International Journal of Heat and Mass Transfer 89 (2015) 749–759

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

# Computational study of gas separation using a hollow fiber membrane

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ARTICLE INFO

*Article history:*
Received 6 March 2015
Received in revised form 20 May 2015
Accepted 20 May 2015
Available online 12 June 2015

*Keywords:*
Hollow fiber membrane
Porous layer
Turbulence model
Membrane performance

ABSTRACT

Computational fluid dynamics simulations are conducted for binary mixture fluid flows in a hollow fiber membrane. The membrane is modeled as a functional surface, where the mass fluxes of each species will be determined based on the local partial pressures, the permeability, and the selectivity of the membrane. Baseline Reynolds Stress (BSL Reynolds Stress) turbulence model and the Brinkman–Forchheimer equations are employed to study spatial structure of the flow inside the lumen and the porous layer for Reynolds number up to 400. The process of separating $CO_2$ from $CH_4$ is improved by the presence of orifices in the membrane system by about 60%. The degree of improvement is greater at higher flow rate. The influence of the momentum mixing induced by orifices strongly depends on the permeability and the thickness of the support layer. It is demonstrated here that altering flow inside the lumen by placing flow restricting devices can be used in the hollow fiber membrane system design in the application of gas–gas separation.



## 1. Introduction

Natural gas consumption has increased significantly in recent years. The impurities found in raw natural gas cause corrosion. Membranes are used to separate these undesired gasses, thereby purifying the natural gas. Increasing membrane performance will reduce capital and operation costs of the purification process.

Enhancing membrane performance by introducing turbulent mixing in the feed flow has been investigated in the water treatment, food industries and gas separation. Several investigators employed the momentum equation only to predict the pressure loss induced by turbulators in spiral wound membrane [1–5]. Fimbres-Weihs et al. [6,7], Al-Sharif et al. [8] and Shakaib et al. [9] determine the flow and concentration field by solving the momentum and the mass transport equation, but still treated the membrane as an impermeable wall. Guillen and Hoek [10], Pal et al. [11], and Subramani et al. [12] improved the process modeling by treating the membrane as a permeable wall with constant flux. Real separation process in these systems requires a proper mass flux model for the membrane. Mass transport through the membrane should be determined as a function of the local pressure and mass fraction. Several investigators determined the membrane mass flux as a function of the local pressure and mass fraction in the desalination process [13–22]. These studies model only flux of water through the membrane in the desalination process, but not the flux of salt. This is because the mass fraction of the salt in the permeate is assumed to be directly proportional to the rejection. This assumption is not valid in the gas–gas separation process since the concentrations of both species are comparable. Recently, the present authors introduced a novel membrane flux model for gas separation process [23]. In their model, the mass flux of each species is determined from the first principle and it is based on the local partial pressures, the permeability, and the selectivity of the membrane.

Kundu et al. [24,25] employed Hagen–Poiseuille approximation to calculate the pressure drop along the lumen side of a hollow fiber membrane (HFM) module. This approximation is not capable of capturing the spatial and temporal characteristics of the flow inside the HFM system. Several investigators just considered only the mass transport through the hollow fiber membrane [26–31]. Ghidossi et al. [32], Marcos et al. [33] and Vinther et al. [34] predicted the flow inside the membrane module by solving the Navier–Stokes equation but neglecting the effect of the porous layer. The present authors demonstrated that the porous layer – the mechanical support layer – should be a part of the flow domain and its effect on the membrane performance should be taken into account [35].

In this work, flows of a binary mixture, $CH_4$ and $CO_2$, in a channel bounded by porous support layer surrounded by a selective

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.05.090
0017-9310/

**Nomenclature**

| | |
|---|---|
| $C$ | concentration [mol/m$^3$] |
| $D$ | diffusion coefficient [m$^2$/s] |
| $D_2$ | hollow fiber membrane |
| $K$ | permeability of porous media |
| $M$ | molecular weight [g/mol] |
| $P$ | permeance [mol/(m$^2$ s Pa)] |
| $S$ | spacing between spacers [m] |
| $Sh$ | Sherwood number [–] |
| $V_w$ | suction rate [m/s] |
| $d$ | orifice diameter [m] |
| $k$ | turbulent kinetic energy [J/kg] |
| $m$ | mass flux [kg/(s m$^2$)] |
| $u$ | $x$-component of velocity [m/s] |
| $x$ | $x$ coordinate [m] |
| $\Delta p$ | pressure difference [Pa] |
| $\alpha$ | mass selectivity [–] |
| $\gamma$ | rate of strain tensor |
| $\rho$ | density [kg/m$^3$] |
| $\sigma$, $\lambda$ | turbulent model parameters [–] |
| $\varphi$ | porosity |
| $C_F$ | drag coefficient of porous media |
| $Dp^*$ | normalized permeability |
| $D_1$ | lumen diameter |
| $J$ | molar flux [mol/m$^2$] |
| $L$ | membrane length [m] |
| $\ddot{P}$ | permeability [mol/(m$^2$ s Pa)] |
| $Re$ | Reynolds number [–] |
| $Sc$ | Schmidt number [–] |
| $U$ | average velocity [m/s] |
| $N$ | mole fraction [–] |
| $hm$ | mass transfer coefficient [m/s] |
| $l$ | membrane thickness [m] |
| $p$ | pressure [Pa] |
| $v$ | $r$-component of velocity [m/s] |
| $r$ | $r$ coordinate [m] |
| $\beta^*$, $\beta_1$, $\beta$ | turbulent model parameters [–] |
| $\upsilon$ | kinematic viscosity [m$^2$/s] |
| $\omega$ | specific dissipation rate [1/s] |
| $u$ | velocity vector |

