The effect of feed spacer geometry on membrane performance and concentration polarisation based on 3D CFD simulations

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Abstract

Feed spacers are used in spiral wound reverse osmosis (RO) membrane modules to keep the membrane sheets apart as well as to enhance mixing. They are beneficial to membrane performance but at the expense of additional pressure loss. In this study, four types of feed spacer configurations are investigated, with a total of 20 geometric variations based on commercially available spacers and selected filament angles. The impact of feed spacer design on membrane performance is investigated by means of three-dimensional (3D) computational fluid dynamics (CFD) simulations, where the solution-diffusion model is employed for water and solute transport through RO membranes. Numerical simulation results show that, for the operating and geometric conditions examined, fully woven spacers outperform other spacer configurations in mitigating concentration polarisation (CP). When designed with a mesh angle of 60° , fully woven spacers also deliver the highest water flux, although the associated pressure drops are slightly higher than their nonwoven counterparts. Middle layer geometries with a mesh angle of 30° produce the lowest water flux. On the other hand, spacers with a mesh angle of 90° show the lowest pressure drop among all the filament arrangements examined. Furthermore, the computational model presented here can also be used to predict membrane performance for a given feed spacer type and geometry.

Keywords: reverse osmosis (RO); spiral wound module; feed spacers; computational fluid dynamics (CFD); membrane performance

1. Introduction

Mass transfer phenomena in reverse osmosis (RO) processes have been studied experimentally and theoretically for many decades in order to understand how water and solute permeation occur within membrane modules [1-16], so as to identify the factors that determine the performance of membrane modules. One of the most critical mass transfer phenomena present in an RO membrane module is concentration polarisation (CP), which is caused by the accumulation of solute(s) rejected by a selective RO membrane, resulting in an elevated solute concentration on the membrane surface [13-16]. In a spiral wound membrane (SWM) module, which is the type of module most widely used in large scale RO plants, spacers are inserted between membrane sheets to keep them apart [37]. Feed spacers also promote mixing by inducing vortices near the membrane surfaces, which can mitigate CP but at the expense of an increased pressure drop [2, 5, 10, 12, 17]. It is therefore important to elucidate the effects of spacers on mass and momentum transfer in an SWM module with the ultimate aim to improve module performance.

In recent years computational fluid dynamics (CFD) has been increasingly used to study mass and momentum transfer in feed spacer-filled channels [1-2, 5, 7-10, 12-20, 22-32]. Early CFD work focussed on flow, solute concentration and pressure distributions in simplified two-dimensional (2D)

geometries [8, 12-16, 18-20, 30, 31], including 2D cross-sectional models for cavity, submerged and zigzag configurations [12, 14, 15, 19]. Different spacer shapes were also examined in several studies [13, 16, 18]. Ahmad *et al.* compared rectangular, cylindrical and triangular spacers and found the triangular shape to be most effective in mitigating CP [16]. Despite the computational efficiency and usefulness of 2D CFD models, they are limited in capturing the complex geometric features of spacers, e.g., the intersection of filaments cannot be incorporated in 2D models.

With the rapid increase in computational power, three-dimensional (3D) CFD models of spacer-filled channels have emerged [1-2, 5, 7, 10, 22-29]. Several studies reported flow patterns and mass transfer in 3D models of nonwoven spacers, with a focus on the effects of geometric parameters such as the filament distance-to-diameter ratio, the mesh angle and flow attack angle [1, 7, 23, 26]. Picioareanu *et al.* improved their 3D CFD model by introducing a more realistic nonwoven spacer geometry based on microscopic images, where variations in filament diameter were captured [29]. Other types of spacers that have been considered in 3D CFD models include ‘Parallel spacer’ [2, 40] and ‘Middle layer spacer’ [31], both consisting of thick filaments with a diameter equivalent to the channel height and thinner filaments piercing through the thick ones. However, 3D models of woven spacers with realistic spacer geometries are lacking. There is clearly a need to investigate flow, pressure and concentration patterns in spacer-filled feed channels for a variety of spacer types accounting for realistic spacer geometries.

In addition to capturing geometric details, it is equally important to specify appropriate boundary conditions, especially those on membrane walls, which have a direct influence on the predicted momentum and mass transfer behaviour in spacer-filled channels [1-2, 5-7, 10-11, 13-16, 21, 38-39]. There are essentially three types of boundary conditions for water flux through membranes: no water permeation, constant water flux and the solution-diffusion model. More options exist for solute flux through membranes. In a number of studies, membranes have been treated as an impermeable wall but with a constant solute concentration to allow for convection-dominated mass transfer near the membrane wall [1-2, 5, 7, 9, 38-40]. Although this approach is relatively simple and provides useful information on enhanced mass transfer due to the presence of feed spacers, simulation results with a constant wall concentration boundary condition cannot be used to predict membrane performance directly. As such, spacers of different types and geometries have been compared in terms of local shear stress and mass transfer coefficient [1-2, 5, 7, 9, 38-40]. A commonly used approach to account for solute permeation is to specify a constant membrane rejection combined with water flux and wall concentration [6, 12, 15, 18, 21, 26, 30, 31]. This can be expressed as: $J_s = J_w c_m (1 - R_s)$ where J_s is the solute flux, J_w the water flux (or flow velocity on the membrane wall), c_m the solute concentration on the membrane wall and R_s the membrane rejection. Introducing the rejection term is clearly more useful than imposing a constant solute concentration on the membrane wall due to the more realistic

representation of membrane [10], but it does not describe accurately mass transport through RO membranes, as this is governed by diffusion due to its small size pores (less than a nanometre) [32-33, 36]. The most widely accepted transport theory for RO membrane is the solution-diffusion model [32-33], where the solute flux is related to the solute permeability and the difference in concentration between the two sides of a membrane. The predicted solute fluxes can then be used to calculate the solute concentration in the produced permeate, thereby obtaining the solute rejection of the membrane.

In this study, the solution-diffusion model is employed in order to provide a more realistic description of water and solute transport phenomena in an RO membrane spacer-filled channel for various spacer geometries by means of 3D CFD simulations. Four spacer types are selected: nonwoven, partially woven, middle layer and fully woven. For each spacer type, the mesh angle and flow attack angle (or filament orientation) are varied according to information available on commercial nonwoven spacers [28]. The influence of spacer type and configuration on membrane performance is assessed quantitatively. In addition to evaluating and comparing direct performance indicators, such as water and solute fluxes and pressure drop, concentration polarisation at the membrane wall is also compared among different spacer configurations.

2. Methods

This study aims to provide not only a qualitative analysis of momentum and mass transfer behaviours but also quantitative results on water and salt permeation in an SWM module with various types of spacers. In this section, we present details of the model geometry, the governing equations required to construct a coupled fluid dynamics and mass transfer model, the boundary conditions and the numerical procedures used.

