Integrated CFD simulation of concentration polarization in narrow membrane channel

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Abstract

Numerous analyses on the mass transfer phenomena and hydrodynamics for the fluid adjacent to the membrane have been studied and visualized by computational fluid dynamics (CFD) mathematical modeling and simulation. The availability of CFD simulation study to reveal the concentration polarization profile in the membrane channel, which considering hydrodynamics and membrane transport properties is found to be limited. The main goal of this paper is targeted to the utilization of CFD simulation using commercial CFD package FLUENT to predict the concentration polarization profile, mass transfer coefficient and wall shear stress under different types of conditions in the empty narrow membrane channel. The permeation conditions such as permeation flux and mass fraction have been taken into account in the solution of the governing equations. Simulation results show that the concentration polarization phenomena can be reduced by increasing feed Reynolds number. The decrease of wall shear stress also contributes to the formation of the concentration polarization layer along the membrane surface. The simulated results were validated and compared with the literature data, showing a satisfactory agreement.

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Keywords: Computational fluid dynamics (CFD) simulation; Concentration polarization; Membranes; Fouling; Hydrodynamics; Mass transfer

1. Introduction

During the past decades, analyses for the hydrodynamics and the fluid flow pattern adjacent to the membrane have been studied and visualized by computational fluid dynamics (CFD) mathematical modeling and simulation. These studies are crucial due to the variation of hydrodynamics condition for the fluid adjacent to the membrane can influence the permeation and solute rejection mechanisms across the membrane (Avlonitis, Sakellaropoulos, & Hanbury, 1995; Costa & Dickson, 1991; Marriott, & Sorensen, 2003; Zimmerer & Kottke, 1996).

Li, Meindersma, de Haan, and Reith (2002) had carried out three-dimensional laminar CFD simulation for the spiral wound membrane (SWM) feed channel to evaluate the mass transfer coefficients and power consumption for commercial net spacers. The authors had investigated on the relation between the Sherwood and power numbers using three-dimensional CFD transient models for low-Reynolds flows in non-woven spacer-filled channel. The study had revealed an optimum ratio for channel height over spacer length to yield maximum mass transfer coefficient with moderate power consumption. Consequent study had also been conducted experimentally to validate the optimum ratio (Li, Meindersma, de Haan, & Reith 2004).

Meanwhile, study on CFD simulation for the spacer-filled channel to evaluate the velocity profile and turbulent kinetic energy distributions had been conducted by Cao, Wiley, and Fane (2001). The study had proven the existence of the spacer is plausible to improve the local shear stress on the membrane surface and produces eddy activities for mass transfer enhancement and fouling reduction. CFD simulations had also been utilized to reveal complex relationships between filament configurations, mesh length, filament diameter and Reynolds number (Schwinge, Wiley, & Fletcher, 2002). The
The availability of CFD simulation study to reveal the concentration polarization profile, which considering hydrodynamics and membrane transport mechanisms in the membrane channel is found to be limited. For the CFD mathematical modeling, it is constraint to the two-dimensional laminar fluid flow for the membrane channel studies. Hence, a comprehensive CFD simulation which considering hydrodynamics and membrane transport properties is crucial as an alternative to portray the actual fluid flow condition in the

study had concluded that the variations in grid size and time steps must be carefully examined to ensure the prediction for time-dependent flow movements in spacer-filled channel not influenced by those factors. Modifications in boundary condition in CFD simulation can offer significant savings in computational time and costs. Hence, periodic boundary conditions in the stream wise direction had been employed as an alternative to portray the actual fluid flow condition in the membrane channel or two-dimensional spacer-filled channel assuming laminar fluid flow condition. However, there are some limitations by employing CFD mathematical modeling method to model spacer-filled membranes channel. Since these numerical codes had been specially developed for two-dimensional domain, CFD mathematical modeling typically is restricted to simple two-dimensional domain. Subsequently, the orientations of spacer in three-dimensional membrane channel tend to be neglected as a result of the employment of two-dimensional domain.

