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Liquid-liquid extraction process for gas separation from water in polymeric membrane: Mathematical modeling and simulation

Nahid Salimi [1], Sadegh Moradi [1], Afsaneh Fakhar [2] and Seyed Mohammad Reza Razavi [*2]

[1] *Department of Chemical Engineering, Faculty of Engineering, Arak University, Arak, Iran*
[2] *Young Researchers and Elite Club, South Tehran Branch, Islamic Azad University, Tehran, Iran*

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Abstract. In this study, application of polypropylene hollow fiber membrane contactors for CO_2 removal from water in liquid-liquid extraction (LLE) mode was simulated. For this purpose, a steady state 2D mathematical model was developed. In this model axial and radial diffusion was considered to CO_2 permeation through the hollow fibers. CO_2 laden water is fed at a constant flow rate into the lumen side, permeated through the pores of membrane and at the end of this process, CO_2 solution in the lumen side was extracted by means of aqueous diethanolamine (DEA) and chemical reaction. The simulation results were validated with the experimental data and it was found a good agreement between them, which confirmed the reliability of the proposed model. Both simulation and experimental results confirmed the reduction in the percentage of CO_2 removal by increment of feed flow rate.

Keywords: carbon dioxide; hollow fiber; DEA; diffusion; liquid-liquid extraction; simulation

1. Introduction

The reasons of the presence of CO_2 in natural water can be atmospheric absorption of CO_2, breathing of sea creatures, marine plant photosynthesis and decomposition of organic compounds in water. Although the presence of CO_2 in water is mostly due to natural phenomena, amount of CO_2 is increased significantly because of pumping industrial sewage into the water. High concentration of CO_2 (> 0 mg/l) in water can threat marine life (Hope *et al*. 1995, Vinci *et al*. 2004). Industrial production of solution and vapor of ammonia and urea also leads to production of sewage with high concentration of CO_2. So CO_2 separation from water is become an important issue in recent years. Industrial and usual processes used for CO_2 separation are faced with some frequently reoccurring problems such as loading, channeling, foaming, flooding and also are not cost-effective (Al-Marzouqi *et al*. 2008). In recent years, researches have been focused on application of hollow fiber membrane contactors (HFMCs) which are able to degasify liquids and resolve the most of the mentioned problems and limitations. Membrane contactor has several advantages compared to common processes such as higher mass transfer rates, independent control of gas and liquid rates, known and constant interfacial area and easy scale up (Mohammadi *et al*. 2016, Miramini *et al*. 2013, IPCC 2005, Wang *et al*. 2004, Razavi *et al*. 2015a, c, Lu *et al*. 2005,

*Corresponding author, Ph.D. Researcher, E-mail: mohammadreza.razavi@ce.iut.ac.ir

