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CFD modeling of porous membranes

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Abstract

Membrane filtration has become firmly established as a primary technology for ensuring the purity, safety and efficiency of treatment of water or effluents. Water desalination is one of the major applications of this technology around the world. Several researches have been performed to develop and design membrane systems in order to increase the process accuracy and performance. In this research, the laminar fluid flow in porous tubes, a mode of crossflow filtration tubular membrane, is simulated numerically using the computational fluid dynamics (CFD) techniques. A two-dimensional numerical solution of the coupled Navier–Stokes, Darcy's law and mass transfer equation has been developed using control volume based finite difference method. Case study was performed for a microfiltration process. Prediction of the growth rate of the concentration polarization boundary layer along the length of tubular membranes has been performed. Effects of various operating conditions (e.g. geometrical dimension, required membrane surface area, Reynolds number and fouling) on the performance of membrane are studied and some comments on designing of such membranes are suggested.

Keywords: Membrane filtration; Water desalination; Computational fluid dynamics (CFD)

1. Introduction

Over the past two decades, membrane filtration processes have played a more and more important role in industrial separation process. Many studies have focused on the best ways of using a particular membrane process. Computational fluid dynamics techniques may provide a lot of interesting information for the development of membrane processes. Numerous improvements of the technology have allowed membrane selection for a particular process to be done more easily and more quickly. The development of this technology is because of the increasing number of different types of applications of these processes in different domains, particularly in the industrial sector. Membrane filtration is used in a broad range of applications [1].

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In membrane separation processes the hydrodynamics of fluid moves upon the membrane is very important. A combination of free flow and flow through porous media occurs in a membrane filtration process. A fluid dynamic description of free flows is usually easy to perform and in most cases the well known Navier–Stokes equations can be used to model this part. The validity of Darcy's law for the representation of non-inertial, incompressible flows in porous media with small porosity is also widely accepted [2]. Therefore, in membrane filtration processes where a combined free and porous flow occurs, the flow regime can be modeled by coupling Darcy's law and the Navier–Stokes equations. The important point is to make sure that the continuity of flow field variables across the interface between laminar flow and porous region is maintained.

Numerous approximate one-dimensional models have been performed [3]. The first simulation of flow in a membrane was undertaken under laminar conditions in channels with porous walls [4]. Investigation of laminar flow in a porous pipe with variable wall suction or variable radial mass flux was done by Galowin and De Santis [5]. A summary of the recent developments, up to 1989, on the role of fluid mechanics in membrane filtration was presented by Belfort et al. [6]. Many authors are very interested in using this method to optimize membrane processes [7]. Nassehi et al. [8] used Darcy's equation to represent the porous wall conditions. They used the finite element method in their simulation and presented a more robust simulation comparing to other previous works. Damak et al. [9] simulated a laminar, incompressible and isothermal flow in a cylindrical tube with a permeable wall using a finite difference scheme.

Several methods have been used for modeling the concentration polarization layer near a membrane surface. In membrane crossflow filtration, particles with the feed stream are convectively driven to the membrane surface and they finally accumulate near the membrane surface, until the equilibrium between convective and diffusive fluxes is reached. The major problem during membrane crossflow filtration is the permeate flux decline caused by concentration polarization phenomena. In order to analyze and predict the problem of concentration polarization one must understand the transport phenomena at the membrane surface. In most cases, model development starts with the fundamental equations of fluid flow and mass transfer [10]. A more precise model was developed by Lee and Clark [11]. The numerical model of cross flow filtration developed in their work successfully explained the fundamental mechanisms involved in flux decline during crossflow ultrafiltration of colloidal suspensions. Wiley [12] modeled the flow and concentration polarization in pressure driven membrane processes with added effects of variable solution properties such as viscosity and diffusion coefficient.

In the present paper a numerical technique based on finite volume method is used to solve the two-dimensional flow field and convective diffusion equation for particle transport in laminar flow over a permeable surface in a tubular membrane. The effect of various physical parameters on the growth of concentration polarization layer along the membrane surface is studied.

