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# CFD modeling and simulation of concentration polarization in microfiltration of oil–water emulsions; Application of an Eulerian multiphase model

Mehrdad Zare, Farzin Zokaee Ashtiani *, Amir Fouladitajar

*Department of Chemical Engineering, Amirkabir University of Technology, No. 424, Hafez Ave., Tehran, Iran*

## HIGHLIGHTS

- CP phenomenon was modeled using CFD technique in microfiltration of oily water.
- An Eulerian multiphase model was used to solve oil concentration for the first time.
- The model showed high capability to predict CP behavior in different conditions.
- The model needs modifications to predict permeate flux accurately.

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## ABSTRACT

In this study, a 2D CFD modeling and simulation of concentration polarization (CP) phenomenon in microfiltration of oil–water emulsion in a narrow rectangular membrane module was presented. As the novelty of this research, an Eulerian based multiphase method was investigated for the first time to capture the concentration of emulsified oil droplets in different extents of membrane module. It was shown that this new model is highly compatible with concentration polarization theory and is highly capable for determining CP profile and mass boundary layer behavior in different operating conditions, as well. In this research it was proved that under developed feed cross-flow shows better performance in terms of membrane surface cleaning. Also it was shown that a small portion of oil droplets accumulates at the roof of membrane module feed channel due to gravity. The simulation results proved that for under developed feed cross-flows, lower feed Reynolds number induces a lower CP profile peak despite increasing the oil droplet concentration on membrane surface and at the feed channel roof.


## 1. Introduction

Oily waste-water is one of the most important pollutants emitted into the environment. These oil contaminated waters are generated daily worldwide in many diverse industries such as petroleum refinery, petrochemical, metal and steel, textile and machine industries [1,2]. For the oily wastewater treatment, the conventional technologies are not efficient enough to treat the stable oil–water emulsions, with oil droplets smaller than 20 μm, especially when the oil concentration is pretty low and the droplets are finely dispersed. To address this problem membrane processes have been increasingly investigated for treating oil–water emulsions. The first attempts to treat oily water by membrane separation processes were made in the beginning of 70's decade [3].

In recent decades pressure driven membrane separation processes have been playing an important role in industrial unit operations due to their moderate operational conditions and cost efficiency [4]. However these processes are suffered by fouling phenomena causing permeate flux decline which is undesirable and in some cases may be irreversible [3]. A solute concentration which is higher in regions close to the membrane surface in comparison to the bulk free stream, leads to the concentration polarization, CP, phenomenon which arises from the nature of microfiltration and ultrafiltration processes [5]. This phenomenon affects the permeate flux negatively by introducing a positive concentration profile toward the membrane surface causing back-diffusion of solute rejectants from membrane surface to the bulk [5].

Therefore, numerous studies have been accomplished by researchers experimentally, mathematically and numerically to achieve insight knowledge about membrane fouling, especially concentration polarization.

Many of these studies employed CFD simulation techniques due to the accuracy of the results which are yielded through the numerical solution of conservation of mass, momentum, and energy [6].

A large number of these studies have been performed over the last two decades and are devoted to investigate the effects of different

* Corresponding author. Tel.: +98 21 6454 3124; fax: +98 2166405847.
*E-mail address:* zokaee@aut.ac.ir (F. Zokaee Ashtiani).

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types of baffles, spacers and other types of turbulent promoters and their orientation and spatial configuration on flow hydrodynamics and concentration boundary layer disruption. These effects have been considered in terms of parameters such as wall sheer stress, mass transfer coefficients, friction factor, power number, etc. [6–17]. Also some researches are about the CFD calculations for new membrane module designs or special turbulence promoting modules such as gas sparged ones to demonstrate their effects on flow hydrodynamics, mass boundary layer, and permeation flux [18–27]. In this category, some authors neglected the effects of low permeate flux by considering the membrane as an impermeable wall and fully focused on studying the effects of the promoted turbulence on flow hydrodynamics [7,12,14,15,17,20,21,23–27]. Consequently the effect of membrane transport mechanism on the flow hydrodynamics was neglected.

Liu et al. [14] conducted a CFD simulation to evaluate the effects of baffles on turbulent flow in a tubular membrane module. They showed that using baffles significantly increases the wall shear stress and improves the separation performance. Furthermore, it was proved that central baffles are more effective than wall baffles in producing wall shear stress and result in a higher permeation flux.

Karode and Kumar [17] visualized the flow in a spacer filled rectangular channel. Despite the previous reports, it was revealed that the bulk of fluid flows along the spacer filaments and does not change direction at each spacer node. Also, it was proved that spacers with unequal filament diameters exert lower pressure drop to the fluid flow.

On the other hand, some researchers made the assumption of a fixed solute concentration, higher than that of the feed bulk, as a boundary condition on the membrane wall (impermeable wall) to consider the mass boundary layer formed due to concentration polarization phenomenon. Then, they evaluated the effects of the promoted turbulence on the mass boundary layer disruption [6,9,11,16]. These assumptions might lead to a more detailed but unrealistic evaluation of concentration polarization phenomenon.