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Jun *et al*. 2015, Zhang *et al*. 2006, Keshavarz *et al*. 2008, Razavi and Miri 2015). Because CO_2 is an acid gas, chemical absorption using organic amines for CO_2 capture has evaluated by many authors (Lu *et al*. 2005, Sayari and Belmabkhout 2010, Hoff *et al*. 2004, Olajire 2010, Mondal *et al*. 2012). The methods that have been widely designed allow the CO_2 separation by absorption in alkanolamines solution in contactor (IPCC 2005, Lu *et al*. 2005, Paul *et al*. 2007). In order to gain a better understanding of CO_2 absorption in a HFMC, some researchers have been working on the modeling and simulation of CO_2 capture and studied some variables which are affective on the removal of CO_2. Since using simulation of CO_2 removal from mixtures is more cost-effective and prevents wasting money on doing different experiments, researchers have been tending to use it for the separation studies (Zhang *et al*. 2006, Hoff *et al*. 2004, Paul *et al*. 2007). Hoff investigated the effect of CO_2 partial pressure, liquid CO_2 loading, liquid velocity and temperature on the flux of the CO_2 absorption rate by using aqueous solutions of monoethanolamine (MEA) and methyldiethanolamine (MDEA) as the absorbents (Hoff *et al*. 2004). A theoretical simulation was performed to study CO_2 capture by three typical alkanolaminesolutions of 2-amino-2-methyl-1-propanol (AMP), diethanolamine (DEA) and methyldiethanoamine (MDEA) in a HFMC. Simulation results indicated that liquid flow velocity, initial liquid concentration, the fiber length and fiber radius affect the CO_2 absorption significantly (Wang *et al*. 2004). In addition, Lu studied the effects of 2-Amino-2-methyl-1-propanol (AMP) and piperazine (PZ) activators on mass-transfer enhancement in a HFMC. The Activators showed effective enhancement in mass-transfer of membrane gas absorption (Lu *et al*. 2007). A two-dimensional mathematical model was developed by Al-Marzouqi for the permeation of CO_2 through HFMCs. That model considered axial and radial diffusion inside the fiber, through the membrane, and within the shell side of the contactor. The modeling results showed that the removal of CO_2 increased by enhancement of solvent concentration and liquid velocity. On the contrary, higher temperatures resulted in little effect on the rate of removal (Al-Marzouqi *et al*. 2008). It is notable that the methods involving gas–liquid contactors have operational drawbacks such as loading and flooding in the column. Therefore, liquid-liquid extraction has received more attention, recently (Agrahari *et al*. 2011). HFMC systems in LLE mode, have been used successfully in refinery systems. For example, Mansourizadeh used polyvinylidene fluoride (PVDF) hollow fiber membrane contactor for CO_2 stripping from water and investigated the effect of different operating conditions on the CO_2 stripping efficiency. In our previous studies, CO_2 capture from gas mixtures and natural gas in nanoporous and porous membranes was simulated (Fazaeli *et al*. 2015, Razavi *et al*. 2013, Tahvildari *et al*. 2015, Razavi *et al*. 2015a). Owing to very few studies done on removal of CO_2 from water under liquid–liquid extraction mode, this object was selected for this research. Since reaction of secondary amines with CO_2 is considerably faster than that with tertiary amines (Rinker *et al*. 1996), in this study secondary amine DEA are used as extractor liquid for CO_2 separation. The effect of operating conditions on the separation was studied and compared with experimental data.

2. Simulation

2.1 Model domain for simulation

In this work a two-dimensional mathematical model was developed for the CO_2 capture from water through hollow fiber membrane contactors (HFMCs). The separation of CO_2 using DEA as an absorbent in a non-aligned flow hollow fiber membrane contactor was studied. The mass

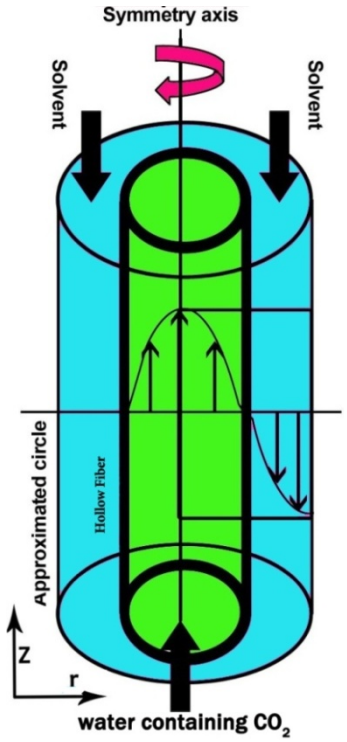


Fig. 1 The mass transfer model used for modeling (Razavi *et al*. 2016)

transfer model used for modelling is shown in Fig. 1. As shown in Fig. 1 hollow fiber is fed by water containing CO_2 from a tank at constant flow rate and shell is fed by DEA at constant flow rate in a non- aligned way. The molecules of CO_2 are separated from water and permeate through the pores filled with air. To keep DEA in high concentration, it is assumed CO_2 molecules are reacted quickly with DEA and make no change in extracting phase resistance. Therefore, CO_2 concentration is decreased exponentially from an initial level in the tank. The output water which is free of CO_2 is recycled continuously and returned to the tank. The HFMC consists of three sections: lumen side, membrane and shell side. The steady state 2- dimensional model is applied for each section.