2. Problem description and formulation

The problem under consideration is schematically shown in Fig. 1. The steady state concentration polarization phenomenon in a crossflow

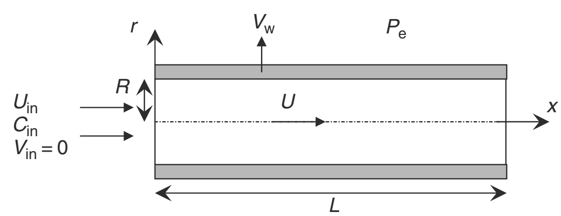

Fig. 1. Simulated geometry for tubular membrane.

filtration process is described by two-dimensional convective–diffusion equations, coupled with the resistance-in-series model for permeation transport. This work deals with the mass transfer phenomenon in a tubular membrane (r, x) with radius R and length L in the case of laminar crossflow. Water is assumed to be the solvent and salt to be the solute in this study. The simulation is based on the following assumptions:

- Steady state, incompressible, isothermal axisymmetric flow.
- Due to the low concentration of particles, constant solution viscosity and density [13].
- Constant diffusion coefficient for the solvent [14].
- A fully developed velocity profile at the tube inlet.
- No slip condition at the membrane surface [15].
- The local wall permeation velocity determined from resistance-in-series model [16].

Governing equations are described as the following:

Continuity equation:

$$\nabla(\rho\vec{V}) = 0 \tag{1}$$

Axial momentum equation:

$$\nabla(\rho u\vec{V}) = -\frac{\partial p}{\partial x} + \nabla(\mu\nabla u) \tag{2}$$

Radial momentum equation:

$$\nabla(\rho v\vec{V}) = -\frac{\partial p}{\partial r} + \nabla(\mu\nabla v) \tag{3}$$

Mass transfer or solute transport equation:

$$\nabla(\rho\vec{V}C) = \nabla(\rho D\nabla C) \tag{4}$$

Boundary conditions:

Inlet boundary condition, $x = 0$:

$$U(0,r) = 2U_{\max}\left(1 - \left(\frac{r}{R}\right)^2\right),\quad V(0,r) = 0,\ C(0,r) = C_0 \tag{5}$$

Outlet boundary condition, $x = L$:

Fully developed flow condition is considered at the tube exit plane.

$$\frac{\partial U(L,r)}{\partial x} = 0,\ \frac{\partial V(L,r)}{\partial x} = 0,\ \frac{\partial C(L,r)}{\partial x} = 0 \tag{6}$$

At axisymmetric axis, $r = 0$:

$$\frac{\partial U(x,0)}{\partial r} = 0,\ V(x,0) = 0,\ \frac{\partial C(x,0)}{\partial r} = 0 \tag{7}$$

At membrane surface, $r = R$:

$$\frac{\partial U(x,R)}{\partial r} = 0,\ V(x,R) = V_w(x),\quad V_w(x)C(x,R) = D\frac{\partial C(x,R)}{\partial r} \tag{8}$$

In the above equation, $V_w(x)$ is determined by Darcy equation, using resistance-in-series model:

$$V_w(x) = \frac{\Delta P}{\mu(R_m + R_p)} \tag{9}$$

where R_p is the resistance of concentration polarization layer and is obtained using the following equation:

$$R_p = \int_{R-\delta_p}^{R} r_p\,\mathrm{d}\delta = r_p\delta_p \tag{10}$$

where r_p is the specific resistance and δ_p is the thickness of concentration polarization layer. The right hand side of the above equation is obtained by the consumption of homogeneous concentration layer. r_p is obtained from Carmen–Kozeny equation:

$$r_p = 180\frac{(1-\varepsilon_p)^2}{a_p^2\varepsilon_p^3} \tag{11}$$

where a_p is the average particle diameter and ε_p is the porosity of the concentration polarization layer.

The concentration polarization layer, δ_p, is approximately equal to the distance from the

