Impact of Reactor Design on Temperature and Concentration Polarization in Direct Contact Membrane Distillation

Yinuo Yao\textsuperscript{a}, Siqin Yu\textsuperscript{a}, Ilenia Battiato\textsuperscript{a,\ast}

\textsuperscript{a}Department of Energy Science and Engineering, Stanford University, Stanford, CA 94305, USA

Abstract

Optimization and design of full-scale membrane distillation (MD) systems remain a challenge due to the disparity in scale with lab-scale setups, used for performance assessment. Entrance effects in lab-scale systems can significantly impact heat, mass and momentum transfer in the reactor and affect experimental Sherwood correlations, used in the design of full scale MD systems. Here, computational Fluid Dynamics (CFD) simulations using OpenFOAM are performed to understand the effects of right-angled bends and inlet design on flow dynamics, temperature and concentration polarization in MD systems. Simulation results show that the presence of right-angled bends and inlets with sudden expansions lead to the formation of Dean vortices. Dean vortices enhance perpendicular mixing in MD systems and reduce both temperature and concentration polarization. Temperature and concentration polarization coefficients in MD systems with right-angled bends and inlets with sudden expansions vary significantly for the same volumetric flow rate. The difference between theoretically predicted and numerically calculated

\textsuperscript{\ast}Corresponding author
correlations can be as high as 40%. This study demonstrates the importance of CFD-informed design of lab-scale systems for model calibration.

Keywords:

1. Introduction

Over the past few decades, desalination processes of unconventional water sources (i.e., seawater, brackish water, treated used-water etc.) have received considerable attention to improve local water supply in the era of climate change [1, 2, 3, 4]. Typical membrane-based desalination processes are reverse osmosis (RO), forward osmosis (FO) and membrane distillation (MD). Nowadays, RO has been widely adopted to separate salt and impurities from water, producing water quality that meets the drinking standard. Although promising, the cost of treating unconventional water sources is still significantly higher than that of treating conventional sources. One challenge associated with desalination is the production of brine [5]. Membrane distillation is proposed to treat the high concentration brine produced.

One of the challenges in operating MD systems is related to membrane fouling. Membrane fouling is a complex phenomenon in which foulant accumulates on the membrane surface due to deposition or adsorption arising from temperature and concentration polarization as a result of the coupling between heat transfer, mass transport and flow dynamics [6, 7, 8]. Severe membrane fouling will reduce permeate flux and increase the maintenance cost in long-term operation. One method of minimizing membrane fouling is to develop models, based on the predicted temperature and concentration, that can be used to optimize MD systems [9, 10, 11]. To establish a rela-
tionship between design, operating parameters and temperature polarization, multiple models have been developed based on the Nusselt number correlation \[12, 13, 14\] which establishes a relationship between the Nusselt number, the Reynolds number and the Prandtl number \[8, 13\]. Similarly to temperature polarization, concentration polarization can be predicted by models based on the Sherwood number correlation which correlates the Sherwood number with Reynolds number and Schmidt number \[15, 16\]. In addition to developing theoretical models, numerous experimental studies have focused on understanding heat and mass transfer in MD systems \[17, 12, 18, 19\].

However, one challenge associated with model development and experiments is the “tyranny of scales” where models and experiments are developed and performed on the laboratory scale (on the order of centimeters) \[20\] while the industrial scale is usually on the order of meters \[21\], resulting in significantly different polarization and flow dynamics. Song \[22\] investigated a novel reactor design on a larger scale (on the order of decimeter), but still smaller than the typical industrial scale. Due to the limited size of experimental laboratory bench modules, the inlet and module designs may have strong influences on the measured temperature and concentration polarization as well as permeate fluxes \[23, 9\]. Dudchenko et al. \[10\] compared different existing Nusselt number correlations with experimental results. They concluded that the best correlation still had significant errors in predicting permeate fluxes and its performance was also highly dependent on module designs. Yet, the underlying physical mechanisms leading to such discrepancy between bench experiments and theoretical correlations are not fully understood.
In general, two typical module designs influence measured quantities in MD systems: right-angled bends and inlets [23, 20]. Over the past few decades, both experiments and simulations have demonstrated the impact of right-angled bends on the flow dynamics [24, 25, 26, 27, 28, 29, 30, 31, 32]. Chen and Zhang [33] investigated the coupling of thermal distribution and flow characteristics. Lira [34] studied the difference in flow dynamics and mass transport between straight and curved channels in a chemical system. In a typical MD system, the inlet is designed with a surface area smaller than the main channel such that impinging jet is generated. Previous studies have shown that impinging jets would result in a high local heat and mass transfer coefficient. Gardon and Akfirat [35] found that the maximum heat transfer would occur at the stagnation point of the jet when the inlet spacing is greater than four times of the inlet diameter. Lytle and Webb [36] observed that the heat transfer coefficient exhibits two local maxima away from the stagnation point. Sparrow and Wong [37] measured the dependence of the mass transport coefficient at the stagnation point on the Reynolds number. Feroz [38] observed that the mass transfer coefficient increases with increasing the inlet diameter. The impinging jet has also been reported to enhance vortex formation and transition to turbulence [39, 40, 41]. To date, the combined effects of right-angled bends and inlets on flow dynamics, temperature and concentration polarization on the membrane in MD systems are still not fully understood. With increasing computational power, high-fidelity CFD simulations have been used to understand the impact of flow dynamics on system operation and optimization [11, 23, 25, 30, 31, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50]. A thorough understanding of the effects will provide quantitative guidelines.
for model development.

