Modeling and simulation of CO_2 stripping from monoethanolamine solution

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Abstract
In this research, a mathematical model based on the finite volume analysis is proposed to simulate the flow and concentration in a hollow fiber Polytetrafluoroethylene (PTFE) membrane contactor for CO_2. To develop this model, the membrane contactor is divided into three parts including the tube, shell and membrane. Then, to validate and test the model, the obtained results are compared with the experimental data reported in open literature. It is confirmed that the simulation results are in good agreement with the actual data. Moreover, by considering the mass transfer resistances in studied system, it is found that the gas phase mass transfer resistance in gas stripping membranes has a minor effect on the CO_2 desorption flux.

Keywords: CO_2 Capture, Modeling & Simulation, membrane contactor

Introduction
Many climate scientists believe that a major cause of climate change is the anthropogenic emission of greenhouse gases (GHGs) such as CO_2 into the atmosphere [1]. In this regard, capturing of CO_2 is probably the most important interests in different industries which can be done by proper management and required technical knowledge. Many sources such as fossil fuel or biomass energy facilities, natural gas processing, and synthetic fuel plants have high potential to capture and stash the CO_2 gas [2]. For example, the natural gas contains significant amounts of CO_2 causing efficiency loss due to the reduction of heating value of gas in power plants. Additionaly, its acidic nature causes corrosion problems in equipment and pipelines [3]. Nowadays, many researchers have proposed the absorption of CO_2 into amine solutions as an effective methods for CO_2 capturing. However, the stripping of CO_2 from amine solvents is the main part of an absorption–stripping process [4-6]. Ghadiri et al. [7] used a polytetrafluoroethylene (PTFE) hollow-fiber membrane for absorption of CO_2 from monoethanolamine solution, and proved that this configuration had a higher CO_2 removal efficiency than the conventional absorption column without any membrane contactors. In fact, using the amine absorption system is the most common way in CO_2 capturing which is applied by Petronas Fertilizer Co. in Malaysia and Sleipner project in Norway capturing

plants [7]. Therefore, modeling and simulating of CO_2 stripping process can be still significant in order to efficiently design and construct such facilities in related industries.
In this study, a system including a membrane contactor for the separation of CO_2 from an amine solution like monoethanolamine is modeled. To do such a task, finite volume scheme as a numerical solution method is applied. Then, in order to validate the proposed methodology, simulation results are compared versus the experimental data reported by Khaisri et al. [8].

Mathematical modeling

To model the transport of CO_2 through the Polytetrafluoroethylene (PTFE) membrane contactors, a mathematical model was derived based on the following assumptions [6,7]:
1. Steady-state and isothermal conditions.
2. The Newtonian fluid with constant physical properties.
3. Constant liquid velocity in the tube side.
4. Henry's law is applicable for gas–liquid interface.
5. Non-wetted condition. It means that the gas phase fills the pores of membrane and liquid cannot penetrate to them.

Fig. 1 shows a schematic diagram for CO_2 stripping in membrane contactor. To develop more simplified model, the single fiber is divided into three parts, i.e. tube side, membrane, and shell side, and then, the 2D mass balances are considered for all of them. The liquid phase enters to the tube side (at z = 0), while the gas phase (pure N_2) is passed through the shell side (at z= L). Therefore, CO_2 is removed from the absorbent by diffusing through the liquid bulk and membrane, and then it is desorbed in the gas phase [7,8]. According to the previous works [5-8], laminar parabolic velocity distribution of liquid phase can be assumed constant due to its meager variation. Therefore, the partial differential equations showing CO_2 transportation through the tube, membrane and shell side can be written as Eq. 1, 2 and 3, respectively.

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

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

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

where i refers to CO_2, and also r and z refer to radial and axial coordinates, respectively.

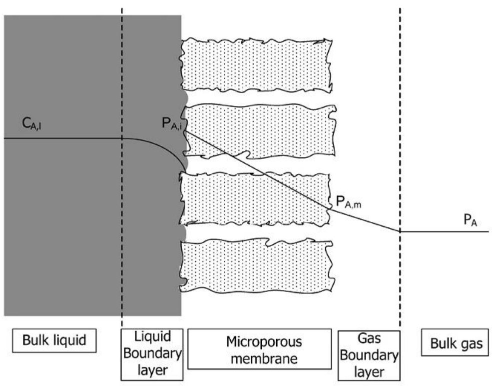


Figure 1. A schematic diagram for CO_2 stripping in membrane contactors [8].