2.1 Feed spacer geometry

There are two basic feed spacer configurations: nonwoven and woven [23], which are commercially available net spacer types. In this study four different spacer configurations are created; these include nonwoven, partially woven, middle layer and fully woven spacers, as shown in Figure 1. The nonwoven configuration is the simplest type, which consists of two layers of straight filaments. The woven configuration can be divided into two different types depending on the extent to which the spacer filaments are woven together: partially woven and fully woven, as shown in Figures 1 (b) and 1 (d), respectively. The fully woven configuration, consisting of curved strands being woven together, has a highly complex geometry. In the partially woven configuration, one set of filaments remains straight, with each strand being in contact with the top and bottom plane alternatingly, while the other set is woven through the gaps between the first set of filaments [30]. The middle layer configuration is built based on the ‘Parallel spacer’ [2, 40] and ‘Middle layer spacer’ [31] in the literature. The filaments are arranged in a similar manner to those in the nonwoven configuration, but one set of

straight filaments has a smaller diameter and pierces through the other set of filaments whose diameter is the same as the channel height.

Figure 1. Filament configurations of feed spacers: (a) nonwoven (b) partially woven (c) middle layer (d) fully woven spacers.

For each spacer configuration, the orientation of the spacers and the intersecting angle between two layers of filaments are also varied. A schematic illustration of nonwoven spacers is shown in Figure 2 where important angles that describe the spacer orientation and filament arrangement are defined. Spacers consisting of two distinct layers of intersecting filaments are the most widely used design in RO modules [42]. Filaments that are oriented along the inflow direction are called axial filaments while those crossing the inflow are transverse filaments. The acute angle between the axial and transverse filaments is defined as the mesh angle, θ_f , which can be calculated from θ_a (angle between the inflow direction and axial filament or attack angle) and θ_t (angle between the inflow and transverse filament), $\theta_f = (\theta_a - \theta_t)$ or $180 - (\theta_a - \theta_t)$, as shown in Figure 2.

Five combinations of θ_t and θ_a are selected in this study, as described in Figure 3. In order to isolate the effect of θ_a and θ_t , the base-case arrangement shown in Figure 3 (a) is modified to form two groups by changing the orientation of the axial or transverse filaments. In the first group, Figures 3 (b) and 3 (c), the transverse filaments stay perpendicular to the inflow direction, while the axial filaments are rotated by -30° (or $+150^\circ$) and -60° (or $+120^\circ$), producing mesh angles of 60° and 30° , respectively. In the second group, the axial filaments are parallel to the inflow direction while the transverse filaments have angles of 60° or 30° with the axial filaments as shown in Figure 3 (d) and 3 (e). Therefore, for a fixed mesh angle, the effects of spacer orientations can be studied by comparing the two groups.

Figure 2. Schematic illustration of the filament arrangement and definitions of key angles: θ_a is the angle between the inlet flow direction and axial filament (attack angle), θ_t the angle between the inlet flow and transverse filament and θ_f the angle between the axial and transverse filaments (mesh angle), which depends on θ_a and θ_t .

By applying these five angular arrangements to the four spacer configurations introduced earlier, a total of 20 different spacer geometries can be created (Table 1). Each spacer configuration has a reference case (or base-case arrangement) where $\theta_a=180^\circ$ and $\theta_t=90^\circ$.

Figure 3. Selected filament arrangements in this study: (a) reference case, and (b)-(e) different variations. Blue and green lines in the upper panels indicate the transverse and axial filaments, respectively, while the corresponding elemental units are shown in the lower panel. All sides of the elemental unit have an equal length.

Table 1. 20 simulation cases consisting of 4 space types and 5 angular combinations.

Case No.	Name	Configuration	θ_t (°)	θ_a (°)	θ_f (°)	
1	NW90	Nonwoven	90	180	90	
2	PW90	Partially woven	90	180	90	Reference cases
3	ML90	Middle layer	90	180	90	
4	FW90	Fully woven	90	180	90	
5	NW60T	Nonwoven	90	150	60	
6	NW30T	Nonwoven	90	120	30	
7	PW60T	Partially woven	90	150	60	Transverse filaments perpendicular to inflow
8	PW30T	Partially woven	90	120	30	
9	ML60T	Middle layer	90	150	60	
10	ML30T	Middle layer	90	120	30	
11	FW60T	Fully woven	90	150	60	
12	FW30T	Fully woven	90	120	30	
13	NW60A	Nonwoven	60	180	60	
14	NW30A	Nonwoven	30	180	30	
15	PW60A	Partially woven	60	180	60	Axial filaments parallel to inflow
16	PW30A	Partially woven	30	180	30	
17	ML60A	Middle layer	60	180	60	
18	ML30A	Middle layer	30	180	30	
19	FW60A	Fully woven	60	180	60	
20	FW30A	Fully woven	30	180	30	

2.2 Computational fluid dynamics (CFD) simulations

2.2.1 Model description

Owing to the repeating pattern in feed spacer geometry as shown in Figure 3, a single unit cell is modelled for each simulation case. Elemental units for 20 geometries are created and representative models are shown in Figure 4. It should be noted that the elemental unit model for the fully woven spacer consists of two units in order to capture a complete repeating pattern. As can be seen in Figure 4 (d), side openings on the left and right side of the geometry are symmetrical only when two units are included.

Figure 4. Elemental units of the 4 reference cases. (a) nonwoven (NW90), (b) partially woven (PW90), (c) middle layer (ML90) and (d) fully woven (FW90). L_f is the distance between filaments, H_c the channel height, D_f the diameter of filaments in the nonwoven and woven configurations and $D_{f,1}$ and $D_{f,2}$ the diameter of transverse and axial filaments in the middle layer configuration, respectively.

The feed stream flows through the elemental unit in a direction normal to the inlet and outlet faces, while natural flow is allowed through side openings. Permeation occurs through the upper and lower membranes in the z -direction. Elemental unit models for Cases 5 to 12, where inlet and outlet faces are perpendicular to the inflow, are built in a similar way to the reference cases. For Cases 13 to 20, however, the transverse filaments are not perpendicular to the inlet flow. Therefore, an artificial section is created to obtain a developed flow velocity profile at the actual inlet, as shown in Figure 5 for Case 19 (FW60A).

Figure 5. Computational model for a fully woven geometry (FW60A) where the transverse filaments are not perpendicular to the inlet flow direction. The artificial section contains a channel with impermeable walls. The middle axial filament in the artificial section has a length of L_f and the dimension of the artificial section is determined accordingly.

2.2.2 Governing equations and boundary conditions

For each elemental unit, the flow is assumed to be laminar, incompressible, Newtonian and steady, and is governed by the continuity and Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} \quad (2)$$

where $\mathbf{u}$ is the fluid velocity vector, ρ the density of the fluid, μ the viscosity of the fluid and p the pressure. The transport of a single solute in the fluid domain can be described by the convection-diffusion equation.

$$\nabla \cdot (D_s \nabla \mathbf{u}) - \nabla \cdot (\mathbf{u}c) = 0 \quad (3)$$

where c is the solute concentration and D_s the diffusion coefficient. The fluid is assumed to have the properties of pure water due to the degree of dilution of typical feed streams in RO processes.

Each elemental unit model consists of 5 types of boundaries: the inlet, outlet, side openings, filament walls and membrane walls. A fully developed velocity profile and a flat concentration profile are imposed at the inlet (artificial inlet for Cases 13 to 20). Since the actual inlet faces are tilted at an angle in Cases 13 to 20, average inlet flow velocities for the permeation units are different from those in Cases 1 to 12. This allows for an investigation of the effects of different spacer orientations in a membrane module. A constant pressure is prescribed at the outlet boundary. Spacer filaments are treated as no-slip walls with zero velocity and zero solute flux. For the side openings through which

fluid can move, periodic conditions for flow and solute transport are imposed. All the walls in the artificial section for Cases 13 to 20 are assumed to be no-slip with no flux conditions.