In this work, we use of computational fluid dynamics (CFD) simulations to study the effects of right-angled bends and inlets on direct-contact membrane distillation (DCMD) system performance. Four designs with different volumetric flow rates will be simulated to evaluate the flow dynamics, and its coupling to temperature and concentration polarization. The paper is organized as follows. In Section 2.1, we describe the governing equations. The verification of the numerical implementation and the setup of the simulations are presented in Sections 2.2 and 2.3, respectively. In Section 3, the effects of right-angled bends and inlets on vortex formation, as well as temperature and concentration polarization are discussed. The relationship between vortex formation and modeling errors is presented in Section 4. We present concluding remarks in Section 5.

2. Methodology

2.1. Governing equations

We consider membrane-desalinating a stream of sodium chloride solution that flows through the feed side of the DCMD systems. The permeate is collected on the draw side while sodium chloride is rejected and retained on the feed side of the DCMD systems. In this study, we incorporate the effects of varying density and temperature by solving the compressible Navier–Stokes equations in a three-dimensional membrane distillation (MD) system

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot \sigma + \rho g,$$  \hspace{1cm} (1)
with $\sigma$ the viscous stress tensor, defined as
\[
\sigma = \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right),
\] (2)
subject to continuity,
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0.
\] (3)

In Equations (1)-(3), $\mathbf{u} [\text{m s}^{-1}] = \begin{pmatrix} u & v & w \end{pmatrix}^T$ is the velocity vector, $\rho [\text{kg m}^{-3}]$ is the fluid density, $p [\text{Pa}]$ is the total pressure, $\mu [\text{kg m}^{-1} \text{s}^{-1}]$ is the dynamic viscosity of the fluid, and $g [\text{m s}^{-2}] = \begin{pmatrix} 0 & 0 & -9.81 \end{pmatrix}$ is the gravitational acceleration vector. The temperature equation is given by the energy equation as
\[
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (k \nabla T) + \frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p,
\] (4)
where $h [\text{kJ kg}^{-1}]$ is the specific enthalpy, $k [\text{W m}^{-1} \text{K}^{-1}]$ is the thermal conductivity and $T [\text{K}]$ is the temperature. The relationship between $h$ and $T$ is given by
\[
\int_{T_{stp}}^{T} c_p(T, C) \, dT = h,
\] (5)
where $c_p [\text{J kg}^{-1} \text{K}^{-1}]$ is the specific heat capacity of the fluid, $T_{stp} = 273.15 \text{ K}$ is the standard temperature and $C [\text{kg m}^{-3}]$ is the concentration of sodium chloride. The transport of sodium chloride is governed by the scalar transport equation such that
\[
\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u} C) = \nabla \cdot (D \nabla C),
\] (6)
where $D [\text{m}^2 \text{s}^{-1}]$ is the molecular diffusion coefficient.
At the inlets for both the feed and draw sides, Dirichlet boundary conditions for velocity, temperature and concentration, and Neumann boundary condition for pressure are applied as

\[ u(x, t) = u_{in,i}, \quad x \in \Gamma_{in,i}, \quad (7a) \]
\[ T(x, t) = T_{in,i}, \quad x \in \Gamma_{in,i}, \quad (7b) \]
\[ C(x, t) = C_{in,i}, \quad x \in \Gamma_{in,i}, \quad (7c) \]
\[ \nabla p(x, t) \cdot n(x) = 0, \quad x \in \Gamma_{in,i}, \quad (7d) \]

where \( i = f \) or \( d \) refers to the feed and draw sides of the MD system, respectively, \( u_{in,i}, T_{in,i} \) and \( C_{in,i} \) are the inlet velocity, temperature and concentration, \( n \) is the normal vector that points outwards of the surface and \( \Gamma_{in,i} \) is the surface of the inlet for subdomain \( i \). At the outlets of the feed and draw channels, we apply a Dirichlet boundary condition to pressure and Neumann boundary conditions to velocity, temperature and concentration as

\[ \nabla u(x, t) \cdot n(x) = 0, \quad x \in \Gamma_{out,i}, \quad (8a) \]
\[ \nabla T(x, t) \cdot n(x) = 0, \quad x \in \Gamma_{out,i}, \quad (8b) \]
\[ \nabla C(x, t) \cdot n(x) = 0, \quad x \in \Gamma_{out,i}, \quad (8c) \]
\[ p(x, t) = 0, \quad x \in \Gamma_{out,i}, \quad (8d) \]

where \( \Gamma_{out,i} \) is the surface of the outlet for the subdomain \( i \). For the walls, the no-slip boundary condition is applied to velocity and zero-gradient boundary conditions are applied to pressure, temperature and concentration such that
\( \mathbf{u}(x, t) = 0, \quad x \in \Gamma_{wall}, \) \hspace{1cm} (9a)