2.2 The characteristics of module and membrane

Hollow fibers membrane contactor was made of PP. Characteristic parameters of the membrane are given in Table 1.

2.3 Equations of the model

2.3.1 Species balance on the lumen side

The fully developed tubular flow of a liquid was assumed. The velocity profile is parabolic that allowing for diffusion in the axial and radial direction on the tube. 2D Geometry and steady state for species balance was considered, Eq. (1) under such condition can be written as follows (Bird *et al*. 1960)

Table 1 HFMC physical properties and set up operation (Criscuoli *et al*. 2003)

Parameter	Value	Reference	Parameter	Value	Reference
Inner fiber radius (μm)	120	-	Solvent flow rate (L/m)	1.5	-
Outer fiber radius (μm)	150		Feed flow rate (L/m)	(0.2, 0.5, 0.8)	-
ε (porosity %)	40				-
τ (tortuosity)[a]	2.5				(Versteeg *et al*. 1998)
Number of fibers	10200		Henry's law constant, $m = 1/H$	$H = 2/82\times10^{-6}$ $\exp(-2044/T)/(RT)$	(Versteeg *et al*. 1998)
Fiber length (cm)	25	-	$D_{co2\text{-}lumen}$	$1.92*10^{-9}$	
Temperature (K)	298	-			

[a] $\tau = 1/\varepsilon$

$$D_{CO_2-tube}\left[\frac{\partial^2 C_{CO_2-tube}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{CO_2-tube}}{\partial r}+\frac{\partial^2 C_{CO_2-tube}}{\partial z^2}\right]=V_{z-tube}\frac{\partial C_{CO_2-tube}}{\partial z} \tag{1}$$

Where r and z denote the radial and axial coordinates, respectively. In Eq. (1) $D^{CO_2\text{-tube}}$ and C refers to diffusion coefficient of CO_2 into water and the concentration of solute (CO_2) in water at the temperature and pressure of system, respectively. The velocity profile in the lumen side under laminar flow is obtained (Bird *et al*. 1960) by

$$v_z(r)=2\overline{V}\left[1-(\frac{r}{r_1})^2\right] \tag{2}$$

Where $\overline{V}$ is the average velocity in the lumen, r is the radial distance, v_z is the velocity of stream at r and r_1 is the inner radius of the lumen. The average velocity in the lumen can be defined as

$$\overline{V}=\frac{Q}{N\pi r_1^2} \tag{3}$$

Where Q is flow rate of feed and N is number of fibers.

Boundary conditions considered for the lumen side are as follows

$$at\ z=0 \quad c_{co2-Lumen}=c_{o,co2} \tag{4}$$

$$at\ z=L \quad Convective\ \ Flux \tag{5}$$

$$at\ r=r_1 \quad c_{co2-lumen}=c_{co2-membrane} \tag{6}$$

$$at\ r=0 \quad \frac{\partial c_{co2-Lumen}}{\partial r}=0 \qquad \text{(symmetry)} \tag{7}$$

2.3.2 Membrane equations

CO_2 transmission into the membrane pores is just conducted by diffusion mechanism. The continuity equation will be simplified by steady state and no reaction assumptions as follows (Bird *et al*. 1960)

$$D_{CO_2-membrane}\left[\frac{\partial^2 C_{CO_2-membrane}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{CO_2-membrane}}{\partial r}+\frac{\partial^2 C_{CO_2-membrane}}{\partial z^2}\right]=0 \tag{8}$$

In which boundary conditions can be written as follows

$$at\ r=r_1 \qquad c_{co2-membrane}=c_{co2-Lumen} \tag{9}$$

$$at\ r=r_2 \quad c_{co2-membrane}=c_{co2-shell/m}\ \ (base\ on\ Henry's\ law) \tag{10}$$

$$at\ z=0 \quad \frac{\partial c_{co2-membrane}}{\partial r}=0 \qquad \text{(isolation)} \tag{11}$$

$$at\ z=0 \quad \frac{\partial c_{co2-membrane}}{\partial r}=0 \qquad \text{(isolation)} \tag{12}$$