In Equation (5) to (7), the required boundary conditions for solving the Eq.1 (i.e. tube side) are presented, and for the others, the related boundary conditions can be defined similarily [6,7].

$$@\, z = 0, C_{CO_2-tube} = C_{CO_2,0} \qquad @\, z = L, \text{Convective Flux} \tag{5}$$

$$@\, r = 0, \frac{\partial C_{CO_2-tube}}{\partial r} = 0 \tag{6}$$

$$@\, r = R_{in}, C_{CO_2-tube} = \frac{C_{CO_2-membrane}}{m_{Henry}} \tag{7}$$

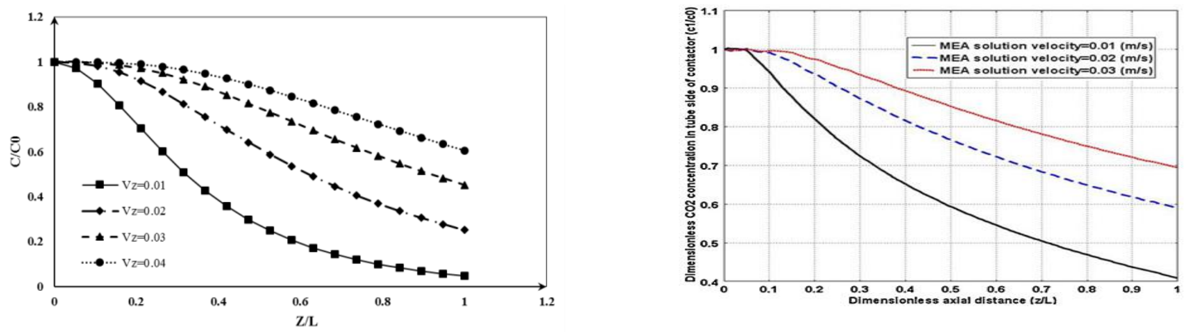
where m is the solubility of gas in the liquid solvent and R_{in}=0.813 is fiber inner radius (mm).

Numerical solution scheme

The presented model were solved using MATLAB software version 2015. In this regard, the finite volume method (FVM) was used for numerical solutions of partial equations proposed in the mathematical model.

Results and discussion

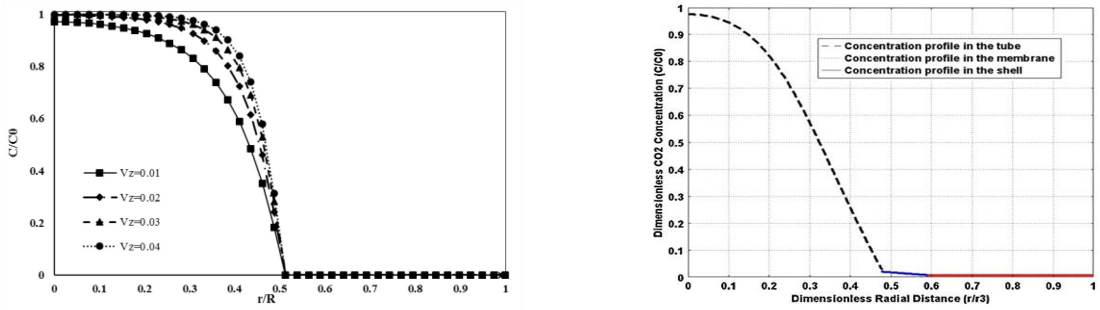
In Fig. 2a, the CO_2 concentration versus the axial length of the system in different values of superficial velocity of MEA is presented. As expected, the increase in the MEA solution velocity reduces the residence time of liquid phase in the module. Also, it reduces the concentration gradient along the length of the module. As seen, the obtained results have a good agreement with experimental data (Fig. 2b).



(a) (b)

Figure 2. concentration of CO_2 in the axial direction (tube side) in different values of MEA solution velocity, numerical solution (a) experimental data (b) [7,8].

Radial concentration profile of CO_2 obtained by solving the model is shown in Fig. 3a. As seen, by increasing the superficial velocity of MEA solution, the radial concentration of CO_2 in the radial axis is ratherly insignificant. Moreover, a sharp decrease in CO_2 concentration can be concluded from this figure. This observation is compatible with the experimental data reported by Ghadiri et al [7] and Khaisri et al [8] (see Fig.3b). The reason for this phenomenon is due to the higher diffusion coefficients of CO_2 inside the membrane pores and the gas phase than those in the tube side (liquid phase). Consequently, mass transfer resistances to CO_2 transport in the membrane and shell sides are much smaller than that of liquid phase. Moreover, these results confirm that the mass transfer resistance of liquid phase is roughly 90% of the overall one. Therefore, the transport phenomena of this system is mainly controlled by the liquid phase which has been proved by the other authors [6-8].



(a) (b)

Figure 3. Concentration of CO_2 in the radial direction in different values of MEA solution velocity, numerical solution (a) experimental data (b) [7,8]

Conclusions

Modeling and simulation are the most important step which should be performed prior to any designing and manufacturing activities. In this work, a mathematical model were applied to simulate CO_2 capturing using the hollow fiber Polytetrafluoroethylene (PTFE) membrane contactors. This model was developed to study stripping of CO_2 from monoethanolamine solutions in which finite volume analysis was adopted to solve the corresponding partial equations. The numerical results showed that the CO_2 stripping flux increased with an increase in the MEA solution velocity. Moreover, by considering the mass transfer resistances in the studied system, it was found that the gas phase mass transfer resistance in gas stripping membranes had a minor effect on the CO_2 desorption flux. Additionally. to validate the model, the simulation results for the stripping of CO_2 using the membrane contactor were also compared versus the reported experimental data in the literature. Results confirmed that the proposed model was capable of simulating the under study sytem with an acceptable accuracy.

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