The availability of CFD simulation study to reveal the concentration polarization profile, which considering hydrodynamics and membrane transport mechanisms in the membrane channel is found to be limited. For the CFD mathematical modeling, it is constraint to the two-dimensional laminar fluid flow for the membrane channel studies. Hence, a comprehensive CFD simulation which considering hydrodynamics and membrane transport properties is crucial as an alternative to portray the actual fluid flow condition in the

Inevitably, the improvements in CFD simulation technique and methodology had accelerated the simulations speed and offer the visualization of fluid flow pattern in the complex three-dimensional spacer-filled domain. However, CFD simulations for fluid flow in the membrane channel developed by researchers mentioned above are found to be restricted to the hydrodynamics condition prediction for the fluid adjacent to the membrane which assuming membrane as an impermeable wall with zero concentration build-up. This assumption has neglected the mass transport across the membrane and might leads to the incorrect assessment of the concentration polarization phenomenon. To overcome this problem, Wiley and Fletcher (2003) had conducted two-dimensional CFD simulation, which involved concentration polarization prediction. They had integrated the wall concentration value with the adjacent fluid hydrodynamics to suit the particular CFD simulation with the commercial finite control volume simulator CFX 4. At the membrane, a constant rejection and constant or variable permeation rate were specified while the tangential velocity was set to zero.

To give a better description of concentration polarization, CFD mathematical modeling had been applied as a rigorous tool to model concentration polarization through the solution of the continuity, Navier-Stokes and solute continuity equations. Film theory, which constructed based on true rejection and permeation flux had been incorporated in the membrane boundary condition. Special numerical code had been developed for two-dimensional domain to yield the fluid flow profile and membrane permeation data (Geraldes, Semiao, & Pinho, 2000). Geraldes et al. (2001) had applied this technique to reveal the hydrodynamics and the membrane transport mechanism in the empty membrane channel. Similar technique had also been utilized by Pinho, Semiao, and Geraldes (2002) to determine and compared the intrinsic rejection coefficients obtained from experiment and simulations. Modified governing equation in stream function and vorticity had also been utilized to link the membrane transport equation for the computation of fluid flow and membrane transport profile in the empty membrane channel (Miranda & Campos, 2001). Besides, membrane channel filled with ladder type spacer had been discretized in two-dimensional and laminar condition to predict the concentration polarization profile by the employment of this CFD mathematical modeling method (Geraldes, Semiao, & Pinho, 2002a, 2002b, 2003). Hence, CFD mathematical modeling methods are excellent solutions for the empty membrane channel or two-dimensional spacer-filled channel assuming laminar fluid flow condition. However, there are some limitations by employing CFD mathematical modeling method to model spacer-filled membranes channel. Since these numerical codes had been specially developed for two-dimensional domain, CFD mathematical modeling typically is restricted to simple two-dimensional domain. Subsequently, the orientations of spacer in three-dimensional membrane channel tend to be neglected as a result of the employment of two-dimensional domain.

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<table>
<thead>
<tr>
<th>Nomenclature</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( d_w )</td>
<td>distance of membrane adjacent node to membrane wall</td>
</tr>
<tr>
<td>( D_{AB} )</td>
<td>binary mass coefficient ((m^2/s))</td>
</tr>
<tr>
<td>( h )</td>
<td>channel height</td>
</tr>
<tr>
<td>( J_p )</td>
<td>permeate volume flux ((m/s))</td>
</tr>
<tr>
<td>( k )</td>
<td>mass transfer coefficient ((m/s))</td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>average mass transfer coefficient ((m/s))</td>
</tr>
<tr>
<td>( l )</td>
<td>narrow membrane channel length ((m))</td>
</tr>
<tr>
<td>( m_A )</td>
<td>solute mass fraction ((kg solute/kg solution))</td>
</tr>
<tr>
<td>( Re )</td>
<td>feed Reynolds number ((Re = \mu u/\rho))</td>
</tr>
<tr>
<td>( Sc )</td>
<td>Schmidt number ((Sc = \mu/\rho D_{AB}))</td>
</tr>
<tr>
<td>( u )</td>
<td>velocity in (x)-direction ((m/s))</td>
</tr>
<tr>
<td>( v )</td>
<td>velocity in (y)-direction ((m/s))</td>
</tr>
<tr>
<td>( x )</td>
<td>(x) coordinate</td>
</tr>
<tr>
<td>( y )</td>
<td>(y) coordinate</td>
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</table>

