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Computational fluid dynamics modeling and experimental studies of oil-in-water emulsion microfiltration in a flat sheet membrane using Eulerian approach

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ABSTRACT

In the present study, microfiltration of oil-in-water emulsion was experimentally and numerically studied in a flat sheet membrane module. Due to the significance of fluid flow hydrodynamics on the concentration polarization phenomenon and membrane performance, 2D computational fluid dynamics modeling was conducted to simulate oil concentration profile in the mass boundary layer and to predict permeate flux. Multi-phase flow equations, based on an Eulerian multiphase model, for continuous and dispersed phase were solved using Navier–Stokes equations coupled with Darcy's law for the porous media. This novel approach considered the interparticle interactions of oil droplets which led to much more accurate results in comparison with other previous works. Besides, the capabilities of this new model in predicting oil concentration profile and mass boundary layer behavior were checked in different operating conditions, in which the predicted data showed good accordance to the experimental results and CP theory.

1. Introduction

Over the past two decades, pressure-driven membrane systems (PDMS) have received much attention for treatment of oily wastewater due to their effectiveness over the conventional technologies. This technology is usually preferred when the oil concentration is relatively low and/or the droplets are finely dispersed [1]. In addition, because of their moderate operation conditions and cost efficiency, PDMS have been widely applied in industrial unit operations [2,3]. Nevertheless, fouling and concentration polarization (CP) have been recognized drawbacks in these processes. Increasing the solute concentration in regions close to the membrane surface leads to formation of a concentrated boundary layer near it and may create a gel layer over the membrane wall. This is known to have negative effects on the permeate flux by causing a positive concentration profile toward the membrane surface and increases the back diffusive transport of the solute to the main stream [4].

In order to understand the complex feature of membrane fouling and CP, many experimental and theoretical researches have been conducted [5–8]. Computational fluid dynamics (CFD) provides a more robust approach capable of considering many parameters and provides accurate results through the numerical solution of mass, momentum and energy conservation [5,9,10]. Most previous attempts have investigated the effects of different kinds of turbulence promoters such as baffles [11,12], spacers [9,13], design of new geometries [14], gas sparged modules [15,16] and operating parameters on flow hydrodynamics, mass boundary layer and permeation flux [17–22]. In some studies, the membrane has been considered as an impermeable wall [11–14,17,20,22–25]. In these studies, the effects of low permeate flux were neglected and only the effects of turbulence on flow hydrodynamics were taken into consideration. Consequently, the effect of membrane transport mechanism on the flow hydrodynamics was neglected.

Monfared et al. [26] carried out a CFD model to investigate six different arrangements of baffles. By comparing permeate flow versus time in six baffle arrangement as well as a simple channel without any baffles, they recommended the central baffling as the most efficient baffle arrangement in a rectangular channel. Koutsou et al. [27] performed a numerical simulation of flow in a channel with a regular array of cylindrical turbulence promoters over a range of Reynolds numbers, to gain insight about transport phenomena in membrane elements. They showed that the flow becomes unstable at a critical Reynolds number. Furthermore, qualitative flow features and quantitative statistical characteristics were investigated.

Later, Schwinge et al. [13] studied the effect of spacer filaments on flow patterns in narrow spacer-filled channel for spiral-wound membrane system using CFD code. They investigated the dependence of the recirculation formation regions on the filament

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configuration, mesh length, filament diameter, and the Reynolds number. In addition, Saeed et al. [28] used CFD tools to analyze the effects of flow patterns through a spacer-filled Reverse Osmosis (RO) membrane with secondary structure of the membranes at various angles to the inlet flow. They observed that the feed spacers in the membrane channel led to secondary flow patterns, which increased the prospects for self-induced backwashing and enhanced the allowable operational time and membrane efficiency.

Many studies have also dealt with the simulation of laminar conditions in empty membrane channels [5,10,14,29–33]. The first simulations of flow in a membrane were undertaken under laminar conditions in channels with porous walls. The calculations of CP have been based on the solution of continuity, Navier–Stokes and solute continuity equations by incorporating film theory, in which the true rejection and permeation flux were considered. The boundary condition for membrane in CFD simulation is regarded by constant rejection and constant or variable permeation flux [5,10,14,33]. In addition, a fixed solute concentration higher than that of the feed bulk is suggested as the boundary condition on the membrane wall for considering the mass boundary layer formed due to CP. However, these simplifying assumptions might lead to unrealistic evaluation of CP [9,26,28,34]. Recently, some CFD studies have also been done which consider both rejection and permeate flux to be variable, where Keir and Jegatheesan reviewed CFD applications in pressure driven membrane filtration [35] and predicted solute rejection and concentration polarization in such processes [36].

Ahmad et al. [5] used CFD simulation to predict the CP profile and mass transfer coefficient in the empty narrow membrane channel. In this study, the permeate flux was assumed to be constant and the effect of different operation condition on CP was studied. It was reported that the simulated results had a satisfactory agreement with the literature data.

