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Mathematical modeling and simulation of carbon dioxide stripping from water using hollow fiber membrane contactors

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ABSTRACT

In the present investigation, removal of carbon dioxide from water was examined theoretically using a hollow fiber membrane contactor. A 2D mathematical model with axial and radial diffusions in the membrane contactor was developed. The finite element method was used to solve the governing equations. The results of modeling were in good agreement on the wide range of liquid velocity and temperature with experimental data. The results indicated that, as liquid phase velocity and carbon dioxide concentration in liquid phase increased, the carbon dioxide stripping increased significantly. Also by the increment of the liquid temperature, carbon dioxide stripping flux increased because of carbon dioxide solubility decrement. By increasing gas velocity from 0.02 to 0.07, CO_2 stripping flux increases by 7.5%. The diffusion coefficient was computed through the equations of Versteeg and Wilke–Chang. The results revealed that since concentration does not change through the tube and diffusion coefficient is a function of concentration in liquids, the Wilke–Chang equation could better predict the diffusion coefficient than the Versteeg equation. The maximum error in this regard was 6% with solution time of 20 second.

1. Introduction

Although the presence of CO_2 in water is mostly due to natural processes, the effluence of industrial wastewater significantly increases the CO_2 content into water bodies. Manufacturing of ammonia and urea industries generate wastewater that has higher CO_2 concentrations, and if left untreated, it may ultimately find its way to natural reservoirs. For decarbonation, i.e., removing CO_2, industries typically employ measures such as aeration, forced draft degasification, and vacuum degasification. Since heavy-duty equipment such as pumps and blowers are employed, these conventional methods involve high costs [1,2].

The hollow fiber membrane contactor can be one of promising alternatives for CO_2 absorption/stripping processes. In this technique, the porous membrane acts as a fixed interface between the gas and liquid phases, which prevents dispersing one phase into another. Qi and Cussler first studied these devices, and since then, extensive studies on the hollow-fiber membrane contactors (HFMCS) have been conducted [3–5]. The membrane contactors have several advantages in comparison with conventional technologies such as: (1) no flooding at high flow rate; (2) no unloading at low flow rates; (3) absence of emulsions (4) no density difference between fluids required, and (5) high interfacial area.

Usually, the stripping units are highly energy-consuming and consequently, the most of the studies have focused on CO_2 absorption using gas–liquid membrane contactors [6–12]. In fact, there are a handful of studies on CO_2 stripping through hollow fiber membrane contactors. Koonaphapdeelert et al., have used ceramic hollow fiber membrane contactors for CO_2 stripping from a monoethanolamine (MEA) solution at high temperature. They found that even in the region of an ordinary column showing flooding or loading, the membrane contactors could operate very well. The maximum capacity factor tested in this experiment was without any sign of flooding at least 2–10 times higher than the flooding line [13].

Albo et al. mathematical modeling was developed for CO_2 removal in hollow fiber membrane contactors. The ionic liquid 1-ethyl-3-methylimidazolium ethylsulfate has been used as the absorption liquid, and has been studied at macroscopic and microscopic scales. They found that there are not any differences between the results considering logarithmic mean concentration profiles through the contactor or a plug flow profile. Investigating their conclusions, it is also realized that the membrane mass transfer coefficient takes a value of $k_m = 3.78 \times 10^{-6}$ (m/s^{-1}), which is about five times higher than that obtained in the macroscopic

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Nomenclature

M_B	The molar mass of the solvent (g/mol)
ν_A	The volume of the solute at its normal boiling point (cm^3/mol)
C_i	Concentration (mol/m^3)
R_i	Reaction term (mol/m^3 s)
$\overline{u}$	Average velocity (m/s)
D_{AB}	Diffusivity of A in B solution (m^2/s)
D_{w,CO_2}	Diffusivity of CO_2 in water (m^2/s)
$D_{CO_2-lumen}$	$D_{CO_2-lumen}$ diffusion coefficient of CO_2 in the lumen (m^2/s)
$D_{CO_2-membrane}$	$D_{CO_2-membrane}$ diffusion coefficient of CO_2 in the lumen (m^2/s)
$D_{CO_2-shell}$	$D_{CO_2-shell}$ diffusion coefficient of CO_2 in the lumen (m^2/s)
m	Solubility (dimensionless)
$V_{z\text{-shell}}$	$V_{z\text{-shell}}$ z-velocity in the shell (m/s)
$V_{z\text{-lumen}}$	$V_{z\text{-lumen}}$ z-velocity in the lumen (m/s)
r	Radial coordinate (m)
r_1	Inner tube radius (m)
r_2	Outer tube radius (m)
r_3	Inner shell radius (m)
n	Number of fibers (dimensionless)

Greek symbols

μ	Viscosity, cp
φ	Module volume fraction

Abbreviations

FEM	Finite element method
HFMC	Hollow-fiber membrane contactor
2D	Two dimensional
PVDF	Polyvinylidene fluoride
CFD	Computational fluid dynamics

study. This means that the influence of the laminar flow is included in the mass-transfer parameter [14].