In order to predict membrane performance, it is critical to have as realistic a set of boundary conditions as possible, particularly with regard to water and solute fluxes for membrane walls. Since water and solute fluxes vary with pressure and concentration on membrane surfaces, boundary conditions for membrane walls should accommodate this and constant water and solute flux boundary conditions should be avoided. The most widely accepted description of water and solute fluxes for RO membranes is the solution-diffusion model, which can be expressed as [32-33].

$$J_w = A(\Delta p - \kappa \Delta c) \quad (4)$$

$$J_s = B \Delta c \quad (5)$$

where J_w is the water flux, J_s the solute flux, A the hydraulic conductivity, κ the osmotic factor which is constant under isothermal conditions, B the solute permeability and Δ indicates that the difference between values of the relevant property (pressure or concentration) in the feed and permeate streams is taken. It is assumed that the intrinsic membrane properties, A and B , are constant. It is apparent that four key variables are required to calculate water and solute fluxes: feed pressure, feed concentration, permeate pressure and permeate concentration. This can be simplified by making appropriate assumptions for the permeate stream to avoid having to solve for permeate pressure and concentration distributions. Two assumptions are made for this purpose: (i) the pressure in the permeate channel is constant, and (ii) the solute concentration at the wall depends on local water and solute fluxes and is not influenced by cross flow [35].

The first assumption can be justified for a model unit which is very small compared to a real size RO module. The second assumption can also be justified owing to the relatively low permeate flowrate in RO membrane modules (less than 10% of feed flowrate). Based on these assumptions, Eqs. (4)-(5) can be rewritten as follows:

$$J_w(x, y) = A \left[\{p_f(x, y) - p_p\} - \kappa \{c_f(x, y) - c_p(x, y)\} \right] \quad (6)$$

$$J_s(x, y) = B [c_f(x, y) - c_p(x, y)] \quad (7)$$

$$c_p(x, y) = \frac{J_s(x, y)}{J_w(x, y)} \quad (8)$$

where subscripts f and p denote feed and permeate stream, respectively, x and y are Cartesian coordinates as defined in Figure 4. The coordinate z is omitted here since the membrane walls are perpendicular to the z -axis. The second assumption is described by Eq. (8) [35]. Since feed pressure and concentration are obtained from the solutions of the governing equations in Eqs. (1) to (3) and

permeate pressure is assumed to be a constant, it is possible to derive an explicit expression for permeate concentration by combining Eqs. (6) to (8).

$$\kappa A c_p^2 + [A(p - \kappa c) + B] c_p - Bc = 0 \quad (9)$$

Subscripts for the feed channel are omitted from now on so as to have consistent notation with that used in Eqs. (1) to (3). The permeate pressure is assumed to be zero for convenience in this study although its absolute value is usually slightly above the atmospheric pressure in a practical operation. The root of Eq. (9) is given by

$$c_p = \frac{-X_1 + \sqrt{X_1^2 + X_2}}{2\kappa A} \quad (10)$$

where $X_1 = A(p - \kappa c) + B$, and $X_2 = 4\kappa ABc$.

The permeate concentration determined by the above equation can then be used to obtain water and solute fluxes using Eqs. (6) and (7).

Under the assumption that water flux is normal to the membrane surface, boundary conditions for the upper and lower membrane walls in the feed channel can be prescribed.

$$\mathbf{u}_{l,up} = [0 \quad 0 \quad J_w] \quad (11)$$

$$\mathbf{u}_{l,low} = [0 \quad 0 \quad -J_w] \quad (12)$$

where $\mathbf{u}_{l,up}$ and $\mathbf{u}_{l,low}$ are the leaking velocity at the upper and lower membrane walls, respectively. As expressed in Eqs. (11) and (12), the only non-zero component is in the z direction, and the negative sign in Eq. (12) indicates the direction of water flux leaving the fluid domain. Solute fluxes through the membrane walls are prescribed as:

$$-\mathbf{n} \cdot (D_s \nabla c - \mathbf{u}c) = -J_s. \quad (13)$$

The formulated boundary conditions for RO membrane walls make it possible to examine the effects of feed spacer types on membrane performance accounting for locally varying water and solute permeation, which is the most important characteristics of RO membrane channels.

Parameter values for boundary conditions and transport properties are listed in Table 2 along with geometric parameters for spacer designs. Permeability parameters are chosen within practical ranges found in the literature [34]. The osmotic factor is based on the assumption that temperature is 25°C and the product of the osmotic coefficient and ionisation number is 2. Geometric parameters are also found in the literature [2, 12]. Inlet velocity, concentration and outlet pressure are within RO operating ranges, and the chosen molar concentration is equivalent to approximately 35 kg/m³ of aqueous sodium chloride solution. Based on the definition of Reynolds number used in [6, 12], the

channel Reynolds number corresponding to the conditions adopted in the present study is 224, which is within the laminar flow regime.

Table 2. List of parameters and boundary conditions

Symbol [unit]	Parameter	Value	Source
A [m/s/Pa]	Hydraulic conductivity	2.50×10^{-12}	[34]
B [m/s]	Salt permeability	2.50×10^{-8}	[34]
κ [m ³ Pa/mol]	Osmotic factor	4958	-
D_s [m ² /s]	Diffusion coefficient	1×10^{-9}	[41]
ρ [kg/m ³]	Density	998.20	-
μ [Pa·s]	Viscosity	8.93×10^{-4}	-
L_f [m]	Distance between filaments	4.5×10^{-3}	[12]
H_c [m]	Channel height	1×10^{-3}	[12]
D_f [m]	Diameter of filaments in nonwoven and woven spacers	0.5×10^{-3}	[12]
$D_{f,1}$ [m]	Diameter of transverse filaments in middle layer spacer	0.5×10^{-3}	[2]
$D_{f,2}$ [m]	Diameter of axial filaments in middle layer spacer	1×10^{-3}	[2]
u_0 [m/s]	Average inlet velocity	0.1	Selected
c_0 [mol/m ³]	Inlet concentration	603.45	within
p_0 [Pa]	Outlet pressure	60×10^5	operating range

2.2.3 Computational details

All CFD simulations included in this study are performed by using COMSOL Multiphysics 5.0, which employs the Galerkin finite element method with linear shape functions and stabilisation methods based on streamline diffusion and crosswind diffusion for the numerical solution of the governing equations. Computational meshes consisting of tetrahedral elements are generated, with local mesh refinement around sharp corners where spacer filaments are in direct contact with membrane walls, and in the vicinity of the membrane walls to allow for adequate resolution of the mass transfer boundary layer. A mesh sensitivity test is carried out by increasing the number of mesh elements until the difference in average water flux between two successive meshes is below 0.2%. The final mesh contains 1.4 - 2.9 million elements depending on the volume of the fluid domain.

