



# Mathematical modeling of gas–liquid membrane contactors using random distribution of fibers

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## ABSTRACT

This work presents a mathematical model for gas absorption in microporous hollow fiber membrane contactors by using a random distribution of fibers. The chemical absorption of carbon dioxide into aqueous amine solutions and sulfur dioxide into water were simulated by this model. The nonlinear mathematical expressions of the component material balance for the liquid, membrane, and gas were solved simultaneously by using a numerical method. The results from the model were compared with four sets of different experimental data in the literature. In addition, the contactors were modeled based on the assumption of regular arrangement of fibers in the shell side by using Happel's free surface as well as plug flow models. The plug flow model was employed to compare the various available equations in the literature for the shell side mass transfer coefficient. The results indicate that the channeling of gas in the shell side decreases the efficiency of contactor significantly. It was found that the random distribution of fibers is a suitable method to simulate the commercial modules. The results also indicate that, the regular Happel's free surface model and the plug flow model are more suitable for handmade modules. The influence of shell side channeling on the contactor performance were investigated in different fiber packing densities, and in various gas and liquid flow rates.

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## 1. Introduction

The capture and utilization of carbon dioxide, as a greenhouse gas, and other acid gases such as sulfur dioxide and hydrogen sulfide from industries is an important process. Some examples are sweetening of natural gas, purification of ammonia and methanol synthesis gas, waste water treatment and hydrogen purifying. The sequestration of these gases by using microporous hollow fiber membrane contactors has gained considerable attention recently and is still a relatively new concept. This hybrid-type process is based on a combination of membrane separation and chemical absorption. The membrane used in this type of contactor is usually a microporous non-selective type, leading to a higher mass transfer rate comparing with a thin selective type. Due to a very small pressure difference between the shell side and the lumen side, the mass transfer driving force in a membrane contactor is the concentration difference rather than the pressure difference. The membrane contactor has some advantages over traditional contactors, including higher mass transfer rates, independent control of gas and liquid rates, a known and constant interfacial area, easy

scale up and no operational problems such as foaming, flooding or entrainment [1,2].

These advantages have led to a number of investigations on the use of this hybrid process for gas absorption and stripping. The absorption of various gases by a number of solvents in a hydrophobic membrane were first carried out by Zhang and Cussler [3,4]. Karoor and Sirkar [5] and Kreulen et al. [6,7] studied the absorption of some acid gases and found that the mass transfer rate is much higher than those typically obtained in packed towers. It was also found that, despite the fact that the membrane wall introduces an additional resistance, the higher surface area in these types of modules offers much higher mass transfer rates.

Other experimental and theoretical studies focused on the absorption of CO<sub>2</sub>, SO<sub>2</sub> and H<sub>2</sub>S from flue gases by using various absorbents such as water, sodium hydroxide, potassium hydroxide or alkanolamines [8–15].

The advantages of the hybrid process over the conventional processes largely depend on gas–liquid systems, types of membranes and operating conditions. For example, the membrane wetting, even at a very low fraction, significantly decreases the module performance [16,17].

Another important parameter affecting the gas absorption is shell side channeling. The flow pattern in the shell side is usually quite complex and most researchers try to overcome it by making

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some simplified assumptions. These assumptions are practically valid only in some cases. For example, if the gas in the shell side is pure, the main mass transfer resistance can be attributed to the liquid and membrane. The same approach can be used for the physical absorption from a gas mixture when the liquid flow rate is low. However, gas resistance is very important if the gas in the shell side is a mixture and is absorbed chemically in the liquid bulk. In such a common case, the channeling might affect the module performance. Therefore, the shell side hydrodynamics cannot be easily ignored.

A few sophisticated models have been proposed in which the shell side effect is considered for gas–liquid systems. Karoor and Sirkar [5] employed the Happel's free surface model [18] to characterize the shell side flow, with the assumption of a regular arrangement of fibers in the shell side. They also assumed a constant gas velocity through the shell side in the axial direction [19,20]. Keshavarz et al. [17] used a plug flow model in the shell side to calculate the velocity and concentration gradient in the axial direction. Although these models have included the shell side characteristics, they are essentially based on the assumption of the regular fiber arrangement in the shell cross-section.