2.3.3 Shell side equations

The steady-state continuity equation in the shell side is expressed as below (Bird *et al*. 1960)

$$D_{CO_2-Shell}\left[\frac{\partial^2 C_{CO_2-Shell}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{CO_2-Shell}}{\partial r}+\frac{\partial^2 C_{CO_2-Shell}}{\partial z^2}\right]=V_{z-Shell}\frac{\partial C_{CO_2-Shell}}{\partial z}-R_{CO_2} \tag{13}$$

As stated before, by solving Navier-Stokes equation, velocity distribution in the shell side can be obtained by (Bird *et al*. 1960)

$$\begin{aligned}&-\nabla.\eta\left(\nabla V_{z-Shell}+\left(\nabla V_{z-Shell}\right)^T\right)+\rho\left(V_{z-Shell}.\nabla\right)V_{z-Shell}+\nabla p=F\\&\nabla V_{z-Shell}=0\end{aligned} \tag{14}$$

V (m/s), P (Pa), ρ (kg m^{-3}), η (kg m^{-1} s^{-1}) and F (N) denote velocity, pressure, density, dynamic viscosity and body force, respectively. The shell radius can be estimate by applying Happel free surface model (Happel 1959)

$$r_3=\left(\frac{1}{1-\phi}\right)^{1/2}\mathrm{r}_2 \tag{15}$$

Where r_2 indicate the tube outer radius. Φ is volume fraction of void section and can be defined by

$$1-\phi=\frac{nr^2}{R^2} \tag{16}$$

Where n and R^2 are the number of fibers and inner radius of modules, respectively.
Boundary conditions used for the shell are as follows

$$at \quad r=r_2 \quad c_{co2-shell}=c_{co2-membrane}*m \tag{17}$$

$$\text{(isolation)} \qquad at \quad r=r_3 \quad \frac{\partial c_{co2-shell}}{\partial r}=0 \tag{18}$$

$$at \qquad z=L \quad c_{co2-shell}=0 \tag{19}$$

$$at \quad z=0 \quad Convective \quad Flux \tag{20}$$

2.3.4 DEA equations in shell side

The steady state continuity equation for DEA absorber is written as follows

$$D_{i-shell}\left[\frac{\partial^2 C_{i-shell}}{\partial r^2}+\frac{1}{r}\frac{\partial C_{i-shell}}{\partial r}+\frac{\partial^2 C_{i-shell}}{\partial z^2}\right]=V_{z-shell}\frac{\partial C_{i-shell}}{\partial z}-R_i \tag{21}$$

R_i denotes the chemical reaction between CO_2 and DEA absorber. Boundary conditions required for solving Eq. (21) is given as follows

$$at \quad z=L \quad c_{DEA-shell}=c_{M0} \tag{22}$$

$$at \quad z=0 \quad Convective\ Flux \tag{23}$$

$$at \quad r=r_2 \quad \frac{\partial c_{DEA-shell}}{\partial r}=0 \qquad \text{(isolation)} \tag{24}$$

$$at \quad r=r_3 \quad \frac{\partial c_{DEA-shell}}{\partial r}=0 \qquad \text{(symmetry)} \tag{25}$$

4. Numerical solution

The equations related to the lumen side, the membrane, the shell side, with the appropriated boundary conditions were solved using COMSOL Multiphysics version 4.2 software, which uses finite element method for numerical solutions of the model equations. The finite element analysis

is combined with adaptive meshing and error using numerical solver of UMFPACK version. The applicability and accuracy of UMFPACK for solving membrane equations have been asserted by some researchers (Ghadiri *et al*. 2013a, b, Bishnoi and Rochelle 2000, Shirazian *et al*. 2009, Tahvildari *et al*. 2015, Fadaei *et al*. 2011).