Since the boundary conditions at the membrane walls are fully coupled with the governing equations as they are a function of pressure and concentration, all simulations are carried out in two steps in order to achieve more robust convergence preferably within 25 iterations. In the first step, the membrane walls are treated as impermeable, i.e. no water and solute fluxes. The obtained solutions are then used as an initial guess for the second step where the aforementioned boundary conditions are applied at the membrane walls. The MULTifrontal Massively Parallel Spacer direct solver (MUMPS) is used to solve the coupled momentum and mass transport problem, with a convergence criterion of 10^{-6} . All computations are performed on an Intel Xeon CPU E5-2665 workstation with 96 GB of RAM at 2.40 GHz. Each simulation takes between 3 to 8 hours depending on the size of the geometry.

2.2.5 Analysis of results

In addition to examining spatial distributions of velocity and solute concentration, the performance of the membrane unit is evaluated in terms of average water and solute fluxes through the upper and lower membrane walls. Other important parameters, such as pressure drop and CP modulus, are also calculated to allow for direct comparisons among different spacer configurations. Pressure drop is calculated as the difference in average pressure between the inlet and outlet pressures. Since the distance between the inlet and outlet pressures in each elemental unit varies depending on the mesh angle, the pressure drop per unit length is calculated by accounting for the filament length (L_f) and axial filament angle (θ_a).

$$\Delta\bar{p} = \frac{\Delta p}{L_f \cos(180 - \theta_a)} \quad (14)$$

The CP modulus has been used to measure the degree of CP on the membrane walls, and it is defined as

$$M_i = \frac{c_{w,i}}{c_b} \quad (i = up, low) \quad (15)$$

where M_i is the CP modulus for i membrane and the bulk concentration c_b is taken from the centroid of the fluid domain. Average CP moduli at the upper and lower membrane walls and for the entire elemental feed channel are also calculated for the purpose of comparison.

3. Results and discussions

Obtained velocity and concentration distributions from the CFD simulations are presented first so that the effects of geometric differences can be examined. In order to determine which spacer design provides superior membrane performance, quantitative comparisons are made of water and solute fluxes, as well as their spatial distributions on membrane walls. In addition, CP moduli and pressure drops in different geometries are compared, which help to explain why membrane performances differ among different spacer types.

3.1 Velocity and concentration distributions within fluid domains

The influence of spacer geometry on flow and mass transfer can be appreciated by comparing velocity and concentration fields in feed channels filled with different spacers. Figure 6 shows velocity magnitude contours for the 4 reference cases which have a fixed filament angle and orientation but different filament configurations. 2D velocity magnitude contours are displayed at selected xz and yz planes, which are parallel and perpendicular to the flow direction, respectively. A common feature is the presence of low-velocity zones near spacer filaments in all cases although their sizes vary. Further examination of velocity vectors near the membrane wall reveals the presence of flow recirculation. Figure 7 shows velocity vectors in the xz plane in NW90 as a representative case, where a recirculation zone is clearly formed behind the front filament. There is hardly any forced flow through the side openings in NW90, PW90 and FW90 since no pressure gradient is applied. Flow patterns in spacer geometries with a mesh angle of 90° are symmetrical with respect to the central xz plane.

Figure 6. Velocity magnitude contours for the reference cases at selected planes. (a) xz planes in NW90, (b) xz planes in PW90, (c) xz planes in ML90, (d) xz planes in FW90 (for $y = [0, L_f]$), (e) yz planes in NW90, (f) yz planes in PW90, (g) yz planes in ML90 and (h) yz planes in FW90 (for $y = [0, L_f]$).

Figure 7. Velocity vectors in the xz plane at $y = 0.5L_f$ for NW90.

Figure 8 shows the concentration contours at selected yz planes. Since the cross-sections of NW90 and ML90 do not change along the flow path, a slice at $x = 0.5L_f$ is chosen as representative. For PW90 and FW90, slices are taken at three locations to observe variations of solute concentration along the channels. By comparing Figure 8 with Figure 6, it can be seen that areas of high concentrations correspond to stagnation zones. In Figure 8(a) for NW90, accumulation of the solute at the side edges is observed with a maximum concentration of $1,342 \text{ mol/m}^3$ since the spacer filaments are in direct contact with the upper membrane wall all the way through the feed channel. An even higher maximum concentration, $1,452 \text{ mol/m}^3$, is observed in ML90, where the thick axial filaments completely block the side openings. In PW90 and FW90, however, solutes are more uniformly distributed according to the concentration contours at $x=0.5L_f$ with a maximum concentration of 829 mol/m^3 and 790 mol/m^3 for PW90 and FW90, respectively, as axial filaments are not in contact with any membrane walls. At $x=0.15L_f$ and $0.85L_f$, axial filaments curve towards either the upper or lower membrane wall so that the gaps between the filaments and membrane walls become very small. This prevents the solute from diffusing back to the bulk solution, leading to accumulation of solutes in the narrow gaps. An interesting observation can be made for FW90 in Figure 8 (d) that there are distinct areas of CP in the middle between axial filaments, where the cross flow velocity is particularly low as the inflow stream is split into four by the front transverse filament as shown in Figure 6 (h).

The concentration contours indicate that although CP occurs predominantly around sharp edges where spacer filaments meet membrane walls, it can also occur in areas of low cross flow velocity due to the geometric feature of spacers.

Figure 8. Concentration contours at selected yz planes for the reference cases. (a) yz plane at $x=0.5L_f$ in NW90, (b) yz planes at $x=0.15L_f$, $0.5L_f$ and $0.85L_f$ in PW90, (c) yz plane at $x=0.5L_f$ in ML90 and (d) yz planes at $x=0.15L_f$, $0.5L_f$ and $0.85L_f$ in FW90 for $y = [0, L_f]$

In order to examine the effects of mesh angle and attack angle on flow and mass transfer, four cases with the fully woven configuration (FW60T, FW30T, FW60A and FW30A) are selected for analysis since they demonstrate the most complex behaviour. Figure 9 presents velocity and concentration contours at selected yz planes in FW60T and FW30T. A similar velocity pattern to that in Figure 6 (h) is observed, which appears to have four distinct regions of high velocity due to the split inlet faces, although velocity contours in FW60T and FW30T are skewed compared to those in FW90. As the flow proceeds towards the exit, the flow velocity becomes more uniform. As a result, the extent of CP is reduced near the exit except in the narrow gaps between the filaments and membrane walls, as shown in Figure 9 (b) and (d) for $x=0.85L_f \sin \theta_f$. Due to the axial filaments being tilted to the positive y -direction, stagnant zones are formed on the opposite side in the negative y -direction near the entrance of the channels as shown in Figure 9 (b) and (d). A similar behaviour is observed in other spacer configurations, that is, stagnant zones tend to form on the left side (negative y -direction) of a single elemental unit due to the tilted axial filaments. Comparing the concentration contours in FW60T and FW30T, the locations where high concentrations appear are similar but their sizes are different; in the contours taken at $x=0.15L_f \sin \theta_f$ and $0.5L_f \sin \theta_f$ CP areas near the central axial filament in FW30T are wider than those in FW60T. In nonwoven, middle layer and partially woven

configurations, areas of high concentration near sharp edges are also larger in geometries with a mesh angle of 30° than 60° .

