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# Modelling of $CO_2$ absorption via hollow fiber membrane contactors: Comparison of pore gas diffusivity models

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## HIGHLIGHTS

- Influence of the different gas diffusivity model in membrane contactor was considered.
- Results of the modelling were improved by assuming realistic values for tortuosity.
- Using Wakao et al. model rather than Bosanquet model the prediction was improved.

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## ABSTRACT

This paper discusses the modelling of $CO_2$ absorption in water as an absorbent via a hollow fiber membrane contactor to predict the performance of the absorption process under various operational conditions. The governing equations are two dimensional. Since, the gas diffusion along the pores is responsible for the mass transfer across the membrane thickness, i.e. both the skin layer and the membrane bulk, how to estimate the effective gas diffusivity has a vital degree of importance. When small pores combined with low pressures are dealt with, a challenging issue appears, i.e. the effective gas diffusivity is a contributive phenomenon, in which, several mechanisms are cooperated. Selecting an inappropriate model, inevitably leads to unrealistic values for the tuning parameters. Conventionally, the Bosanquet equation has been widely used for modelling the gas diffusivity through the membrane pores. In the current paper, it is intended to prove that the Bosanquet model is a limiting form of Wakao et al. model, when we are far enough from the continuum region. The modelling results are compared with six sets of different membranes from the open literature including high and low pressures. The results show that, ignoring the viscous flow contribution in $D_{g,eff}$ (the Bosanquet gas diffusivity model) causes underestimation of the absorption flux. Based on the observations, there is a meaningful consistency between the model and the experimental data once the contribution of the viscous flow in $D_{eff}$ (the Wakao et al. gas diffusivity model) is considered.



## 1. Introduction

Development of industrial movement during the last decades resulted in a boundless increase in greenhouse gases best exemplified by carbon dioxide ($CO_2$) which in turn accelerated global warming and severe environmental impacts (Herzog et al., 2000; Rongwong et al., 2013). Several technologies have been used for $CO_2$ removal, namely absorption, adsorption, calcium looping (CaL), chemical looping combustion (CLC) and membrane processes (Mansourizadeh and Ismail, 2009; Gabelman and Hwang, 1999; Li and Chen, 2005). In the field of membrane processes, membrane contactor (MC) as an alternative technology, due to proposing high contact area and independence of gas and liquid flow rates exhibits superior potential with respect to the conventional processes (Sea and Park, 2002). The modelling of MC hollow fibers is important because it is aimed at better understanding the unseen parameters which affect the final performance of MCs, such as pore wetting, gas diffusivity along the skin pores and so forth. The gas absorption via a MC based on diffusion-reaction model was studied by Karror and Sirkaras as an initiative research group. They investigated a series of comprehensive experiments of

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gas-liquid absorption in a shell and tube MC in a parallel flow configuration by using pure $CO_2$, pure $SO_2$, $CO_2$-$N_2$ and $CO_2$-air mixtures and pure water as absorbent. They simulated this absorption processes with numerical model considering a laminar flow velocity profile for liquid in lumen side and the Happel model for gas in shell side. In final, a good agreement between the modelling results and the experimental data was reported in most cases (Karoor and Sirkar, 1993). In another work, Bakhshali et al. proposed a model for simulation of $CO_2$ absorption in a MC in a non-wetting mode, considering an axial and radial diffusion simultaneously in both the lumen and the shell side in a counter-current gas-liquid contact. They considered a turbulent velocity profile for the liquid. Their results by employing computational fluid dynamics (CFD) showed that the removal efficiency of $CO_2$ in water in turbulent flow conditions is much more than that of laminar flow conditions (Bakhshali et al., 2013). Also, Zhang et al. developed a general mass transfer 2-D numerical model for $CO_2$ absorption in a non-wetting mode in methyldiethanolamine and 2-(1-piperazinyl)-ethylamine. The results of their modelling presented that an increase in the fiber length, number of the fibers as well as the porosity of the considered membranes showed a positive effect on the absorption flux. Also, they concluded that increase of the membrane thickness, inner fiber radius and inner module radius had a negative effect on $CO_2$ capture. (Zhang, et al., 2014). After that, Ameri et al. performed a comprehensive mathematical model for simultaneous absorption of $CO_2$ and $H_2S$ via Monoethanolamine (MEA) in a hollow fiber MC. They simulated the effects of various parameters such as wetting fraction, gas and liquid inlet velocities, inlet temperature of the solvent, MEA concentration, and $CO_2$ and $H_2S$ compositions by utilizing Computational Fluid Dynamics (CFD) techniques to solve the governing equations by finite element method. Their results indicated that for large values of gas velocity or small values of liquid velocity, the thermal energy equation can play an important role in the model predictions (Amrei et al., 2014). In addition, Motahari et al. simulated $CO_2$ absorption from a mixture of $CO_2$-$N_2$ in water by employing a polyvinylidene fluoride (PVDF) MC. They investigated the effect of temperature and velocity of liquid phase and velocity of gas phase on $CO_2$ absorption by solving the governing equations using finite element method (two dimensional model by considering dry mode). The results of their work demonstrated that the resistance of liquid phase is the controller of mass transfer during $CO_2$ absorption and temperature of liquid phase has a negative effect on $CO_2$ absorption due to the reduction of gas solubility in liquid phase. (Motahari et al., 2016). Finally, Farjami et al. proposed a two dimensional model under steady state condition for absorption of $CO_2$ by employing a PVDF hollow fiber MCs by employing CFD in a non-wetting mode. They studied the effects of fiber length, flow direction and absorbent temperature on the performance of $CO_2$ absorption. Simulation results presented that increasing fiber length and membrane porosity had a positive effect on the CO2 removal efficiency and counter-current flow arrangement was better than co-current at the same operating conditions (Farjami et al., 2015).