The commercial hollow fiber modules consist of randomly packed fiber bundles in the shell cross-section. To calculate the hydrodynamics of such modules, Chen and Hlavacek [21] distributed the fibers based on an exponential probability density function. Each fiber was considered to be surrounded by a polygonal cell defined by a Voronoi tessellation. More recently, Rogers and Long [22], and Wu and Chen [23] employed the Voronoi tessellation method to analyze the shell side mass transfer performance of hollow fiber modules. A new method for the distribution of flow in the shell side was proposed by Zheng et al. [24] based on the application of the exponential density function for fiber distribution and the Happel's free surface model for flow distribution. Their method has the advantage of the hydrodynamics in each cell, which can be described according to Happel's free surface model. The random distribution model has also been used for the modeling and analysis of some membrane transport processes such as membrane distillation and liquid–liquid extraction [25,26]. These studies indicate that the random packing of fibers causes a serious flow maldistribution and significantly decreases the mass transfer performance of the mentioned processes. Therefore, the application of the random distribution technique would be suitable for the gas–liquid systems with fast reactions in the liquid.

In this work a mathematical model based on the random distribution technique for the gas–liquid systems accompanied by chemical reactions in the liquid has been developed for the prediction of module performance, and to investigate the importance of shell side channeling in these types of processes. The systems, including the absorption of carbon dioxide into monoethanolamine (MEA) and diethanolamine (DEA) aqueous solutions, and the absorption of sulfur dioxide into water were investigated. The proposed diffusion–reaction model contains chemical reactions in the liquid bulk in the lumen side as well as governing equations for the gas in the shell side. A numerical scheme was employed to solve the nonlinear mathematical expressions obtained in the liquid, membrane and gas. Because of the sophisticated nature of the model, the results of the model were compared with two simpler models: the plug flow model and Happel's free surface model. The outcomes of these models were checked with four sets of experimental data in the literature [5,8,16,27]. The performance of the commercial and handmade membrane contactors and the effects of some parameters on the recovery were also investigated by this model. The outcomes of this study provide a more accurate analysis of absorption of acid gases in commercial modules.

## 2. Model development

The governing equations in the liquid, membrane and gas involve a set of partial and ordinary differential equations as well as a number of algebraic equations. These coupled mathematical formulations of the phases are described in the following sections. The major assumptions involved in developing the model include: (a) laminar parabolic velocity profile within the fibers; (b) isothermal condition; (c) ideal gas behavior; (d) uniform pore size distribution and uniform thickness of membrane wall. The method used in this study assumes that the liquid runs inside the fibers, countercurrent to gas flow inside the shell. The specification of contactors modeled in this study and their references are given in Table 1.

### 2.1. Diffusion–reaction model in liquid

Applying a component material balance on the liquid within the fibers for each diffusing component leads to the following two-dimensional partial differential equation:

$$U_z \frac{\partial C_{jL}}{\partial Z} = D_{jL} \left( \frac{\partial^2 C_{jL}}{\partial r^2} + \frac{1}{r} \frac{\partial C_{jL}}{\partial r} \right) - R_j \quad (1)$$

where  $R_j$  is the rate of reaction for component  $j$ . The liquid flow rate inside the fiber is laminar and can be given by

$$U_z = 2U_{avL} \left[ 1 - \left( \frac{r}{r_i} \right)^2 \right] \quad (2)$$

Eq. (1) should be repeated for all necessary components in the liquid. Since the reaction rate ( $R_j$ ) is normally a function of concentration of different species, the partial differential equations are not independent. The initial condition for each diffusing species in the lumen is specified as

$$C_{jL} = C_{jL,i}, \quad \text{for } Z = 0 \quad (3)$$

At the center of each fiber, symmetry is assumed in the radial direction, which results in the following boundary condition:

$$\frac{\partial C_{jL}}{\partial r} = 0, \quad \text{for } r = 0 \text{ and all } Z \quad (4)$$

At the liquid–membrane interface, material balance for the diffusing species leads to the following boundary condition:

$$D_{jL} \frac{\partial C_{jL}}{\partial r} = D_{jm} \frac{\partial C_{jm}}{\partial r}, \quad \text{for } r = r_i \text{ and all } Z \quad (5)$$

Consequently, for non-diffusing species to the membrane such as MEA and DEA, we have

$$D_{jL} \frac{\partial C_{jL}}{\partial r} = 0, \quad \text{for } r = r_i \text{ and all } Z \quad (6)$$

For a hydrophobic membrane with gas-filled pores, Henry's law can be applied at the membrane–liquid interface as follows:

$$C_{jL} = HC_{jm}, \quad \text{for } r = r_i \text{ and all } Z \quad (7)$$

The reaction of carbon dioxide with monoethanolamine and diethanolamine solutions is normally described by zwitterions mechanism. The reaction scheme and the rate of reactions can be obtained from the literature and are given in Appendix A. This appendix also contains the reaction scheme of water and sulfur dioxide.

### 2.2. Mass transfer in microporous membrane

At high membrane porosity (greater than 10%), the diffusion process is essentially one-dimensional [5,28]. Therefore, the trans-

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