Figure 9. Velocity and concentration contours at selected yz planes for FW60T and FW30T. (a) Velocity contour in FW60T, (b) concentration contour in FW60T, (c) velocity contour in FW30T and (d) concentration contour in FW30T

Simulation results for FW60A and FW30A are presented in Figure 10 in the same manner as in Figure 9. Concentration contours are displayed at locations where the transverse and axial filaments overlay. There are stagnation zones near the spacer filaments as found in other geometries. Pronounced CP areas can be seen immediately behind the front transverse filaments as shown in cross-sections (1) and (2) in Figure 10 (b). A similar trend of concentration build-up near the front transverse filament is also found in FW30A as displayed in Figure 10 (d), although the corresponding cross-sectional areas are much smaller than those in FW60A. Other configurations exhibit similar behaviours due to the tilted transverse filaments as can be observed in the fully woven configurations, i.e., larger concentration build-up on the right-hand side (positive y -direction) of the single elemental unit than on the left-hand side.

Figure 10. Velocity magnitude and concentration contours at selected yz planes for FW60A and FW30A. (a) velocity contour in FW60A, (b) concentration contour in FW60A, (c) velocity contour in FW30A and (d) concentration contour in FW30A

3.2 Water and solute fluxes through membrane walls

Due to the complex geometrical arrangements of feed spacers, water and solute fluxes through membrane walls are not uniformly distributed. Lower water flux and higher solute flux are expected at locations of large CP. Spatial distributions of water and solute fluxes in different spacer geometries are presented first and are discussed in relation to the geometric features of each case. Average fluxes are calculated for the upper and lower membrane wall separately, as well as for the total membrane area in a unit channel.

3.2.1 Distributions of local water and solute fluxes

Distributions of water flux through the upper and lower walls for the reference cases (NW90, PW90, ML90 and FW90) are presented in Figure 11 where flow is in the x -direction, that is, from left to right. For all four cases, water flux is relatively low in areas where spacer filaments are in direct contact with membrane walls, implying a strong association between CP and reduced water flux. In NW90, the transverse filaments are placed on the lower membrane causing CP to occur at the left and right edge as illustrated in the lower panel in Figure 11 (a). The front and rear transverse filaments in PW90, which are straight cylinders, are in contact with the lower and upper walls, respectively. As a result, low water flux mainly affects one side as seen in Figure 11 (b). The curved axial filaments in PW90

create spots where CP is exacerbated due to the narrow gap between the filaments and membrane walls. Distributions of water fluxes through the upper and lower walls in ML90 are almost identical since the thick axial filaments are in contact with both the upper and lower walls, while the transverse filaments do not touch any membrane walls. Comparing distributions at the upper walls of NW90 and ML90, areas of low water flux are much larger in ML90 than in NW90, which is caused by the thicker axial filaments in ML90 and the absence of side openings. For FW90 shown in Figure 11 (d), distribution patterns are partially similar to those in PW90 in that there are isolated corners of low water flux on the upper and lower walls. Interestingly, there are bands of moderate water flux (yellow coloured) in the middle of each unit channel in FW90, even though there are no spacer filaments in the vicinity of the walls. These are regions where the velocity is very low due to the nature of the fully woven configuration as explained previously with Figure 6 (h).

Average water fluxes obtained in NW90, PW90, ML90 and FW90 are 6.57×10^{-6} m/s, 6.69×10^{-6} m/s, 6.60×10^{-6} m/s and 6.97×10^{-6} m/s, respectively; with FW90 achieving the highest water flux and ML90 the lowest. When water fluxes through the upper and lower walls are considered separately, differences between the upper and lower membranes are very small, with the largest discrepancy being observed in NW90 where water fluxes through the upper and lower membranes are 6.75×10^{-6} m/s and 6.41×10^{-6} m/s, respectively.

Figure 11. Contours of water flux at the upper and lower membrane walls for the reference cases. (a) $J_{w,up}$ (top) and $J_{w,low}$ (bottom) in NW90 with a range between $1.42 \times 10^{-7} - 7.55 \times 10^{-6}$ m/s, (b) $J_{w,up}$ (top) and $J_{w,low}$ (bottom) in PW90 with a range between $1.79 \times 10^{-7} - 7.55 \times 10^{-6}$ m/s, (c) $J_{w,up}$ (top) and $J_{w,low}$ (bottom) in ML90 with a range between $7.20 \times 10^{-8} - 7.55 \times 10^{-6}$ m/s, (d) $J_{w,up}$ (top) and $J_{w,low}$ (bottom) in FW90 for $y = [0, L_f]$ with a range between $1.41 \times 10^{-7} - 7.55 \times 10^{-6}$ m/s.

Figure 12 shows distributions of solute fluxes through the upper and lower membranes in NW90, PW90, ML90 and FW90. Patterns in Figure 12 are almost identical to those in Figure 11 except that the colour code is reversed, meaning that high water fluxes coincide with low solute fluxes, and vice versa. Average solute fluxes are 1.70×10^{-6} mol/(m² s), 1.68×10^{-6} mol/(m² s), 1.70×10^{-6} mol/(m² s) and 1.62×10^{-6} mol/(m² s) for NW90, PW90, ML90 and FW90, respectively; with FW90 having the lowest solute flux and ML90 the highest.

Figure 12. Contours of solute flux at the upper and lower membrane walls for the reference cases. (a) $J_{s,up}$ (top) and $J_{s,low}$ (bottom) in NW90 with a range between $1.50 \times 10^{-5} - 3.00 \times 10^{-5}$ mol/(m² s), (b) $J_{s,up}$ (top) and $J_{s,low}$ (bottom) in PW90 with a range between $1.50 \times 10^{-5} - 2.99 \times 10^{-5}$ mol/(m² s), (c) $J_{s,up}$ (top) and $J_{s,low}$ (bottom) in ML90 with a range between $1.50 \times 10^{-5} - 3.01 \times 10^{-5}$ mol/(m² s), (d) $J_{s,up}$ (top) and $J_{s,low}$ (bottom) in FW90 for $y = [0, L_f]$ with a range between $1.50 \times 10^{-5} - 3.0 \times 10^{-5}$ mol/(m² s).

The effects of mesh angle and attack angle are also analysed by using the fully woven geometries. Figure 13 shows spatial distributions of water fluxes through the upper and lower membranes in FW60T, FW30T, FW60A and FW30A. By comparing Figure 13 (a) and (b) with the reference case shown in Figure 11 (d), it is clear that areas of low water fluxes appear more irregularly and their sizes are larger as the mesh angle becomes smaller. Isolated areas of low water flux near the middle axial filament also tend to shift towards the right-hand side from the centre axial filament (negative y -direction) as the mesh angle decreases. On the other hand, the low water flux spots in FW60A and FW30A are slightly skewed to the left-hand side from the centre axial filament (positive y -direction). Visual comparisons between different mesh angles reveal that a larger fraction of the total membrane area is exposed to low water flux at a smaller mesh angle. Other configurations also react similarly to

different angles; different mesh angle and attack angles lead to asymmetric contours compared to those presented in Figures 11 and 12.

