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Effect of porosity on mass transfer of gas absorption in a hollow fiber membrane contactor

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ABSTRACT

A mathematical model was proposed to elucidate the mass transfer of a hollow fiber membrane absorption process taking the effect of membrane porosity into account. This model was derived based on the mass transfer differential equation and discretized considering the micropores on the membrane wall. The model was numerically solved by using upwind difference technique, and the solute concentration profiles were obtained. Effects of porosity under various conditions, including membrane pore size, fiber length, pH of absorbent and liquid velocity on the mass transfer process, were quantitatively investigated. The results indicated that the porosity plays an important role in forming the solute concentration profile, and thus influenced the mass transfer performance. Low porosity (or high pH and liquid velocity, or low fiber length) corresponded to the heterogeneous profiles, while opposite conditions led to the homogeneous profiles. The model gave calculation results in good agreement with experimental results.

1. Introduction

Artificial lungs have been actively developed to replace or supplement the respiratory function of human lungs, which are very important for the patients suffering from acute lung failure [1]. The hollow fiber type artificial lung has been proved as an effective and biocompatible device, and therefore has been receiving much more attention in the recent decades [2,3]. The mass transfer characteristics of the hollow fiber type artificial lungs were extensively investigated by many researchers, which can be analogous to the gas absorption process in the hollow fiber membrane contactor (HFMC) [4].

Membrane gas absorption is an effective, energy-saving and environment-friendly process. Many researchers attempted to elucidate its mass transfer mechanism experimentally and theoretically [5–13]. Kreulen et al. [5,6], Al-Marzouqi et al. [8,9] and Keshavarz et al. [14] and many other researchers investigated the membrane absorption process in the HFMC, and developed various mathematical models for different operation modes and membrane structures. Admittedly, the models are significant tools for us to understand the mass transfer of the membrane gas absorption process. However, the membrane porosity, an important parameter of porous media, was simply categorized in their works as “high”, “medium” and “low” scenarios, leading to the controversial explanation for some experimental results. In order to design and optimize the HFMCs for various application fields, especially in the field of artificial lungs, a more accurate model should be developed. In such model, the effect of porosity should be quantitatively included and evaluated.

Zhang et al. [15,16] were aware of the controversies on the membrane porosity and studied the mass transfer mechanism and characteristics of the membrane absorption process with taking the effect of porosity into account. For a flat-sheet membrane, a mathematical model was proposed to reveal the mass transfer mechanism of the membrane absorption process. The modeling prediction was reasonably good, and the results showed that the effect of porosity could be essentially attributed to the various solute concentration profiles near the membrane surface under different operating conditions. Nevertheless, their model cannot be directly applied to a HFMC, because of the mathematical complexity. Considering the effect of porosity, the complexity of a hollow fiber type porous structure should be properly handled regarding the specific flow field and concentration profile.

In this work, in consideration of the effect of membrane porosity, a novel modeling study was developed to analyze the absorption of carbon dioxide in a HFMC. The mathematical model was established to describe the effect of membrane porosity on

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the mass transfer performance. Effects of various parameters, including membrane pore radius, fiber length, pH of liquid absorbent, and liquid velocity on the mass transfer coefficient were studied. In addition, relevant experiments were conducted to verify the model. The model results were in good agreement with the experimental results.

2. Modeling approaches

2.1. Mass transfer characteristics near the surface of porous media

As a typical membrane-based separation technique, the porous membrane in a gas absorption process can be considered as a "barrier" with no separation and selection capabilities. After diffusion via membrane pores, gaseous solute is absorbed by liquid absorbent at the gas–liquid interface located on the membrane surface.

The previous work on the flat-sheet membrane contactor [17] demonstrated that the porous micro-structure plays an important role in the formation of the solute concentration profile near the membrane surface, and thus influences the mass transfer performance. The gaseous solute diffuses through the membrane pores to the gas–liquid interface, followed by diffusing along the vertical direction and parallel direction in the absorbent aqueous phase on the membrane surface simultaneously. Two important physical parameters, the diffusion distances in the vertical direction (related to the absorption systems and operating conditions, such as liquid velocity and absorbent concentration, etc.) and the parallel direction (related to the membrane micro-structure, such as membrane porosity and pore radius) are taken as the thickness of the concentration boundary layer l and the half distance between neighboring pores a, respectively.

Obviously, there are two typical scenarios corresponding to the vertical diffusion dominant state ($l/a \gg 1$) and the parallel diffusion dominant state ($l/a \ll 1$), resulting in different concentration profiles near the membrane surface. The schematic views of the two states are illustrated in Figs. 1(a) and (b), showing the different influence on mass transfer performance.