<table>
<thead>
<tr>
<th>Greeks letters</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{\Gamma} )</td>
<td>concentration polarization factor, defined by ( \bar{\Gamma} = (m_{uH}/m_{uA}) - 1 )</td>
</tr>
<tr>
<td>( \tau_w )</td>
<td>wall shear stress ((Pa))</td>
</tr>
<tr>
<td>( \rho )</td>
<td>density ((kg/m^3))</td>
</tr>
<tr>
<td>( \mu )</td>
<td>viscosity ((kg/m s))</td>
</tr>
<tr>
<td>( \Delta P )</td>
<td>transmembrane pressure ((Pa))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta )</td>
<td>feed solution</td>
</tr>
<tr>
<td>( p )</td>
<td>permeate side</td>
</tr>
<tr>
<td>( w )</td>
<td>solution adjacent to the wall</td>
</tr>
</tbody>
</table>
membrane channel. The objectives of this paper are aimed to the manipulation of CFD simulation using commercial CFD package FLUENT v6 to anticipate the concentration polarization profile, mass transfer coefficient and wall stress under different types of conditions in the narrow membrane channel. The permeation conditions such as permeation flux and mass fraction have been taken into account in the solution of the governing equations.

2. Computational fluid dynamic methodology

2.1. Governing equations

The hydrodynamics of the fluid flow condition can be discretized by the solution of the governing equations. The governing Eqs. (1)–(4) shown below were used to solve laminar fluid flow for two-dimensional membrane channel domain with the consideration of solute concentration variation.

Continuity equation:
\[ \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0 \]  

(1)

Navier–Stokes equation in x-direction:
\[ \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} \right) \]  

(2)

Navier–Stokes equation in y-direction:
\[ \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left( \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial v}{\partial y} \right) \]  

(3)

Solute conservation equation:
\[ \frac{\partial (\rho u m_A)}{\partial x} + \frac{\partial (\rho v m_A)}{\partial y} = \frac{\partial}{\partial x} \left( \rho D_{AB} \frac{\partial m_A}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D_{AB} \frac{\partial m_A}{\partial y} \right) \]  

(4)

Section 2.6 would be discussing the detail solution methods for these equations. The turbulence effects can be incorporated by employing CFD simulation but it was neglected in this CFD simulation due to the absence of spacers, which potentially create turbulence in the narrow channel. Hence, steady state and laminar condition was assumed for fluid flow in the narrow empty membrane channel.

2.2. Computational domain generation

The computational domain was shown in Fig. 1. The simulated domain was 200 mm in length and 0.7 mm height. In order to eliminate the effect of mesh quality and size on the results, initial simulations were carried out with four mesh resolutions, 50 × 40, 50 × 50, 100 × 100 and 200 × 200. Fig. 2a shows the grid dependency test, which determined the optimum simulation grid size for the simulation domain. Based on the results, when the resolution was increased above 50 × 50, it had little effect on the solution in terms of membrane wall mass fraction. Hence, the computational grid was constructed with 50 × 50 cells. Approximately 80% of the
the channel was assumed to be exist in a fully developed condition where all changes for the flow parameters was equal to zero. No-slip condition where \( u = 0 \) was fixed for the wall and membrane interface. Due to the limitation of the solver, wall boundary condition (refer to Eq. (9)) with the incorporation of user defined function (UDF) was used to model the concentration profile for the membrane interface (assuming \( v = 0 \)). The special functions for UDF will be explained in Section 2.5. Permeate flux \( (J_m) \) and mass fraction \( (m_{AP}) \) is assumed to be constant along the flow channel. The permeate volume flux \( (J_v) \) and mass fraction \( (m_{AP}) \) values were obtained from literature (Pinho et al., 2002).