Figure 13. Contours of water flux at the upper and lower membrane walls for fully woven configurations. (a) $J_{w,up}$ (left) and $J_{w,low}$ (right) in FW60T with a range between $1.38 \times 10^{-7} - 7.55 \times 10^{-6}$, (b) $J_{w,up}$ (left) and $J_{w,low}$ (right) in FW30T with a range between $1.08 \times 10^{-7} - 7.55 \times 10^{-6}$, (c) $J_{w,up}$ (left) and $J_{w,low}$ (right) in FW60A with a range between $1.39 \times 10^{-7} - 7.54 \times 10^{-6}$, (d) $J_{w,up}$ (left) and $J_{w,low}$ (right) in FW30A with a range between $1.18 \times 10^{-7} - 7.54 \times 10^{-6}$.

3.2.2 Comparison of average fluxes

Figures 14 and 15 depict average water and solute fluxes for all the spacer geometries included in this study. While the upper and lower membrane fluxes are presented separately, the average values for the total area of membrane in a unit channel are also given in order to compare the performance of different spacer designs.

For the 20 spacer geometries examined here, average water fluxes in a unit channel range between $6.1 - 7.3 \times 10^{-6}$ m/s. It is clear that fully woven spacer geometries achieve higher water fluxes than other configurations; this is followed by partially woven, nonwoven and middle layer configurations. When transverse filaments are perpendicular to the inflow direction (case names ending with T), reducing the mesh angle seems to lower water fluxes although there is little difference between FW60T and FW30T. An interesting finding is that differences between the nonwoven and middle layer configurations are amplified at small mesh angles. These trends are consistent with the observations that velocity and concentration distributions on membrane walls are less uniform in geometries with a smaller mesh angle.

Figure 14. Comparison of average water fluxes in a unit channel for different spacer geometries. Colour bars display the upper and lower membrane fluxes separately, while stars show the corresponding average water flux through the total membrane area of each unit channel.

Comparisons of results for the upper and lower membranes show that the most notable differences are found in nonwoven configurations, with the upper membrane achieving about 5 % higher water flux than the lower membrane in NW90. This is due to asymmetric mixing patterns near the upper and lower membranes. On the other hand, middle layer geometries behave symmetrically regardless of mesh angles and attack angles. While partially woven geometries show small differences between water fluxes through the upper and lower membranes, those in fully woven spacers are almost identical although FW60T and FW30T show little difference between the upper and lower membranes.

For each spacer type, the highest average water flux is achieved with a mesh angle of 60° and the axial filaments aligned parallel to the inflow (case names ending with 60A). However, fixed geometric parameters such as the filament distance and diameter are used here for all configurations and therefore the results might not be the same for a different set of geometric parameters.

Results for average solute fluxes show the opposite trend to those for water fluxes in that spacer geometries that achieve higher water fluxes have lower solute fluxes (Figure 15). Therefore comparing solute fluxes for all the spacer geometries also leads to the same conclusion that NW60A, PW60A, ML60A and FW60A are the best performers for each spacer type in terms of the least solute flux produced.

Figure 15. Comparison of average solute fluxes in a unit channel for different spacer geometries. Colour bars display the upper and lower membrane fluxes separately, while stars show the average solute flux through the total membrane area of each unit channel.

Although water and solute fluxes are direct indicators of membrane performance, it is also useful to evaluate other parameters related to transport phenomena near membrane walls, such as the CP modulus which is presented in the next section.

3.3 Concentration polarisation (CP) modulus

As defined in Eq. (15), CP modulus measures the extent of accumulating solutes on membrane surfaces relative to the bulk concentration. The spatial distribution of CP moduli is similar to that of solute fluxes shown in Figure 12, with regions of high solute fluxes near the edges of membranes corresponding to high CP moduli. This is in keeping with the solution-diffusion model where solute flux is proportional to the concentration difference between feed and permeate. The average and maximum CP moduli for each of the 20 spacer geometries are given in Figure 16 which shows that FW60A achieves the lowest average CP modulus at 1.04 while ML30A shows the most severe CP with an average CP modulus of 1.22. Although fully woven spacers generally have low average CP moduli, the lowest maximum CP modulus is found with PW90 at 2.26. On the other hand, middle layer geometries with a mesh angle of 30° show much greater maximum CP modulus, as a result of solute accumulation in the larger stagnant zone than those in other geometries.

Figure 16. Comparison of CP moduli for all cases. Average CP moduli in a unit channel are presented in bars (M_{ave} on the left vertical axis) and the maximum CP moduli are indicated by stars (M_{max} on the right vertical axis).

CP moduli obtained from other CFD studies in the literature are compared with those from this study. Lyster and Cohen investigated CP in an empty rectangular RO cell with a channel height of 1 mm experimentally and numerically using CFD [21]. By employing the solution-diffusion model for water flux at the membrane wall, together with an imposed concentration gradient for solute flux, they found that the average CP modulus varied from 1.33 to 1.42 for 80-100% membrane rejection. Song and Ma studied the impact of spacer geometry on CP and permeate flux using 2D CFD simulations [14]. They assumed that the solute was completely rejected by the membrane while water could pass through, with its flux being determined by the solution-diffusion model. They found that the average CP modulus achieved in an empty channel was approximately 2.5 while those in spacer-filled channels were 2.10, 2.33 and 1.73 for filament thickness of 0.5mm, 0.25mm, and 0.75mm, respectively. For a spacer-filled channel with a filament thickness of 0.5mm, which is the spacer size used in the present study, CP would be mitigated by a factor of 0.84 according to the study by Song and Ma [14]. By applying the mitigation factor to the results of Lyster and Cohen [21], the average CP modulus in a spacer-filled channel would be approximately 1.2.

The average CP moduli obtained in this study are in the range of 1.04–1.2, which are slightly lower than those in the aforementioned studies [14, 21]. This can be attributed to differences in boundary conditions and spacer geometries. The assumption of a constant solute rejection by the membrane, as was done in the aforementioned study [14, 21] and in others [6, 12, 15, 18, 26, 30, 31], may need to be revisited since membrane rejection is not an intrinsic property of membranes but an output of an RO process. It would be desirable if this could be predicted as part of a CFD simulation. For this purpose, more realistic boundary conditions are implemented in the present study by employing the solution-

diffusion model for water and solute transport through RO membranes without assuming a constant rejection rate. Combined with 3D geometric representations of spacer-filled channels, the CFD models presented here are expected to offer more faithful predictions of membrane performance than previous models.

3.4 Comparison of pressure drop

Pressure drop is an important parameter since it is directly related to energy consumption in an RO process in which hydraulic pressure is the main driving force for water permeation. Figure 17 shows pressure drop and pressure drop per unit length in different spacer geometries. The pressure drop per unit length is included due to the different length of spacer geometries. It is clear that ML30T has the highest pressure drop among all cases while nonwoven geometries have relatively low pressure drops compared to other spacer types for a given attack angle and mesh angle. The reference cases where the mesh angle is 90° result in the lowest pressure drop. The effect of mesh angle is more notable in cases where transverse filaments are perpendicular to the inflow while axial filaments are at an angle with inflow (case names ending with T). Results in Figure 17 show that smaller mesh angles lead to higher pressure drops, due to disturbances caused by the obstruction of axial filaments in the flow path. It is also observed that the difference in pressure drop between NW60T and NW30T is much larger than that between NW60A and NW30A, implying that pressure drop is more sensitive to the alignment of axial filaments than that of transverse filaments.

Figure 17. Comparison of pressure drop (P_{drop} on the left vertical axis) and pressure drop per unit length (P_{drop} on the right vertical axis) along a unit spacer-filled channel for all cases.