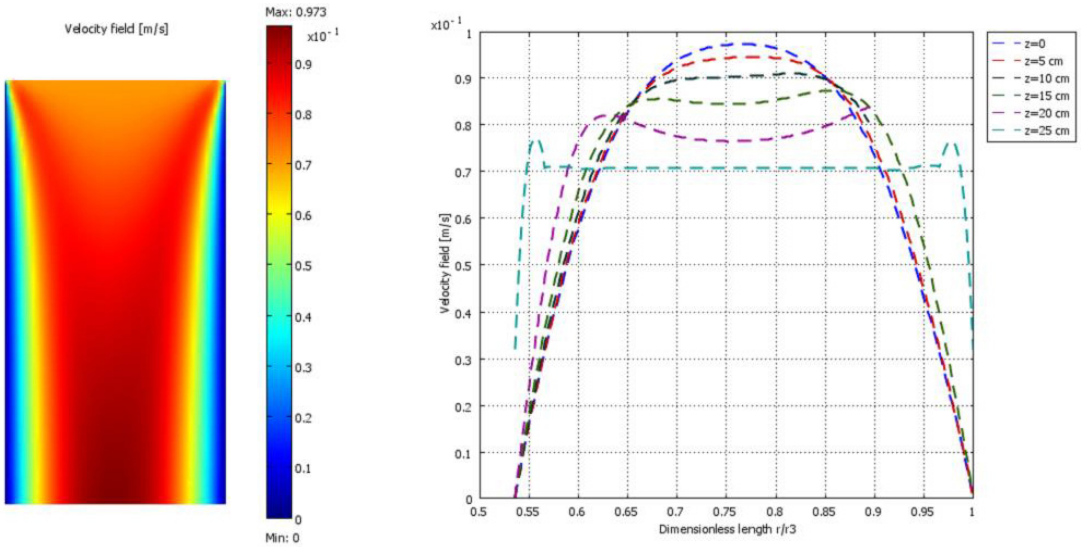
5. Result and discussion

5.1 Model validation

Simulation results for CO_2 removal from water has been compared with experimental data based on Table 2. This comparison was done by using experimental data of Agrahari's research (Agrahari *et al*. 2011) for 300 ppm CO_2 concentration contained feed. The percent removal of CO_2 decreases with increasing feed flow rate. The maximum removal (approximately 95%) obtained at the lowest feed flow rate (0.2 L/min) (The removal decreases to approximately 90% at 0.8 L/min) (Agrahari *et al*. 2011). Furthermore, according to Table 2 good correlation is seen between

Table 2 Compression between the percent removal of CO_2 by simulation and experimental study (Agrahari *et al*. 2011)

Solvent flow rate (L/min)	Feed flow rate (L/min)	Experimental (Co_2%)	Simulation (Co_2%)
1.5	0.2	0.95	0.92
1.5	0.5	0.92	0.88
1.5	0.8	0.9	0.87



(a) (b)

Fig. 2 (a) Velocity field in the shell side of HFMC; (b) Velocity profiles in the shell side along the membrane different length. Feed flow rate = 0.5 L/min; solvent(DEA) flow rate = 1.5 L/min; CO_2 inlet concentration = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/ L; T = 298 K

simulation and experimental results of percent removal of CO_2 and there is a same trend in variation of CO_2 capture by changing feed flow rate in both studies. This agreement ensures the efficiency of this model for larger scales.

5.2 Velocity distribution

The velocity field and its profile in the shell side of hollow fiber membrane, where the absorbent flows, are shown in Figs. 2(a) and (b). The velocity profile in the shell side was simulated by solving the Navier-Stoks equations. The velocity profile is almost parabolic and the maximum velocity is appeared at the center of the shell. Moreover, velocity is zero on the two shell walls due to assumed no-slip conditions. Figs. 2(a) and (b) also display that velocity profile becomes fully developed after a short distance from the entrance of the shell side.