Mathematically, these boundary conditions are expressed as follows:

For \( x = 0 \) and \( 0 < y < h \),

\[
\begin{align*}
\frac{\partial u}{\partial x} &= 0; \\
\frac{\partial v}{\partial x} &= 0; \\
\frac{\partial m_A}{\partial x} &= 0
\end{align*}
\]

(7)

For \( x = l \) and \( 0 < y < h \),

\[
\begin{align*}
\frac{\partial m_A}{\partial x} &= 0
\end{align*}
\]

(8)

For \( y = 0 \) and \( 0 < x < l \),

\[
\begin{align*}
u &= 0; \\
\frac{\partial v}{\partial x} &= 0; \\
J_m \frac{\partial m_A}{\partial y} + J_v \times m_A &= J_v \times m_{AP}
\end{align*}
\]

(9)

For \( y = h \) and \( 0 < x < l \),

\[
\begin{align*}
u &= 0; \\
\frac{\partial v}{\partial x} &= 0
\end{align*}
\]

(10)

2.5. User defined function (UDF)

Basically, UDF is written in ‘C’ programming language. It can access FLUENT solver data using predefined macros or function supplied by the simulator. The UDF would be interpreted and hooked to the solver during simulation. This UDF would access the solver data, perform calculation on the data and update the solver data repeatedly for every iteration.

Under normal simulation without UDF integration, there is only one way to define boundary condition for membrane interface. Typically, Dirichlet boundary condition will be used to simulate the concentration profile for this semi-permeable surface. This constant boundary condition value is not suitable to model the membrane interface since the concentration on the membrane interface will varies according to the fluid hydrodynamics and the membrane transport properties. By integrating UDF file in current simulation domain, boundary condition for the concentration profile in the membrane interface would be more accurately predicted. This was due to the incorporation of Robin boundary condition which describing the film theory for the concentration profile in the membrane boundary condition. ‘Define Profile’ macro would be utilized parallel with the adjacent cell index to represent the film theory which links the relation between the hydrodynamics and the membrane transport phenomena.

---

### Table 1

<table>
<thead>
<tr>
<th>Feed Reynolds number ( (Re = \mu_0 u_0/K) )</th>
<th>1</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>400</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>700</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>400</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1000</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1300</td>
<td></td>
</tr>
</tbody>
</table>

**Simulation conditions for feed concentration, 0.2 g/kg**

Table 1: Solution physical transport properties for NaCl, valid for \( m_A < 0.0091 \) kg kg\(^{-1}\)

<table>
<thead>
<tr>
<th>Viscosity, ( \mu ) (10(^{-3}) Pa s)</th>
<th>0.891 x 1.63(mA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Binary diffusion coefficient, ( D_{AB} ) (10(^{-9}) m(^2)/s)</td>
<td>1.61 x 14(mA) for ( m_A &lt; 0.006 )</td>
</tr>
<tr>
<td>Density, ( \rho ) (kg/m(^3))</td>
<td>997.1 x 0.94(mA)</td>
</tr>
</tbody>
</table>

Geraldes et al. (2001).

---

### Table 2

<table>
<thead>
<tr>
<th>( \Delta P ) (MPa)</th>
<th>Feed Reynolds number ( (Re = \mu_0 u_0/K) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>400</td>
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<tr>
<td>1</td>
<td>700</td>
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<tr>
<td>1</td>
<td>400</td>
</tr>
<tr>
<td>1</td>
<td>1000</td>
</tr>
<tr>
<td>1</td>
<td>1300</td>
</tr>
</tbody>
</table>

| 2 | 100 |
| 2 | 400 |
| 2 | 700 |
| 2 | 1000 |
| 2 | 1300 |

| 3 | 100 |
| 3 | 400 |
| 3 | 700 |
| 3 | 1000 |
| 3 | 1300 |

---

2.3. Simulation conditions

For the feed material condition, solute (A)–solvent (B) system, which consist of sodium chloride (NaCl) and water were defined before executing the simulation loops. Three different types of transmembrane pressure (\( \Delta P \)) were utilized in this simulation. The permeate volume flux \( (J_v) \) and mass fraction \( (m_{AP}) \) under these transmembrane pressure were obtained from literature (Pinho et al., 2002). The length and the height of the membrane channel were identical with the dimensions reported in the literature (Pinho et al., 2002). The details of the simulation conditions and transports properties were summarized in Tables 1 and 2.