As can be seen, a number of valuable studies with various themes associated with asymmetric hollow fiber MCs have been performed. To the best of our knowledge, few research about the role of the gas diffusivity models through the membrane pores can be found. Considering the gas diffusion along the pores is responsible for the mass transfer across the membrane thickness through both the skin layer and the membrane sub layer, therefore; how to estimate the effective gas diffusivity have a vital degree of importance. When small pores combined with low pressure condition are dealt with, a challenging issue appears. The effective gas diffusivity in fact is a contributive phenomenon, which in, several mechanisms are cooperated. Sometimes, oversimplification of the systems may leads to unrealistic results of the modelling. Accordingly, once an inappropriate model is applied, inevitably unrealistic values for the tuning parameters, such as tortuosity should be selected. From the present literature review, the Bosanquet equation has been widely used for modelling the gas diffusivity through the membrane pores. In the current paper, it is intended to model the gas diffusivity by the aid of the Wakao et al. model as a more comprehensive model. Then an analysis is introduced to present the direct influence of the gas diffusion through the pores on the $CO_2$ absorption flux as well as the concentration profile, applying finite difference method. Moreover, the results generated from the proposed modelling are tested against the experimental data performed at low and high pressures (1 to 30 bar) extracted from the open literature.

## 2. Modelling

Fig. 1 presents the element that is modelled for the gas absorption in a hollow fiber MC. The liquid phase is entered in the lumen side at z = 0, while the gas phase is counter-currently introduced in the shell side. The mass transfer is started from the gas side, then across the membrane and finally is absorbed in the absorbent. Here, the element is divided into four separate parts, namely: (i) the gas in the shell side, (ii) the membrane skin layer, (iii) the bulk of the membrane filled with gas and (iv) the liquid in the lumen side. The following required assumption are considered: the absorption is under isothermal and steady state condition, the gas phase is considered to act as an ideal gas, the Henry's law is applied for calculating the gas-liquid interface concentration, the gas and liquid velocity profile are assumed to be fully developed and the axial diffusion is neglected as stated by (Karoor and Sirkar, 1993; Bakhshali et al., 2013; Farjami et al., 2015).

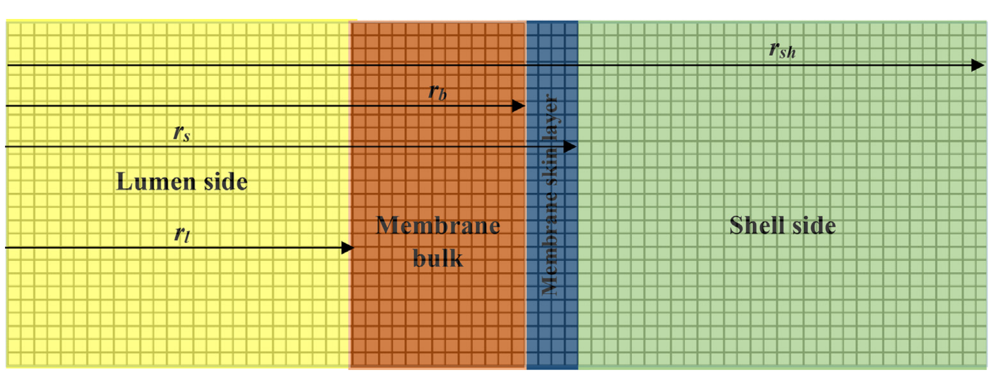


**Fig. 1.** Geometry of the element and the four regions considered for the gas absorption modelling in hollow fiber MC.