5.3 Concentration distribution of CO_2 in the HFMC

The dimensionless concentration of CO_2 (c/c_0) in the lumen side, the membrane and the shell side of the HFMC are shown in Fig. 3. The feed containing CO_2 flows from one side of the HFMC (z = 0) where the concentration of CO_2 is the maximum. Liquid solvent (DEA) flows from the other side ($z = L$) where the concentration of feed is assumed to be zero. As the CO_2 flows through the lumen side, it is transferred towards the membrane due to concentration difference (driving force) (Shirazian *et al*. 2009). The mechanisms of mass transfer in the lumen and shell sides are convection and diffusion. The mechanism of convection in the z-direction is axial, while the mechanism of diffusion in the r- direction is radial. Gas mixture is transferred to the other side through the membrane pores and the mobile solvent in the shell side can absorb the CO_2.

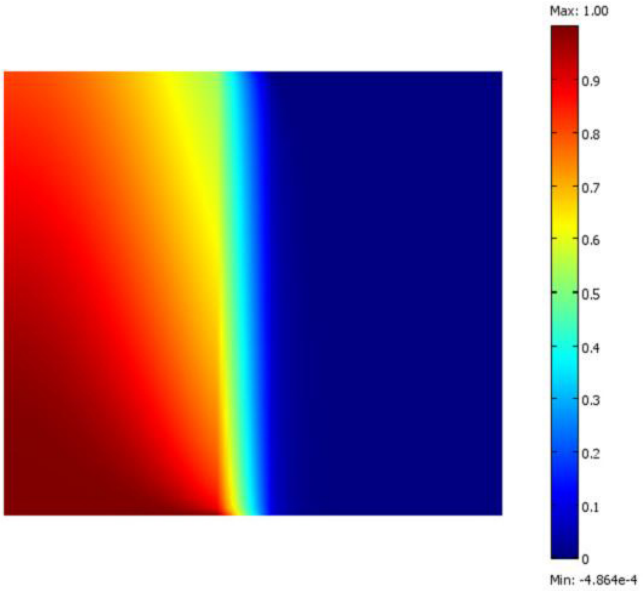


Fig. 3 Concentration distribution of CO_2 in the HFMC, feed flow rate = 0.5 L/min; solvent flow rate = 1.5 L/min; CO_2 inlet concentration = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/ L; T = 298 K

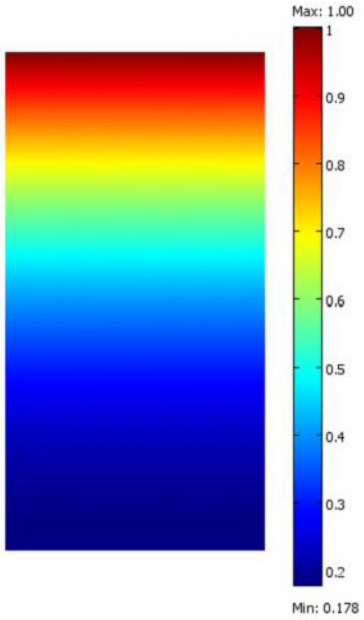


Fig. 4 Dimensionless concentration distribution of DEA in the shell side of the HFMC, feed flow rate = 0.5 L/min; solvent flow rate = 1.5 L/min; CO_2 inlet concentra-tion = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/L; T = 298 K