On the other hand, for the cases where axial filaments are aligned parallel to the inflow direction (case names ending with A), spacers with a mesh angle of 60° generate higher pressure drops than those with 30° . This is due to different average inlet velocities at the actual inlet faces, which are calculated

based on the imposed average velocity at the artificial inlet. The average velocity at the actual inlet in FW60A is 0.19 m/s, which is higher than that in FW30A (0.14 m/s). For the same reason, cross-comparisons between the two groups whose names end with T and A might not be appropriate since pressure drop is strongly influenced by the flow rate in a unit feed channel. Nonetheless, it is clearly demonstrated that spacer type and mesh angle have a strong impact on pressure drop in a spacer-filled channel.

3.5 Limitations of the current study

The current CFD model involves a number of assumptions. Firstly, a single unit cell is modelled with periodic boundary conditions, which ignores the development of fluid flow and mass transfer from the inlet along the channel. It has been reported that fluid flow becomes fully developed after 4–5 cells in the presence of spacers [43]. Secondly, the flow is assumed to be laminar and steady. Although this assumption is justifiable for the relatively low Reynolds number examined here, flow in a narrow spacer-filled channel can become unsteady and transitional at high inlet velocities [10, 44-45]. Thirdly, physical properties of the fluid are assumed to be constant and the adopted diffusion coefficient corresponds to a relatively low temperature range. Finally, the number of parameters assessed is limited. It would be important to determine the effects of key parameters on membrane performance, especially the effect of inlet flow velocity on concentration polarisation in future studies.

4. Conclusions

This study presents the analysis of various feed spacer geometries where three geometric features are varied: filament configuration, mesh angle and attack angle. 3D CFD simulations of 20 spacer geometries are performed in order to investigate the effects of spacer geometry on membrane performance (water and solute fluxes), CP and pressure drop. A unique feature of the CFD model used in this study is the incorporation of realistic boundary conditions for the RO membrane using the solution-diffusion model, allowing for predictions of membrane performance. Based on the numerical results for the operating condition and spacer geometries studied, the following conclusions can be drawn:

1. Fully woven geometries outperform other spacer configurations in terms of higher water flux and lower CP, although the associated pressure drops are slightly higher than their nonwoven counterparts.
2. Reducing mesh angle leads to reduced water flux and larger CP.
3. The pressure drop is very sensitive to the angle between axial filaments and the direction of inflow (attack angle).

It is hoped that the CFD model presented here can be used to predict membrane performance for a given spacer type and geometry. Results on CP can also help to assess the likelihood of membrane

fouling since areas with concentration build-up are vulnerable to the deposition of large particles. In this regard, fully woven configurations would be the preferred choice in situations when energy consumption is not a major limiting factor. Although a mesh angle of 60° is likely to produce the highest water flux among the angles studied, it should be noted that all simulations are undertaken at a fixed operating condition and model parameters. Results could vary depending on parameters specified in simulations.

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References

- [1] C.P. Koutsou, S.G. Yiantsios, A.J. Karabelas, A numerical and experimental study of mass transfer in spacer-filled channels: Effects of spacer geometrical characteristics and Schmidt number, *J. Membr. Sci.* 326 (2009) 234–251
- [2] M. Shakaib, S.M.F. Hasani, M. Mahmood, CFD modelling for flow and mass transfer in spacer-obstructed membrane feed channels, *J. Membr. Sci.* 326 (2009) 270–284
- [3] M.F.A. Goosen, S.S. Sablani, S.S. Al-Maskari, R.H. Al-Belushi, M. Wilf, Effect of feed temperature on permeate flux and mass transfer coefficient in spiral-wound reverse osmosis systems, *Desalination* 144 (2002) 367–372
- [4] M. Khayet, J.I. Mengual, Effect of salt type on mass transfer in reverse osmosis thin film composite membranes, *Desalination* 168 (2004) 383–390
- [5] J.L.C. Santos, V. Geraldes, S. Velizarov, J.G. Crespo, Investigation of flow patterns and mass transfer in membrane module channels filled with flow-aligned spacers using computational fluid dynamics (CFD), *J. Membr. Sci.* 305 (2007) 103–117
- [6] K. Darcovich, M.M. Dal-Cin, B. Gros, Membrane mass transport modelling with the periodic boundary condition, *Comput. Chem. Eng.* 33 (2009) 213–224
- [7] G.A. Fimbres-Weihs, D.E. Wiley, Numerical study of mass transfer in three-dimensional spacer-filled narrow channels with steady flow, *J. Membr. Sci.* 306 (2007) 228–243
- [8] G.A. Fimbres-Weihs, D.E. Wiley, Numerical study of two-dimensional multi-layer spacer designs for minimum drag and maximum mass transfer, *J. Membr. Sci.* 325 (2008) 809–822
- [9] C.P. Koutsou, A. J. Karabelas, Shear stresses and mass transfer at the base of a stirred filtration cell and corresponding conditions in narrow channels with spacers, *J. Membr. Sci.* 399–400 (2012) 60–72
- [10] G.A. Fimbres-Weis, D.E. Wiley, Review of 3D CFD modelling of flow and mass transfer in narrow spacer-filled channels in membrane modules, *Chem. Eng. & Process.* 49 (2010) 759–781

- [11] R. Salcedo-Díaz, P. García-Algado, M. García-Rodríguez, J. Fernández-Semprere, Visualization and modelling of the polarization layer in crossflow reverse osmosis in a slit-type channel, *J. Membr. Sci.* 456 (2014) 21–30
- [12] A. Subramani, S. Kim, E.M.V. Hoek, Pressure, flow, and concentration profiles in open spacer-filled membrane channels, *J. Membr. Sci.* 277 (2006) 7–17
- [13] A.L. Ahmad, K.K. Lau, Impact of different spacer filaments geometries on 2D unsteady hydrodynamics and concentration polarization in spiral wound membrane channel, *J. Membr. Sci.* 286 (2006) 77–92
- [14] L. Song, S. Ma, Numerical studies of the impact of spacer geometry on concentration polarization in spiral wound membrane modules, *Ind. Eng. Chem. Res.* 44 (2005) 7638–7645
- [15] S. Wardeh, H.P. Morvan, CFD simulations of flow and concentration polarization in spacer-filled channels for application to water desalination, *Chem. Eng. Res. & Design.* 86 (2008) 1107–1116
- [16] A.L. Ahmad, K.K. Lau, M.Z. Abu Bakar, Impact of different spacer filament geometries on concentration polarization control in narrow membrane channel, *J. Membr. Sci.* 262 (2005) 138–152
- [17] R. Ghidossi, D. Veyret, P. Moulin, Computational fluid dynamics applied to membranes: State of the art and opportunities, *Chem. Eng. & Process.* 45 (2006) 437–454
- [18] G. Guillen, E.M.V. Hoek, Modeling the impacts of feed spacer geometry on reverse osmosis and nanofiltration processes, *Chem. Eng. J.* 149 (2009) 221–231
- [19] J. Schwinge, D.E. Wiley, D.F. Fletcher, A CFD study of unsteady flow in narrow spacer-filled channels for spiral-wound membrane modules, *Desalination* 146 (2002) 195–201
- [20] V.M. Geraldes, V.A. Semião, M.N. de Pinho, Flow management in nanofiltration spiral wound modules with ladder-type spacers, *J. Membr. Sci.* 203 (2002) 87–102
- [21] E. Lyster, Y. Cohen, Numerical study of concentration polarization in a rectangular reverse osmosis membrane channel: Permeate flux variation and hydrodynamic end effects, *J. Membr. Sci.* 303 (2007) 140–153
- [22] V.V. Ranade, A. Kumar, Fluid dynamics of spacer filled rectangular and curvilinear channels, *J. Membr. Sci.* 271 (2006) 1–15
- [23] F. Li, W. Meindersma, A.B. de Haan, T. Reith, Optimization of commercial net spacers in spiral wound membrane modules, *J. Membr. Sci.* 208 (2002) 289–302
- [24] Y.L. Li, K.L. Tung, M.Y. Lu, S.H. Huang, Mitigating the curvature effect of the spacer-filled channel in a spiral-wound membrane module, *J. Membr. Sci.* 329 (2009) 106–118
- [25] A.S. Saeed, R. Vuthaluru, Y. Yang, H.B. Vuthaluru, Effect of feed spacer arrangement on flow dynamics through spacer filled membranes, *Desalination* 285 (2012) 163–169
- [26] K.K. Lau, M.Z. Abu Bakar, A.L. Ahmad, T. Murugesan, Feed spacer mesh angle: 3D modelling, simulation and optimization based on unsteady hydrodynamic in spiral wound membrane channel, *J. Membr. Sci.* 343 (2009) 16–33