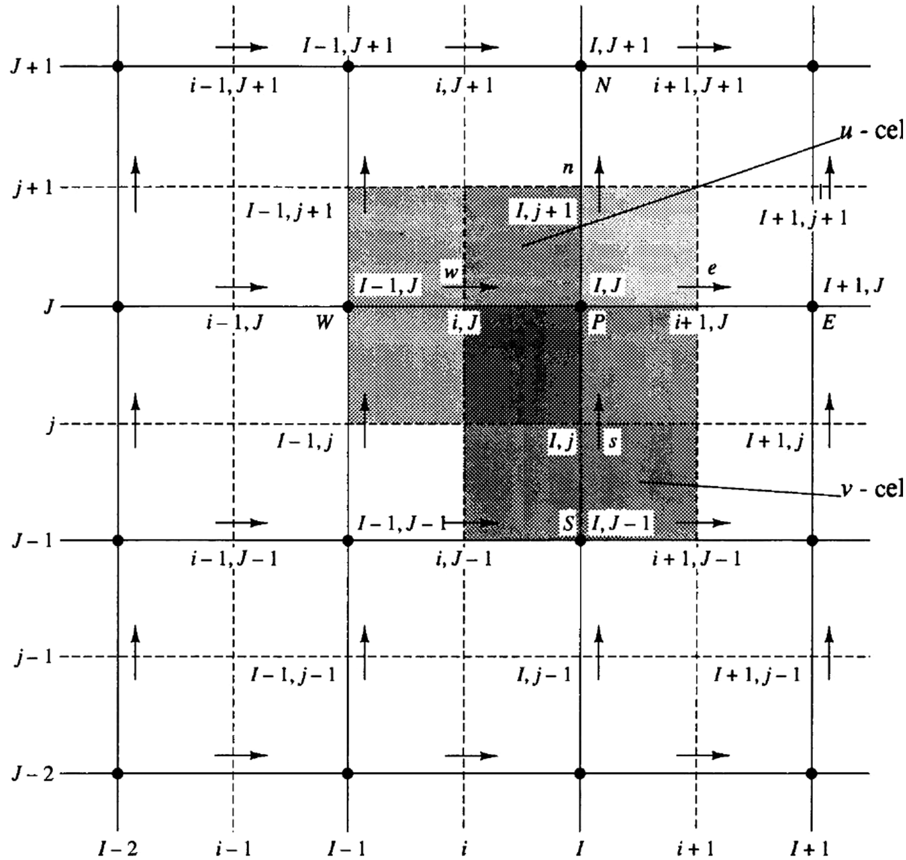

Fig. 2. Staggered grid.

membrane surface where value of concentration is close enough to the inlet value of concentration, so the equilibrium between convective and diffusive fluxes is reached when $\dfrac{C - C_0}{C_0} < 0.001$.

3. Discretization of equations and numerical solution

Navier–Stokes equations together with a mass transfer equation are solved using SIMPLE algorithm based on finite volume method. In discretization of the equations, we used power law scheme. Staggered grid is used for the computational domain (Fig. 2), which is usually used in SIMPLE algorithm [17]. Several researches have been done using finite difference method [9]. Finite volume methods and especially SIMPLE algorithm are commonly used in problems dealing with fluid flow.

In the concentration polarization layer, near the membrane surface, a very refined grid is needed due to the small thickness of concentration polarization layer. To save computational time, this refinement can be applied only for mass transfer equation. For this problem, 70 control volumes in r-direction and 200 control volumes in x-direction were needed to achieve accurate results from solving domain.

A very fine grid was used near the membrane surface in order to capture the mass boundary layer.

In this work, a finite volume based code has been developed with DIGITAL Visual FORTRAN V6.0. The following condition was used for checking the convergency of the numerical solution:

Convergence criterion in interation no.

$$k+1 = \max\left(\left|\frac{\Phi_{i,j}^{k+1} - \Phi_{i,j}^{k}}{\Phi_{i,j}^{k}}\right|\right) < 10^{-10} \qquad (12)$$

4. Results and discussion

The effects of various operating conditions such as geometrical dimensions and Reynolds number on the concentration polarization boundary layer along the length of tubular membrane and as so on the membrane performance are studied. For more understanding of operating conditions, we define non-dimensional quantities as the followings:

$$Re = \frac{\rho u_{\text{ave}} 2R}{\mu},\ Re_{\text{w}} = \frac{\rho V_{\text{w}0} 2R}{\mu},$$
$$Sc = \frac{\mu}{\rho D},\ V_{\text{w}0} = \frac{k}{\mu}\frac{P_0 - P_{\text{e}}}{e} \qquad (13)$$

The tube length is one of the major geometrical characteristic in a tubular membrane. Fig. 3 presents the variation of concentration polarization layer growth along the tube length. As it is shown in the figure, choosing a proper length for membrane is important for having an acceptable performance of the membrane. As it is shown in the figure, the growth rate of mass boundary layer is almost constant at $\frac{x}{R} > 150$.

Increasing Re number by increasing the inlet axial velocity can improve the performance of a tubular membrane. This is because of the decreasing mass boundary layer and so increasing the wall filtration velocity. Fig. 4 presents the numerical results for $250 < Re < 1100$.

The effect of Sc number on the growth of concentration polarization layer is also studied and the results are depicted in Fig. 5.