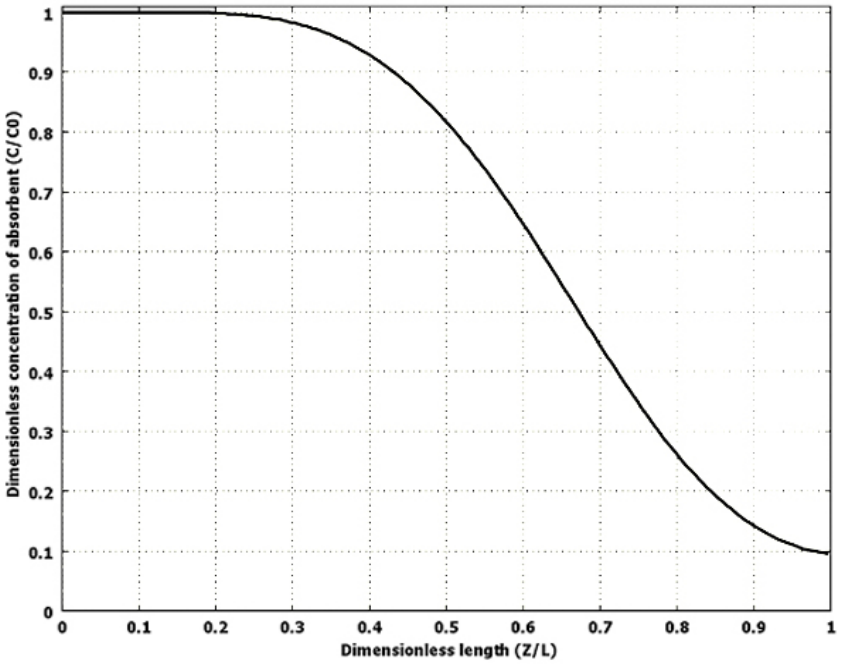


Fig. 5 Axial concentration distribution of DEA along the HFMC, feed flow rate = 0.5 L/min; solvent flow rate = 1.5 L/min; CO_2 inlet concentration = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/L; T = 298 K

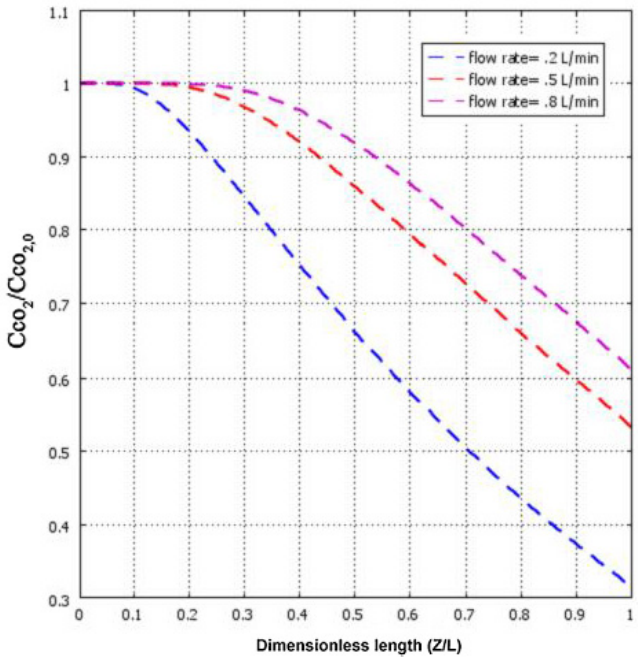


Fig. 6 Dimensionless CO_2 outlet concentration profile of at the different flow rate of feed; solvent flow rate = 1.5 L/min; CO_2 inlet concentration = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/L; T = 298 K

5.4 Concentration distribution of DEA in the HFMC

Fig. 4 represents dimensionless concentration distribution of amine (DEA) in the shell side of the HFMC. The amine solution flows through the shell side and reacts with CO_2 which come from the membrane pores due to the concentration difference between the two sides of the membrane. The amine concentration decrease significantly in the interface zone. Fig. 5 indicates axial concentration distribution of DEA along the contactor. Since CO_2 concentration in the entrance of shell side is negligible, the absorber concentration is reduced in the middle of HFMC length faster than the entrance region of HFMC.

5.5 Effects of feed flow rate on CO_2 outlet concentration

Fig. 6 displays dimensionless concentration of CO_2 along the tube side at different flow rates of feed stream. Enhancement of feed flow rate results in reduction of feed residence time in the tube and as a result absorption rate of carbon dioxide declines. C_{outlet} (mol/m^3) is calculated by integrating the local concentration at the outlet of the lumen side ($z = L$)

$$c_{outlet} = \left. \frac{\int_{r=0}^{r=r_1} \int c(r) dA}{\int_{r=0}^{r=r_1} \int dA} \right|_{z=L} \tag{26}$$