2.4. Boundary conditions

The boundary conditions which describing the current simulated computational domain was represented by Eqs. (7)–(10). A plug flow velocity inlet was applied in the entrance of the membrane channel. Top part of the channel was assumed to be impermeable wall. Fluid flowing out of the channel was assumed to be impermeable wall. Fluid flowing out of the channel was assumed to be impermeable wall.
and concentration data from the published literature (Pinho et al., 2002) would be used to construct the film theory relationship which links the concentration value for membrane adjacent cell and the membrane boundary condition. Any changes in the fluid flow adjacent to the membrane interface will be computed by the UDF with the prediction of new membrane wall concentration. This specific UDF would update the solver data with this new membrane wall concentration. Fig. 3 shows the mechanism for UDF to access and update the solver data.

2.6. Solution method

FLUENT v6 was used as the CFD simulation package in this work to visualize the flow condition in this narrow membrane channel. Discretization of the governing equations was carried out based on control volume technique. The discrete velocities and pressures were stored by a non-staggered system, which consists of cells and faces. These values were stored in the cells center. The velocity and pressure parameters would be linked and solved by SIMPLE algorithm and accelerated by algebraic multigrid solver (AMG).

The detailed of the simulation procedures were demonstrated in Fig. 4. Fluid properties were updated, based on the current solution. If the calculation has just begun, the fluid properties would be updated based on the initialized solution. The Navier–Stokes equations (Eqs. (2) and (3) in x and y directions were solved in turn using current values for pressure and face mass fluxes, in order to update the velocity field. Since the velocities obtained earlier might not satisfy the continuity equation (Eq. (1)) locally, SIMPLE algorithm would be used as the pressure correction equation to obtain the necessary corrections to the pressure and velocity fields and the face mass fluxes such that continuity was satisfied. Equation for scalars such as solute conservation (Eq. (4)) was solved using the previously updated values of the other variables. A check for convergence of the equation set was made. These steps were continued until the convergence criteria were met.

Due to the laminar conditions in the membrane channel, steady state simulation was used. The convergence criterions for the velocity and temperature parameters were fixed to 0.001%. Higher convergence criterion was set for solute NaCl (0.00001%) to offer sufficient iteration for complete convergence between boundary grid and the interior mesh grid.

2.7. Predicted parameters

Concentration polarization layer thickness, \( \delta \) will be evaluated from the simulated solute mass fraction adjacent to membrane, \( m_{AW} \) according to the film theory:

\[
\delta = \ln \left( \frac{m_{AW} - m_{AP}}{m_{AW} - m_{A0}} \right) \times D_{AB} \frac{J_v}{F_e} \tag{11}
\]

Average concentration polarization layer thickness, \( \bar{\delta} \) will be evaluated by numerical integration over the membrane channel length.

\[
\bar{\delta} = \frac{1}{L} \times \int_0^L \delta(x) \, dx \tag{12}
\]
Mass transfer coefficient, \( k \) will also be determined according to this relation:

\[
k = \frac{D_m}{\delta}
\]  \( \quad (13) \)

Average mass transfer coefficient, \( \bar{k} \) will be evaluated by numerical integration over the membrane channel length.

\[
\bar{k} = \frac{1}{l} \int_0^l k(x) \, dx
\]  \( \quad (14) \)

Wall shear stress, \( \tau_w \) will be evaluated from the simulation data which can be represented by:

\[
\tau_w = \frac{\partial u}{\partial y}
\]  \( \quad (15) \)

Concentration polarization factor, \( \Gamma \) will be evaluated from the simulated solute mass fraction adjacent to membrane, \( m_{AW} \) according to this relation:

\[
\Gamma = \frac{m_{AW}}{m_{A0}} - 1
\]  \( \quad (16) \)

Average concentration polarization factor, \( \bar{\Gamma} \) will be evaluated by numerical integration over the membrane channel length.

\[
\bar{\Gamma} = \frac{1}{l} \int_0^l \Gamma(x) \, dx
\]  \( \quad (17) \)

### 3. Results and discussion

Fig. 5 shows the NaCl concentration factor, \( (m_{AW}/m_{A0} - 1) \) at the distance of 1, 5, 10, 15 and 20 cm from the channel entrance. The NaCl concentration factor increases along the narrow membrane channel from 1, 5, 10, 15 and 20 cm as shown in Fig. 5(a-e). The concentration factor is inversely proportional to the dimensionless channel height \( z/h \) indicating that the concentration polarization profile is being built up at the laminar region adjacent to the membrane. Higher feed Reynolds number (1300) will generate less concentration build-up on the membrane surface as compared to lower feed Reynolds number (100). The difference of concentration build-up phenomena for two extreme feed Reynolds number becomes more obvious with the increment in the horizontal distance from the channel entrance. This trend is found to be in agreement with the literature data reported by Pinho et al. (2002).