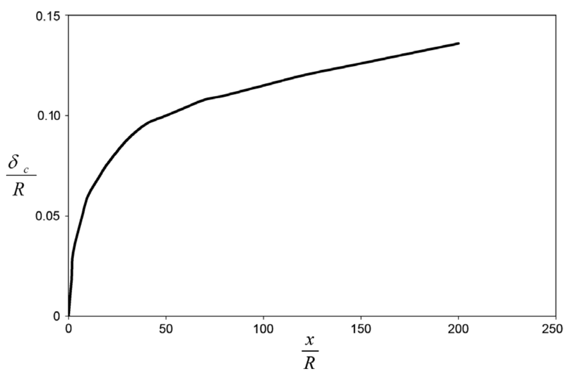

Fig. 3. Growth of concentration polarization layer: $Re = 1000$, $Re_{\text{w}} = 0.1$, $Sc = 1000$.

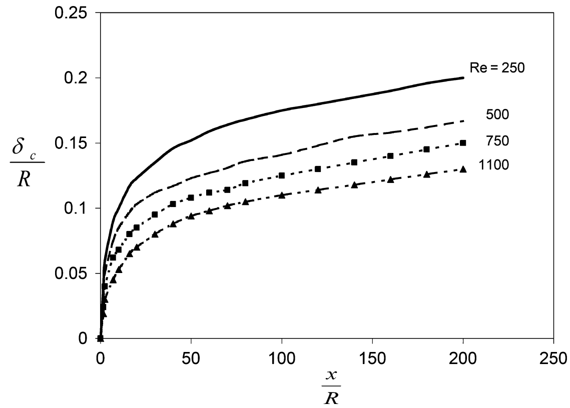

Fig. 4. Variation of mass boundary layer growth along the tube length for different Re numbers: $Re_{\text{w}} = 0.015$, $Sc = 1000$.

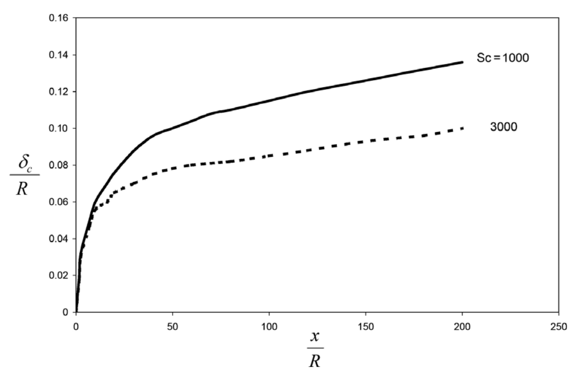

Fig. 5. Variation of mass boundary layer growth with Sc: $Re = 1000$, $Re_{\text{w}} = 0.1$.

5. Conclusions

In the present work, the effects of different operating conditions on the concentration polarization layer have been studied. This has done with developing a numerical finite volume code, using SIMPLE algorithm, for solution of flow and concentration fields. A two-dimensional microfiltration membrane with permeable walls in cylindrical system was considered as the case study. The developed numerical model successfully predicts the fundamental mechanisms involved in flux decline behavior during crossflow filtration. The axial concentration profiles present the important influence of the membrane length which is a very important factor in designing a microfiltration crossflow membrane. The concentration polarization under a wide range of operating conditions has been analyzed in terms of the concentration boundary layer thickness. These numerical results show that a higher axial Reynolds number leads to a decrease of the thickness of the local concentration boundary layer and that a higher Schmidt number leads to a decrease of the thickness of the local concentration boundary layer. It is generally accepted that approaching to turbulent conditions can improve the performance of the membrane.

Nomenclature

a_p	average solute particle diameter
C	solute concentration
C_0	feed concentration
D	diffusion coefficient
e	membrane thickness
L	length of tubular membrane
P	pressure
P_0	inlet pressure
P_e	external pressure
R	radius of the tubular membrane
R_p	the resistance of concentration polarization layer
R_m	the resistance of membrane
r	radial coordinate
r_p	specific resistance of concentration polarization layer
u	axial velocity
u_0	inlet average axial velocity
U_{av}	radial velocity
V_w	local permeation flux
V_{w0}	inlet local permeation flux
x	axial coordinate
δ_p	thickness of concentration polarization layer
κ	permeability
μ	fluid viscosity
ρ	fluid density
ε_p	porosity of cake layer

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