concentration profile of $CO_2$ and velocity plots are shown. At the end the effect of gas and liquid flow rates indicates that by increasing liquid flow rate the percentage of $CO_2$ removal increases too, but by increasing gas flow rate the $CO_2$ removal percentage





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decreases. This simulation can be provided for complex chemical reaction schemes.

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