Santos et al. [6] performed a CFD simulation to investigate the flow pattern for 12 different flow-aligned using cyclic boundary condition. They analyzed the results in terms of shear rate, mass transfer and a modified form of friction factor. It was proved that the modified friction factor can be used to determine the best spacer configuration to achieve higher mass transfer.

Shakaib et al. [9] carried out a CFD simulation to investigate the flow and mass transfer in spacer filled channel of a spiral wound membrane module. They proved that axial and transverse spacer filaments exert higher shear stress at the top membrane wall but the mass transfer rate remained almost the same.

In contrast, some studies have been conducted to model the empty membrane channel with laminar flow condition [13,28–38]. In these studies the attempt was to consider the impact of membrane transport mechanism on flow hydrodynamics. The calculations of concentration polarization were conducted through the solution of continuity, Navier–Stokes and solute continuity equations by incorporating "Film Theory" which is based on true rejection and permeation flux. In these studies the impact of membrane transport mechanism on flow hydrodynamics was calculated by considering constant rejection and constant or variable permeation flux as a boundary condition for membrane in CFD calculations [30,32,33,38].

Ahmad et al. [32] performed a CFD modeling of concentration polarization in a narrow rectangular membrane channel by assuming fixed permeate flux for the membrane. They investigated the effects of different operating conditions on CP and showed that there was a good agreement between simulation results and literature data.

But the assumption of fixed/variable permeation-rejection might lead to introducing errors to the calculation of concentration polarization. Hence some authors tried to improve the accuracy of these calculations by introducing the Darcy's permeation law to the CFD codes to predict the membrane permeate flux locally, based on local pressure distribution profile on the membrane surface in the computational domain [29,31,34–37].

Pak et al. [29] developed a 2D CFD code to simulate concentration polarization for a porous membrane using Darcy's permeation law as a boundary condition for the membrane. They showed that with this assumption the CFD model may have a better agreement with experiment results.

Following this, some researchers employed Darcy's permeation law, solute continuity equation and film theory in conjunction with turbulence promoters to calculate a more accurate solution of turbulent dominated membrane modules [8,10,13]. Using Darcy's permeation law, Wardeh and Morvan [13] carried out a CFD simulation of a spacer-obstructed rectangular membrane module. They proved that zigzagging type spacers are more efficient in concentration polarization disruption.

Since the first attempts for treating oily wastewater by membrane in early 1970's, several studies have been done to achieve insight knowledge about different membrane separation of oil–water emulsion systems and concentration polarization. Most of these studies are limited to experiments and mathematical modeling where valuable results have been achieved; however numerical modeling of such systems has received less attention [3,39–47]. Besides, the availability of CFD modeling and simulations of concentration polarization in membrane separation of oil–water emulsion was found to be limited.

Addressing this problem, in the current study, a 2D finite volume model was developed for CFD modeling of laminar flow in cross flow microfiltration of oil–water emulsion in an empty rectangular channel. 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 oil was intended to be dispersed in water in the form of spherical micelles. As the novelty of this study, multi-phase flow equations based on Eulerian multiphase model were investigated in CFD calculations to yield more accurate and realistic results.

## 2. Theory

### 2.1. Module geometry and problem description

In the current study, the focus was on CFD modeling and simulation of concentration polarization in cross-flow microfiltration of oil–water emulsion in an empty rectangular membrane module. The feed channel was a rectangular slit with dimensions of $0.3 \times 5 \times 10$ cm as height, width and length of the rectangle, respectively. The porous membrane was as the lower $5 \times 10$ cm wall of the slit. The permeate channel was at the same shape and dimensions, as well. The feed was a mixture comprising water as continuous phase, containing emulsified oil as dispersed phase in the form of micelles of diameters of about 1 μm. The oil density and viscosity were intended to be 850 kg/m$^3$ and 0.00332 kg/ms, respectively. The membrane module was fed by different oil concentrations of 200, 1000, 5000 and 20,000 ppm. Also different operating conditions in terms of trans-membrane pressure (TMP) and cross-flow velocity were applied in the problem. The process was conducted in different TMPs of 0.5, 1, and 2 bar, and cross-flow velocities corresponding to the Reynolds numbers of 500, 1300 and 2200.

### 2.2. Geometry reconstruction and grid generation

According to geometry dimensions noted in previous section, the ratio of height to width of the feed channel of membrane module was far less than unity (H/W ≅ 0.06). Hence the effects of side walls on flow hydrodynamics were neglected, and in order to reduce computational costs, the model was intended to be two-dimensional for CFD calculations. Therefore, a $0.3 \times 10$ cm rectangle (longitudinal cross-section of feed channel) was considered as the computational