A number of authors have used numerical methods based on solving conservation equations for the specie in all phases using computational fluid dynamics (CFD) techniques to simulate the gas separation and solvent extraction carried out in HFMCs. Their results showed good agreements between the experimental and simulation results [15–17]. The importance of the stripping process using membranes and the good agreement between experimental and simulation results have made researchers pay much more attention to simulation the membrane processes [18,19]. Therefore, in the shortest period of time with the lowest cost, the optimal conditions for the process to be implemented will be achieved.

In this study, the modeling of CO_2 stripping from water using polyvinylidene fluoride (PVDF) hollow-fiber membranes were investigated through numerical methods. The main purpose was to develop a 2D mathematical model for striping CO_2 in HFMCs. The governing equations such as mass-transfer and momentum equations were solved through a numerical procedure based on finite element method.

Finally, the simulation results are validated with experimental data reported by Mansourizadeh and Ismail [20]. The aim of this simulation was to predict the influence of operating conditions including gas and liquid velocities, CO_2 concentration in the liquid phase, and rich solution temperature on the mass transfer of CO_2 in HFMCs. Also, the effect of liquid phase velocity on the diffusion coefficient of CO_2 in pure water is studied at constant temperature of 80 °C.

2. Theory

A 2D mathematical model was developed to predict the transfer of CO_2 through the membrane contactors in the stripping process. In this model, the stripping of CO_2 from the water using N_2 in a hollow-fiber membrane contactor (HFMC) was examined. The model was based on "non-wetted" mode. According to this model, the pores of the membrane were filled with gas phase and liquid could not penetrate the membrane pores. This model assumes that the fibers are distributed evenly in the module space, therefore the obtained results with a single fiber can be generalized to the entire module [21]. The liquid stream containing water was fed through the lumen (tube)-side of contactor and the gas phase flew inside the shell in counter-current manner. For the liquid to flow in the lumen side, laminar parabolic velocity distribution was applied. The steady-state 2D mass balances were taken for all three sections, i.e., lumen side, membrane, and shell side.

2.1. Equations of model

2.1.1. Equations of lumen side

The continuity equation for all species in desorption system can be expressed as [18]:

$$\nabla \times (-D_i C_i + C_i u) + \frac{\partial C_i}{\partial t} = R_i \tag{1}$$

where C_i denotes the concentration of solute (mol/m^3), D_i denotes its diffusion coefficient (m^2/s), u denotes the velocity vector (m/s) and R_i denotes the reaction term (mol/m^3 s). By applying Fick's law for estimation of diffusive flux, the steady-state continuity equation for CO_2 transport in the lumen side is written as follows:

$$D_{CO_2-tube}\left[\frac{\partial^2 C_{CO_2-tube}}{\partial r^2} + \frac{1}{r}\frac{\partial C_{CO_2-tube}}{\partial r} + \frac{\partial^2 C_{CO_2-tube}}{\partial z^2}\right] = V_{z-tube}\frac{\partial C_{CO_2-tube}}{\partial z} - R_{CO_2} \tag{2}$$

where r and z represent the radial and axial coordinates, respectively. Because there is no chemical reaction, the reaction term in the lumen side is not discussed.

The convective mass transfer in radial direction is neglected because the feed and solvent are flown in axial direction (z-direction). The velocity distribution in the lumen side is assumed to follow the Newtonian laminar flow [22]:

$$V_{z-tube} = 2\overline{u}\left[1 - \left(\frac{r}{r_1}\right)^2\right] \tag{3}$$

where u (m/s) is the average velocity in the lumen and r_1 is the fiber inner radius. The boundary conditions assumed for the lumen are given below:

$$\text{At}: Z = 0, C_{CO_2-tube} = C_{CO_2-0}(\text{Inlet boundary}) \tag{4}$$

$$\text{At}: Z = \text{L}, \text{convective flux} \tag{5}$$

$$\text{At}: r = 0, \frac{\partial C_{CO_2-tube}}{\partial r} = 0(\text{Axial symmetry boundary}) \tag{6}$$

$$\text{At}: r = r_1, C_{CO_2-tube} = C_{CO_2-membrane}/\text{m}(\text{Henrys law}) \tag{7}$$