Since fully developed region has been defined in the channel outflow, the flow tends to approach fully developed profile along the narrow channel. The velocity will decrease rapidly near the wall entrance region and the rate of decline reduces when it is approaching the fully developed region. For this reason, concentration build-up will increase rapidly near the wall entrance region due to the rapid decrease in velocity. When the fluid flow is approaching the fully developed region, the velocity reduction rate becomes constant. The moderate reduction of velocity has constrained the growth rate of concentration polarization layer at the membrane interface. This phenomenon has contributed to the evolution trend as depicted in Fig. 6 for the dimensionless concentration polarization layer thickness \( (\delta/h) \) versus the dimensionless channel length \( (z/h) \). Higher Reynolds number is responsible for the generation of higher cleaning effect on the concentration polarization layer and directly deters its formation. Thus, higher feed Reynolds tends to produce less concentration polarization profile than lower feed Reynolds number as shown in Fig. 6.

Fig. 7 demonstrates the evolution of mass transfer coefficient in the narrow membrane channel. Mass transfer coefficient, \( k \), which is a function of Schmidt \( (Sc = \mu/\rho D_A k) \) and Reynolds number, tends to decrease with the reduction of Reynolds number when the Schmidt number is assumed to be constant. The rapid decline in the velocity near the wall entrance region causes the \( k \) value to be reduced drastically at smaller channel length \( (z) \) as depicted in the Fig. 7. After this region, \( k \) value reduces gradually along the narrow membrane channel due to the constant reduction of velocity. Besides, the increment of the magnitude of feed Reynolds number exhibits its influence on \( k \) value. The variation in feed Reynolds number from 100 to 1300 will yield \( k \) values in ascending manner. The detail results are tabulated in Table 3.

The increase in transmembrane pressure will promote the formation of concentration polarization layer. This has been shown in Fig. 8. When the feed Reynolds number and feed concentration are constant, higher transmembrane pressure leads to the formation of concentration polarization layer. The increase in transmembrane pressure will generate higher permeation flux, which subsequently promotes the development of concentration polarization layer. This phenomenon is found to be in accordance with the literature data reported by Pinho et al. (2002). Table 4 shows the variation of feed Reynolds number and transmembrane pressure towards the development of concentration polarization profile. According to Table 4, the average concentration polarization factor, \( \bar{\Gamma} \) decreases from 0.364 to 0.119 with the increment in the feed Reynolds number from 100 to 1300 under 1 MPa transmembrane pressure. Similar trend has been observed for transmembrane pressure of 2 and 3 MPa. For average concentration polarization layer thickness \( (\delta) \), the simulated data demonstrates a similar trend where by the increment in the feed Reynolds number has deterred formation of the concentration polarization layer under different transmembrane pressure.

Based on Fig. 9, wall shear stress, \( \tau_w \), decreases rapidly near the wall entrance region and exhibit a nearly constant trend when it is approaching fully developed region. Wall shear stress plays a key role in generating scouring effect on the membrane interface and reduces the potential of the formation of concentration polarization. Rapid decrease in the wall shear stress near the wall entrance region promotes the formation of concentration polarization layer. Higher feed Reynolds number tends to produce higher wall shear stress.
Fig. 5. Dimensionless channel height vs. NaCl concentration factor for feed Reynolds number 100 and 1300 in the narrow membrane channel at \( x = 1, 5, 10, 15 \) and 20 cm. Inlet feed concentration, \( m_{A0} = 0.2 \) g/kg and \( \Delta P = 1.0 \) MPa.

and minimize the formation of concentration polarization layer as depicted in Fig. 9.

