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ORIGINAL ARTICLE

Modeling and simulation of membrane separation process using computational fluid dynamics

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Abstract Separation of CO_2 from air was simulated in this work. The considered process for removal of CO_2 was a hollow-fiber membrane contactor and an aqueous solution of 2-amino-2-metyl-1-propanol (AMP) as absorbent. The model was developed based on mass transfer as well as chemical reaction for CO_2 and solvent in the contactor. The equations of model were solved using finite element method. Simulation results were compared with experimental data, and good agreement was observed. The results revealed that increasing solvent velocity enhances removal of CO_2 in the hollow-fiber membrane contactor. Moreover, it was found that counter-current process mode is more favorable to achieve the highest separation efficiency.

1. Introduction

Design and development of novel separation processes for reduction of emissions of carbon dioxide as the major greenhouse gas is of great importance. It has been reported that emission of CO_2 in atmosphere has adverse environmental effects such as global warming. Therefore, there is a definite need for development of efficient and novel separation processes for removal of CO_2 from gas streams. The main criteria for development of efficient separation processes for capture of carbon dioxide include consumption of low energy and high removal rate (Le Moullec et al., 2014; Razavi et al., 2013; Shirazian et al., 2012a). Currently, gas absorption is the most commonly used method for removal of CO_2 from gas streams which is used extensively at industrial scale. The process involves selective absorption of CO_2 into chemical solvents such as aqueous solutions of NaOH or amines.

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Nomenclature

a	inner radius of fiber (m)	D	diffusion coefficient (m^2/s)
b	outer radius of fiber (m)	D_{CO2}	diffusion coefficient of CO_2 (m^2/s)
c	radius of free surface (m)	L	length of fiber (m)
C	concentration (mol/m^3)	m	partition coefficient
C_{gas}	CO_2 concentration in the gas phase (mol/m^3)	p	pressure (Pa)
C_m	CO_2 concentration inside the membrane (mol/m^3)	T	temperature (K)
C_0	inlet concentration of CO_2 in the gas phase (mol/m^3)	r	radial distance (m)
		z	axial distance (m)

Gas absorption is carried out using conventional contactors such as columns and towers in which some usual technical problems are encountered in these contactors. The most common encountered problems in conventional contactors include flooding, foaming, entraining, and channeling (Shirazian and Ashrafizadeh, 2010; Shirazian et al., 2011, 2012b; Sohrabi et al., 2011a,b). These problems detract efficiency of CO_2 capture using conventional separation processes. Therefore, development of alternative separation processes for removal of CO_2 from gas mixtures is of great importance.

Membrane technology can be used for CO_2 capture. CO_2 removal using membrane technology can be accomplished either by porous or by nonporous membranes. Nonporous membranes are usually polymeric which provide low permeation flux. Porous membranes can be used for removal of CO_2 from gas mixtures in which high permeation flux can be obtained that enhances the efficiency of process (Moghadassi et al., 2011; Sohrabi et al., 2011c,d). One of important membrane processes which can be used for CO_2 capture is membrane contactor. Membrane contactors are porous membranes which are used to keep in contact two specific phases such as gas–liquid or liquid–liquid (Gabelman and Hwang, 1999; Mansourizadeh and Ismail, 2009).

Membrane contactors can be used for absorption of CO_2 in which the problems of conventional contactors are not observed in membrane contactors. The most common and useful classes of membrane contactors are hollow-fiber membrane contactors. These novel devices have attracted much attention recently in separation of gas and liquid mixtures (Fadaei et al., 2011a; Fasihi et al., 2012; Ghadiri et al., 2012, 2013a,b,c, 2014; Ghadiri and Shirazian, 2013; Marjani et al., 2012a,b; Marjani and Shirazian, 2010). The main characteristic of hollow-fiber membrane contactors is provision of high surface area per unit volume for separation and reaction. The latter can increase the efficiency of process drastically which in turn makes the process attractive for CO_2 capture. In gas–liquid hollow-fiber membrane contactors, a feed gas is passed through one side while the chemical solvent is passed either co-currently or counter-currently in other side of membrane module.

The main aim of the present work was to develop a mass transfer model for description of CO_2 removal from air in a hollow-fiber membrane contactor. Aqueous solution of 2-amino-2-metyl-1-propanol (AMP) is considered as chemical solvent in the simulations. Computational fluid dynamic technique is used for numerical simulation, and the results of simulations are then compared with the experimental data reported in the literature.

2. Theory

The separation process studied in this work involves a microporous hollow-fiber membrane contactor, a feed gas containing CO_2 and N_2, and an aqueous solution of 2-amino-2-metyl-1-propanol (AMP). The gas mixture flows through the shell side of membrane contactor while the AMP solution is passed through the tube side (see Fig. 1). A gas–liquid interface is formed at the inner side of fiber due to the hydrophobicity of membrane. The latter means that the aqueous solution cannot wet the membrane pores and the membrane pores are filled by the gas phase. The characteristics of the hollow-fiber contactor and operational conditions are the same as those reported in the literature (Kim and Yang, 2000).

A single hollow fiber is considered as model domain in the simulations. The geometry of model is illustrated in Fig. 1. It should be pointed out that the equations of model are derived in cylindrical coordinate while axial symmetry is assumed.

2.1. Equations of gas phase

In the gas phase, feed containing CO_2 and N_2 is contacted with the solvent. Concentration distribution of CO_2 in the gas phase is obtained by numerical solution of mass transfer equation:

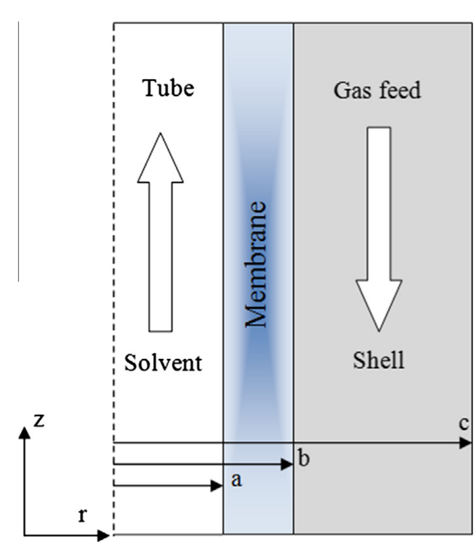

Figure 1 Geometry of hollow-fiber considered in modeling and simulation.