The parallel diffusion dominant state forms when the porosity is relatively small and pore radius is large. Additionally, this state also occurs when the solute enters the liquid bulk in the vertical direction before reaching the half distance between the neighboring pores in the parallel direction (chemical absorption). In this state, the solute concentration profile near the membrane surface is heterogeneous, *i.e.* "fast mass transfer system" [15].

On the contrary, the vertical diffusion dominant state forms when the porosity is large and the pore radius is small. In addition, this state also occurs when the solute concentration profile is homogeneously spread along the parallel direction anterior to reaching the liquid bulk, *i.e.* "slow mass transfer system" (physical absorption) [15]. In this case, the effect of porosity on the mass transfer coefficient can be neglected, implying that the mass transfer performance with varying porosities is almost consistent.

When l is comparable to a, it corresponds to the transitional situation at which the influence of porosity on the effect of mass transfer coefficient appears to be converted from the parallel diffusion dominant state (linear dependence) to the vertical diffusion dominant state (linear independence).

Therefore, the impact of porosity on mass transfer performance can be qualitatively characterized as high (parallel diffusion dominant state), medium (transitional state) and low (vertical diffusion dominant state). In this work, the influence of porosity on mass transfer performance of a HFMC is quantitatively evaluated under difference operating conditions.

2.2. Model development

In this work, the mathematical model was developed for a hollow fiber membrane gas absorption process with pure CO_2-deionized water (weak chemical reaction condition or slow mass transfer system)/NaOH solution (strong chemical reaction condition or fast mass transfer system) as feeding gas and absorbents, respectively. CO_2, as the gaseous solute, diffuses across the membrane pores, following by the absorbing/reacting process on the gas–liquid interface located on the membrane surface [15]. For a HFMC, normally, gas phase is fed to the lumen side, and absorbent countercurrently flows through the shell side. However, the non-ideal flow of liquid fluid on the shell side deteriorates the mass transfer performance [18]. In order to eliminate this influence, in this work, gas and liquid phases flowed through the shell and lumen side of the HFMC, respectively.

Membrane pores have been schematically shown by Zhang et al. [15]. Porosity is represented by r_P/a, the ratio of pore radius (r_P) to the half distance between adjacent pores (a). The value of r_P/a is proportional to the square root of membrane porosity.

Assumption (1) to (7) were used in the weak chemical reaction condition and assumption (1) to (8) were used in the strong chemical reaction condition.

(1) The wall structure of micro-porous membrane was assumed as the repetition of a certain pore-polymeric body system, which is shown in Fig. 2. The liquid phase flowed along the axial direction of the fiber. $z=0$ and $z=L$ represent the inlet and outlet of liquid phase, respectively. At the radial direction of the fiber, $r=0$ and $r=R$ represent the center and wall of the fiber, respectively.

(2) For a gas-aqueous system, a strong hydrophobic membrane should be used and it can be assumed that the micropores would not be wetted if an appropriate gas pressure was maintained. Therefore, the gas–liquid interface is located at the inner surface of the hollow fiber. Because pure gas was used in this work, the solute concentration at the gas–liquid interface can be calculated by using Eq. (1).

$$c^* = pH \tag{1}$$

where H is the Henry's constant of CO_2 and the value is of 3.2×10^{-4} mol m^{-3} Pa^{-1} [19].

(3) In order to simplify the model, pure gas was used in the simulation process. Therefore, based on the *resistance-in-series* theory, the mass transfer resistances of gas and membrane phases can be neglected, while the mass transfer resistance of the liquid phase was dominant [20].

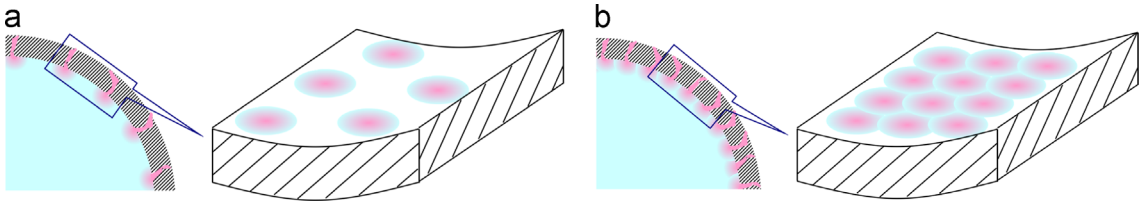

Fig. 1. Schematic diagram of the solute diffusing in liquid near hollow fiber membrane surface. (a) $l/a \ll 1$ (b) $l/a \gg 1$.