Fig. 10 shows the comparison between simulated data and the literature data reported by Pinho et al. (2002) for the concentration polarization factor, \( \Gamma \) versus dimensionless channel length \((x/h)\). The simulated data demonstrates the similar evolution trend as the literature data. The permeation flux has been considered in the film theory but ignored hydrodynamically (assuming wall boundary condition for membrane) due to the limitation of the simulator as mentioned in Section 2.4.
The existence of hydrodynamic permeation flux is capable of reducing the formation of concentration polarization profile on the membrane surface. This has been proven by De and Bhattacharya (1997). In the absence of hydrodynamic permeation flux, the simulated data is postulated to be larger in term of magnitude if compared to the literature data (Pinho et al., 2002). At lower transmembrane pressure simulation, the effect of the permeation flux towards the hydrodynamics is small due to the smaller permeation rate. Hence, the simulated data is seemed to agree very well with the literature data. However, the simulated data is found to be slightly lower as compared to the literature data. This might be due to the variation in the calculation method, which is applied.

Table 3
Average value for mass transfer coefficient, $k$ for $\Delta P = 1\text{ MPa}$, $J_f = 0.73 \times 10^{-5}\text{ m/s}$, $m_{AP} = 5.4 \times 10^{-5}$

<table>
<thead>
<tr>
<th>Feed Reynolds number</th>
<th>$k \times 10^{-5}\text{ m/s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>10.34</td>
</tr>
<tr>
<td>400</td>
<td>7.18</td>
</tr>
<tr>
<td>700</td>
<td>4.12</td>
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<tr>
<td>1000</td>
<td>3.61</td>
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<tr>
<td>1300</td>
<td>3.27</td>
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</table>

Table 4
Average value for concentration polarization layer thickness, $\delta$ and concentration polarization factor, $\Gamma$ for feed concentration 0.2 g/kg

<table>
<thead>
<tr>
<th>Feed Reynolds number</th>
<th>$\delta \times 10^{-5}\text{ m}$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta P = 1\text{ MPa}$, $J_f = 0.73 \times 10^{-5}\text{ m/s}$, $m_{AP} = 5.4 \times 10^{-5}$</td>
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<td></td>
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<tr>
<td>100</td>
<td>8.70</td>
<td>0.364</td>
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<tr>
<td>400</td>
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<td>0.193</td>
</tr>
<tr>
<td>700</td>
<td>4.12</td>
<td>0.132</td>
</tr>
<tr>
<td>1000</td>
<td>3.61</td>
<td>0.119</td>
</tr>
<tr>
<td>1300</td>
<td>3.27</td>
<td>0.081</td>
</tr>
</tbody>
</table>

| $\Delta P = 2\text{ MPa}$, $J_f = 1.36 \times 10^{-5}\text{ m/s}$, $m_{AP} = 3.7 \times 10^{-5}$ | | |
| 100                  | 10.14                            | 1.191   |
| 400                  | 7.38                             | 0.587   |
| 700                  | 4.44                             | 0.382   |
| 1000                 | 3.85                             | 0.322   |
| 1300                 | 3.47                             | 0.285   |

| $\Delta P = 3\text{ MPa}$, $J_f = 1.99 \times 10^{-5}\text{ m/s}$, $m_{AP} = 2.9 \times 10^{-5}$ | | |
| 100                  | 12.31                            | 3.723   |
| 400                  | 9.17                             | 1.046   |
| 700                  | 6.81                             | 0.720   |
| 1000                 | 5.13                             | 0.591   |
| 1300                 | 3.70                             | 0.514   |

Table 5
Average value for mass transfer coefficient, $k$ for $\Delta P = 1\text{ MPa}$, $J_f = 0.73 \times 10^{-5}\text{ m/s}$, $m_{AP} = 5.4 \times 10^{-5}$

<table>
<thead>
<tr>
<th>Feed Reynolds number</th>
<th>$k \times 10^{-5}\text{ m/s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>2.37</td>
</tr>
<tr>
<td>400</td>
<td>4.17</td>
</tr>
<tr>
<td>700</td>
<td>5.23</td>
</tr>
<tr>
<td>1000</td>
<td>6.05</td>
</tr>
<tr>
<td>1300</td>
<td>6.73</td>
</tr>
</tbody>
</table>

Fig. 6. Effect of feed Reynolds number on the concentration polarization profile.