*Subscripts and superscripts*

| | |
|---|---|
| $a$ and $b$ | species: $CO_2$ or $CH_4$ |
| $i$ and $j$ | index notation |
| $CH_4$ | properties of $CH_4$ |
| $tot$ | total properties |
| $w$ | properties at the membrane |
| T | eddy properties |
| $CO_2$ | properties of $CO_2$ |
| – | average property |

membrane are studied for a range of Reynolds numbers from 100 to 400. Number of orifices was placed inside the tubular channel to enhance mixing in the feed channel by serving as turbulators. The steady flow is characterized by a Baseline Reynolds Stress turbulent model. The membrane is modeled as a functional surface, where the mass fluxes of each species will be determined based on the local partial pressures, the permeability, and the selectivity of the membrane.

## 2. Governing equation

The schematic of the flow geometry is illustrated in Fig. 1. It consists of an open tubular channel surrounded by a porous layer which is bounded by a dense membrane. The diameter of the open tubular channel is $D_1$, the diameter of the module consisting of the porous support layer is $D_2$, and the length of the membrane module is $L = 35D_2$, as shown in Fig. 1. Uniformly spaced orifices are placed in an open channel. The orifice is a ring or a washer-like insert that restricts flow inside the empty tube. The diameter of the orifice is $d = 0.5D_1$ and the spacing between two consecutive orifices is $S$. The binary mixture of $CH_4$ and $CO_2$ is treated as an incompressible fluid with uniform physical properties. The flow is axisymmetric and isothermal. The diffusion coefficient is assumed to be independent of the concentration. The permeability of the porous layer is constant. The porous layer is considered to be saturated and the membrane selectivity and permeability are assumed to be constant.

Baseline Reynolds Stress turbulence model is employed to simulate flow inside the tubular channel. Recently, the present authors showed that the BSL Reynolds Stress turbulence model accurately predicts flow past a cylinder confined in a channel for a range of Reynolds number from 250 to 1500 [23]. They documented that their predicted results agree well with the experimental measurement reported in Ref. [36]. The equation governing the fluid motion is given by

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nabla\cdot((\upsilon+\upsilon_T)\nabla\boldsymbol{u}) \tag{1}$$

where $\boldsymbol{u}$ is velocity vector, $p$ is the pressure, $\rho$ is the density of the mixture and $\upsilon$ is the kinematic viscosity of the mixture. $\upsilon_T = k/\omega$ is the eddy viscosity and is determined using the BSL Reynolds Stress turbulence model

$$\frac{\partial k}{\partial t} + \boldsymbol{u}\cdot\nabla k = \nabla\cdot((\upsilon+\upsilon_T)\nabla k) + \boldsymbol{\tau}:\nabla\boldsymbol{u} - \beta^* k\omega \tag{2}$$

$$\frac{\partial \omega}{\partial t} + \boldsymbol{u}\cdot\nabla\omega = \nabla\cdot((\upsilon+\sigma\upsilon_T)\nabla\omega) - \beta_1\omega^2 + \lambda\frac{\omega}{k}\boldsymbol{\tau} : \nabla\boldsymbol{u} + 2(1-F_1)\frac{\sigma}{\omega}\nabla k\cdot\nabla\omega \tag{3}$$

Here $k$ is the turbulent kinetic energy, $\omega$ is the specific dissipation rate, and $\boldsymbol{\tau}$ is the residual stress tensor. The model constants are selected to be $\sigma = 0.5$, $\beta^* = 0.09$, $\beta_1 = 0.075$ and $\lambda = 0.556$ [37]. The detailed description of the blending function, $F_1$, and other model parameters is given in Ref. [37]. In Eqs. (2) and (3) both $j$ and $n$ are summation indices.

In the porous layer, the mechanical support layer, the Brinkman–Forchheimer equation is employed [38]

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nabla\cdot((\upsilon+\upsilon_T)\nabla\boldsymbol{u}) - \phi\frac{\upsilon}{K}\boldsymbol{u} - \frac{C_F}{K^{0.5}}|\boldsymbol{u}|\boldsymbol{u} \tag{4}$$

where $C_F$, $K$, and $\phi$ are drag coefficient, permeability, and porosity of the porous layer, respectively.

The species equation for the BSL Reynolds stress model is of the form

$$\frac{\partial CN_a}{\partial t} + \boldsymbol{u}\cdot\nabla(CN_a) = \nabla\cdot((D+\sigma D_T)\nabla(CN_a)) \tag{5}$$

where $D_T$ is the eddy diffusion coefficient and $Sc_T = \upsilon_T/D_T$ is the turbulent Schmidt number. $Sc_T$ and $\beta$ are selected to be 0.85 and 0.09 in