In order to gain more accurate results and reduce errors, some studies were conducted considering Darcy's permeation law. They could predict the membrane permeate flux locally, based on local pressure distribution profile on the membrane surface in their computational domain [29,30,37–39]. Rahimi et al. [40] developed a 3D CFD simulation to predict water flux through a microfiltration membrane. They obtained the localized permeate flux by using local pressures in Darcy's equation. The experimental results indicated that the CFD flux prediction is more accurate with this assumption. It should be noted that the CFD study was done for a single-phase and the dispersed phase equations were not considered.

Gas–liquid two-phase flow regimes have also been also modeled using a Volume of Fluid (VOF) method and have been reviewed in a recent paper [41]. These studies have mostly modeled flow hydrodynamics in both phases and predict shear stress and mass transfer coefficients on the membrane surface and around the gas slugs. In other two phase flow systems containing solid as the solute and/or oil droplets as the dispersed liquid phase, CFD modeling has been usually done based on the single-phase equations. In other words, no conservation law has been considered for the dispersed phase, which leads to more errors. Besides, the availability of CFD modeling and simulations of CP in membrane separation of oil-in-water emulsion was found to be limited.

In the previous work [8], a 2D CFD modeling and simulation was conducted to predict fluid flow hydrodynamics and CP of oil-in-water emulsion in a flat sheet microfiltration module using Mixture model. Although the velocity profile was successfully modeled in different Reynolds numbers and flow patterns, the Mixture model failed to predict CP layer accurately. It was concluded that the failure might have been the result of assumptions made to simplify the model such as neglecting the inter-particle interactions of oil droplets and neglecting the interaction between oil droplets and the membrane surface.

To address this problem, multi-phase flow equations based on Eulerian multiphase model were solved for both continuous and dispersed phase. The oil was dispersed in water in the form of spherical micelles (diameter = 1 μm). The membrane actual permeation flux and its effect on flow hydrodynamics were considered based on the Darcy's permeation law through the calculation of local pressure distribution in the computational domain. The effect of different operating conditions on the growth of concentration polarization layer along the membrane surface was also successfully modeled.

2. Development of the CFD modeling

2.1. Problem description and model geometry

The channel geometry generated as a solution domain and the imposed boundary conditions for this model is schematically shown in Fig. 1a. As depicted, the feed channel was a rectangular slit with dimensions of $0.3 \times 5 \times 10\ cm^3$ as height, width and length of the rectangle, respectively. The membrane active surface area was the lower $5 \times 10\ cm^2$ wall. Since the ratio of height to width of the feed channel of membrane module was far less than unity ($H/W \cong 0.06$), the model was considered to be two-dimensional for CFD calculations (Fig. 1b). Therefore, a $0.3 \times 10\ cm^2$ rectangle (longitudinal cross-section of feed channel) was considered as the computational domain. In addition, a rectangle with dimension of $0.1 \times 10\ cm^2$ as permeate channel was considered under the feed channel. This consideration was made only due to membrane transport phenomena calculations.

2.2. Governing equations

The fluid flow hydrodynamics on the membrane surface in a cross-flow microfiltration process can be discretized by solving the governing equations. The flow was assumed to be laminar, incompressible, having constant physical properties, and isothermal. The governing equation involves continuity Eq. (1) and Navier–Stokes Eq. (2) which are expressed as

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \vec{u}) = 0 \tag{1}$$

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla(\rho \vec{u}\,\vec{u}) = \nabla P + \rho \vec{g} + \rho \vec{F} \tag{2}$$

where ρ is density, $\vec{u}$ is the velocity vector and $\vec{F}$ is the body forces. These equations were coupled with Darcy's law for permeation transport as a momentum source term. In other words, the effects of porous media were modeled by the addition of a momentum source term to the standard fluid flow equations. The source term is composed of two parts: a viscous loss term, and an inertial loss term. Therefore the momentum and continuity equation are as follows:

$$\frac{\partial(\gamma\rho u)}{\partial x} + \frac{\partial(\gamma\rho v)}{\partial x} = 0 \tag{3}$$

$$u\frac{\partial(\gamma\rho u)}{\partial x} + v\frac{\partial(\gamma\rho v)}{\partial y} = -\gamma\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}\mu\gamma\left(\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\mu\gamma\left(\frac{\partial u}{\partial y}\right) - \left(\frac{\mu}{k} + \frac{C_{2y}\rho}{2}|u|\right)\vec{u} \tag{4}$$

$$u\frac{\partial(\gamma\rho v)}{\partial x} + v\frac{\partial(\gamma\rho v)}{\partial y} = -\gamma\frac{\partial P}{\partial y} + \frac{\partial}{\partial x}\mu\gamma\left(\frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\mu\gamma\left(\frac{\partial v}{\partial y}\right) - \left(\frac{\mu}{k} + \frac{C_{2y}\rho}{2}|v|\right)\vec{v} + \gamma\rho g \tag{5}$$

where ρ is density, μ is viscosity, γ is the porosity of the membrane, P is the field pressure, k is the permeability, C_2 is the inertial resistance factor, and u and v are velocity components in x and y directions, respectively. In the porous media, the velocity in the x