Fig. 7. Effect of feed Reynolds number on the mass transfer coefficient.

Fig. 8. Effect of transmembrane pressure on the concentration polarization profile.

Fig. 9. Variation of wall shear stresses with concentration polarization layer for different types of feed Reynolds number.
to the formulation of both data respectively. For higher trans-
membrane pressure data (3 MPa), the simulated data tends to
exceed the values reported in the literature. Under this cir-
cumstance, the effect of permeation flux towards the fluid’s
hydodynamics is significant due to the higher permeation
rate. The absence of this hydrodynamic permeation flux in the
membrane surface has promoted the formation of higher con-
centration polarization profile in the simulated data at higher
permeation flux as depicted in Fig. 10.

4. Conclusion

Limitation of commercial CFD simulator has been over-
come by the integration of modified boundary condition in
the simulation code to predict the concentration polarization
profile that developed at the membrane interface. This has
been proven from the simulated data, which exhibit a well
accordant trend with the published literate data. According
to the current CFD simulation, the concentration polarization
profile tends to increase along the narrow membrane channel.
The decrease in wall shear stress would promote the forma-
tion of concentration polarization profile. The increase in feed
Reynolds number might contribute to the increment in mass
transfer coefficient. By assuming a constant Schmidt num-
ber (Sc = µ/µD), the concentration polarization profile is
only affected by two factors: feed Reynolds number and the
transmembrane pressure. The decrease in Reynolds number
and increment in transmembrane pressure would promote
the formation of concentration polarization layer and vice
versa. Although this study is conducted for two-dimensional
domain, there is a potential extending it to three-dimensional
spiral wound membrane due the flexibility and func-
tionalty of the CFD simulator.

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References

mal design of spiral wound modules: Analytical method. Transac-
tion IChemE, 73, 375–381.
type turbulence promoters in a narrow channel. Journal of Mem-
brane Science, 185, 157–176.
in reverse osmosis. Part I: Theoretical system design model develop-
ment. Desalination, 60, 251–274.
De, S., & Bhattacheray, P. K. (1997). Prediction of mass-transfer coeffi-
cient with suction in the applications of reverse osmosis and ultrafil-
modules I. Numerical method. Chemical Engineering Commu-
nications, 72, 62.
of mass transfer in slits with semi-permeable membrane walls. Engineer-
ing Computations—International Journal for Computer-aided Engi-
fer modeling of nanofiltration. Journal of Membrane Science, 191,
109–128.
transfer of momentum and concentration boundary layers at the
entrance region of a slit with a nanofiltration membrane wall. Clini-
cal Engineering Science, 188, 735–748.
ladder-type spacers configuration in NF spiral-wound modules on the
Geraldes, V., Semiao, V., & Pinho, M. N. (2003). Hydrodynamics and
concentration polarization in RO/NF spiral wound modules with lad-
simulation of the flow in a plane-channel containing a periodic array
of cylindrical turbulence promoters. Journal of Membrane Science,
231, 81–90.
Li, F., Meindersma, W., de Haan, A. B., & Reith, T. (2002). Optimiza-
tion of commercial net spacers in spiral wound membrane modules.
Li, F., Meindersma, W., de Haan, A. B., & Reith, T. (2004). Experimen-
tal validation of CFD mass transfer simulations in flat channels with non-
membrane modules. Chemical Engineering Science, 58, 4975.
scheme to study mass transfer over a separation membrane. Journal
of Membrane Science, 198, 40–59.
Pinho, M. N., Semiao, V., & Geraldes, V. (2002). Integrated modeling of
transport processes in biultrafiltration membrane systems. Journal of
unsteady flow in narrow spacer-filled channels for spiral-wound mem-
fluid dynamics modeling of flow in membrane channels. Journal of
Membrane Science, 211, 127–137.
Zimmerer, C. C., & Korkes, V. (1996). Effect of spacer geometry on
pressure drop, mass transfer, mixing behavior, and residence time
distribution. Desalination, 104, 129.