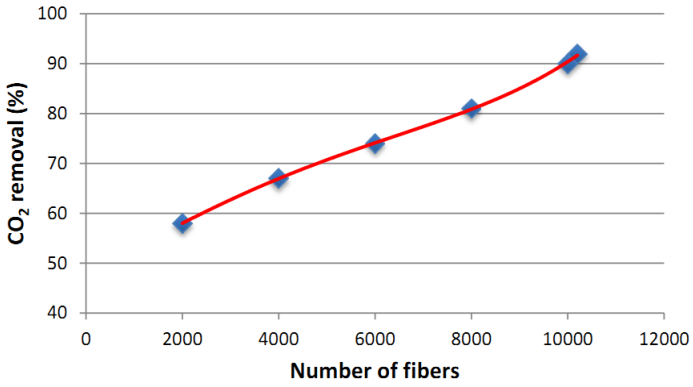


Fig. 7 Effect of fiber number on CO_2 removal(%). solvent flow rate = 1.5 L/min; CO_2 inlet concentration = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/L; T = 298 K

Based on Fig. 6, CO_2 concentration drops suddenly due to high reaction with the solvent (DEA) and by reduction of feed flow rate, decline in dimensionless concentration is enhanced.

5.6 Effect of Number of Fibers on the Removal of CO_2

Number of fibers as an important factor on performance of membrane contactors has been shown in Fig. 7. In this Figure, CO_2 removal on outlet increases by grows in number of fibers. As in number of 10200, maximum amount of CO_2 removal has been obtained. This is due to increase of mass transfer area between CO_2 and DEA, by increase in number of fiber.

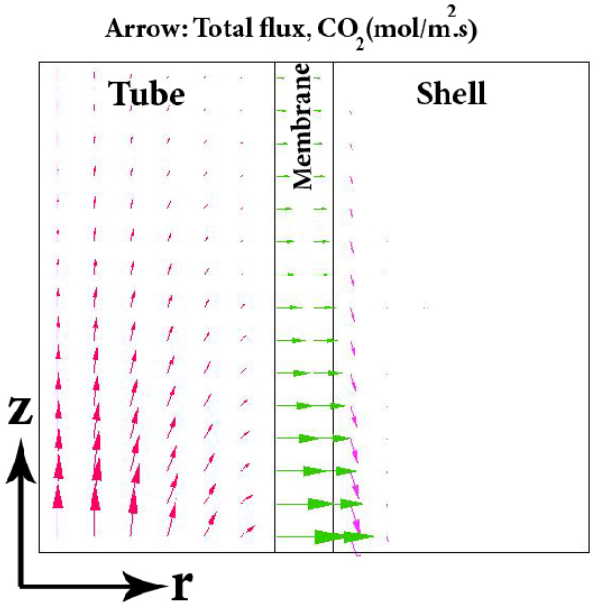


Fig. 8 Vector of total flux for CO_2 in the membrane contactor. solvent flow rate = 1.5 L/min; CO_2 inlet concentration = 6×10^{-3} mol/L; DEA inlet concentration = 1 mol/L; T = 298 K

5.7 Total flux for CO_2 in the three section of membrane contactor

Fig. 8 mention the vector of carbon dioxide concentration in the membrane contactor. It is clearly illustrated that CO_2 mass transfer flux reduces along the membrane module that due to carbon dioxide removal by DEA. Moreover, variation rate of CO_2 concentration along the contactor is significant which confirms the capability of membrane contactor as a good process for CO_2 capture.

4. Conclusions

In this study chemical absorption of CO_2 in amine solution DEA in hollow fiber membrane contactor was investigated. A 2-dimensional geometry was used to describe CO_2 removal process. Simulation results showed that CO_2 removal was completely done by DEA, and the results were validated with the experimental data. The modeling showed a good agreement between simulation and experimental results. The effect of feed flow rate on CO_2 removal from water was also studied. Absorption rate of carbon dioxide declined by increase of feed flow rate, enhancement of feed flow rate results in reduction of feed residence time in the tube and as a result absorption rate of carbon dioxide declines. This agreement ensures the efficiency of this model for larger scales.

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