- [27] Y.L. Li, K.L. Tung, CFD simulation of fluid flow through spacer-filled membrane module: selecting suitable cell types for periodic boundary conditions, *Desalination* 233 (2008) 351–358
- [28] S.K. Karode, A. Kumar, Flow visualization through spacer filled channels by computational fluid dynamics I. Pressure drop and shear rate calculations for flat sheet geometry, *J. Membr. Sci.* 193 (2001) 69–84
- [29] C. Picioreanu, J.S. Vrouwenvelder, M.C.M. van Loosdrecht, Three-dimensional modelling of biofouling and fluid dynamics in feed spacer channels of membrane devices, *J. Membr. Sci.* 345 (2009) 340–354
- [30] A.I. Radu, L. Bergwerff, M.C.M. van Loosdrecht, C. Picioreanu, A two-dimensional mechanistic model for scaling in spiral wound membrane systems, *Chem. Eng. J.* 241 (2014) 77–91
- [31] A.I. Radu, J.S. Vrouwenvelder, M.C.M. van Loosdrecht, C. Picioreanu, Modeling the effect of biofilm formation on reverse osmosis performance: Flux, feed channel pressure drop and solute passage, *J. Membr. Sci.* 365 (2010) 1–15
- [32] J.G. Wijmans, R.W. Baker, The solution-diffusion model: a review, *J. Membr. Sci.* 107 (1995) 1–21
- [33] M. Soltanieh, W.N. Gill, Review of reverse-osmosis membranes and transport models, *Chem. Eng. Commun.* 12 (1981) 279–363
- [34] G. Patroklou, K.M. Sassi, I.M. Mujtaba, Simulation of boron rejection by seawater reverse osmosis desalination, *Chem. Eng. Trans.* 32 (2013) 1873–1878
- [35] K. Jamal, M.A. Khan, M. Kamil, Mathematical modelling of reverse osmosis systems, *Desalination* 160 (2004) 29–42
- [36] K.P. Lee, T.C. Arnot, D. Mattia, A review of reverse osmosis membrane materials for desalination – Development to date and future potential, *J. Membr. Sci.* 370 (2011) 1–22
- [37] J. Schwinge, P.R. Neal, D.E. Wiley, D.F. Fletcher, A.G. Fane, Spiral wound modules and spacers: Review and analysis, *J. Membr. Sci.* 242 (2004) 129–153
- [38] A. Saeed, R. Vuthaluru, H.B. Vuthaluru, Impact of feed spacer filament spacing on mass transport and fouling propensities of RO membrane surfaces, *Chem. Eng. Commun.* 202 (2015) 634–646.
- [39] A. Saeed, R. Vuthaluru, H.B. Vuthaluru, Investigations into the effects of mass transport and flow dynamics of spacer filled membrane modules using CFD, *Chem. Eng. Res. Des.* 93 (2015) 79–99
- [40] M. Shakaib, S.M.F. Hasani, M. Mahmood, Study on the effects of spacer geometry in membrane feed channels using three-dimensional computational flow modeling, *J. Membr. Sci.* 297 (2007) 74–89
- [41] M. Taniguchi, S. Kimura, Estimation of transport parameters of RO membranes for seawater desalination, *AIChE J.* 46 (2000) 1967–1973

- [42] J. Johnson, Engineering aspects of reverse osmosis module design, *Desalin. Water Treat.* 15 (2010) 236–248
- [43] A. Saeed, Effect of feed channel spacer geometry on hydrodynamics and mass transport in membrane modules, PhD Thesis in Chemical Engineering, Curtin University (2012)
- [44] G.A. Fimbres-Weihs, D.E. Wiley, D.F. Fletcher, Unsteady flows with mass transfer in narrow zigzag spacer-filled channels: a numerical study, *Ind. Eng. Chem. Res.* 45 (2006) 6594–6603
- [45] J. Schwinge, D. Wiley, D.F. Fletcher, Simulation of the flow around spacer filaments between channel walls, *Unsteady flows*, *Ind. Eng. Chem. Res.* 42 (2003) 4962–4977

Nomenclature

Symbols

A	water permeability [m/(Pa s)]
B	solute permeability [mol/(m ² s)]
c	concentration [mol/m ³]
D_f	filament diameter in nonwoven and woven spacers [m]
$D_{f,1}$	filament diameter of thin filaments in middle layer spacers [m]
$D_{f,2}$	filament diameter of thick filaments in middle layer spacers [m]
D_s	diffusion coefficient [m ² /s]
H_c	channel height [m]
J_w	water flux [m ³ /m ² s]
J_s	solute flux [mol/m ² s]
L_f	filament distance [m]
M	concentration polarisation modulus [-]
$\mathbf{u}$	velocity vector [m/s]
$\mathbf{n}$	normal vector [-]
$\mathbf{N}$	flux [mol/m ² s]
p	pressure [Pa]
$\Delta\bar{p}$	pressure drop per unit length [Pa/m]
R	gas constant [J/(mol K)]
R_s	membrane rejection [-]
T	temperature [K]
x	Cartesian coordinate or ratio of reduced water flux to bulk water flux [-]
X_1	term used in Eq. (10)
X_2	term used in Eq. (10)
y	Cartesian coordinate

z Cartesian coordinate

Greek letters

θ_a angle between inflow direction and axial filaments (attack angle) [°]

θ_f angle between transverse and axial filaments (mesh angle) [°]

θ_t angle between inflow direction and transverse filaments [°]

ρ density of fluid [kg/m³]

μ viscosity of fluid [Pa s]

π osmotic pressure [Pa]

κ osmotic factor [m³ Pa/mol]

Subscripts

b bulk

f feed side

l leaking

low at lower membrane wall

m at membrane wall

p permeate side

up at upper membrane wall