\( \nabla T(x, t) \cdot \mathbf{n}(x) = 0, \quad x \in \Gamma_{wall}, \) \hspace{1cm} (9b)

\( \nabla C(x, t) \cdot \mathbf{n}(x) = 0, \quad x \in \Gamma_{wall}, \) \hspace{1cm} (9c)

\( \nabla p(x, t) \cdot \mathbf{n}(x) = 0, \quad x \in \Gamma_{wall}, \) \hspace{1cm} (9d)

where \( \Gamma_{wall} \) are the surfaces of the channels.

To simulate flow through the membrane and its effects on temperature and concentration polarization, we adopt the boundary condition formulation by Lou et al. [43, 44] and extend it to three-dimensions. Transmembrane permeate flux \( J_w \) [kg m\(^{-2}\) s\(^{-1}\)] is modeled as

\[ J_w = A (p_{m,f} - p_{m,d}), \] \hspace{1cm} (10)

where \( A \) [m\(^3\) s\(^{-1}\)] is the vapor permeability and \( p_{m,f} \) [Pa] and \( p_{m,d} \) [Pa] are the vapor pressure on the feed and draw sides, respectively. Without resolving the transport in the membrane pores [43, 44, 11], we determine the local vapor pressure \( p_{m,i} \) [Pa] with respect to temperature and concentration as

\[ p_{m,i}(C, T) = a_w(C) p_{sat}(T), \] \hspace{1cm} (11)

with \( a_w \) [-] the water activity

\[ a_w = 1 - 0.03122m + 0.001482m^2, \] \hspace{1cm} (12)

and \( m \) [mol kg\(^{-1}\)] the sodium chloride molality. The vapor saturation pressure \( p_{sat} \) [Pa] is calculated with the Antoine equation [51] as

\[ p_{sat} = \exp \left( 23.238 - \frac{3841}{T_m - 45} \right), \] \hspace{1cm} (13)
where $T_m$ [K] is the temperature on the membrane surface.

Heat transport on the membrane is modeled as a balance between convective and conductive heat transfer. Transmembrane heat conduction $q_m$ [W m$^{-2}$] is modeled as

$$q_m = h_m (T_{m,f} - T_{m,d}), \quad (14)$$

where $T_{m,f}$ [K] and $T_{m,d}$ [K] are the membrane temperature of the feed and draw sides, respectively, and $h_m$ [W m$^{-2}$ K$^{-1}$] is the conductive heat transfer coefficient of the membrane. A balance between diffusive and convective fluxes provides the boundary condition for mass transport on the membrane \[53, 48, 49\]. In general, the boundary conditions for the membrane on the feed side are given by

$$u(x,t) = \frac{J_w}{\rho_f} n_f, \quad x \in \Gamma_{m,f} \quad (15a)$$

$$k \nabla T(x,t) \cdot n_f(x) = -\lambda J_w - h_m \Delta T_m, \quad x \in \Gamma_{m,f} \quad (15b)$$

$$D \nabla C(x,t) \cdot n_f(x) = -\frac{J_w}{\rho_f} C_{m,f}, \quad x \in \Gamma_{m,f} \quad (15c)$$

$$\nabla p(x,t) \cdot n_f(x) = 0, \quad x \in \Gamma_{m,f} \quad (15d)$$

where $\Delta T_m = (T_{m,f} - T_{m,d})$ is the membrane temperature difference between feed and draw sides, $n_f$ is the normal vector that points outward of the feed-side membrane, $\rho_f$ [kg m$^{-3}$] is the feed-side fluid density, $C_{m,f}$ [kg m$^{-3}$] is the sodium chloride concentration on the feed side, $\lambda$ [J kg$^{-1}$] is the latent heat of water and $\Gamma_{m,f}$ is the surface of feed-side membrane. For the draw side,
the boundary conditions are given by

\[ u(x, t) = -\frac{J_w}{\rho_d} n_d, \quad x \in \Gamma_{m,d} \quad (16a) \]

\[ k \nabla T(x, t) \cdot n_d(x) = \lambda J_w + h_m \Delta T_m, \quad x \in \Gamma_{m,d} \quad (16b) \]

\[ D \nabla C(x, t) \cdot n_d(x) = \frac{J_w}{\rho_d} C_{m,d}, \quad x \in \Gamma_{m,d}, \quad (16c) \]

\[ \nabla p(x, t) \cdot n_d(x) = 0, \quad x \in \Gamma_{m,d}, \quad (16d) \]

where \( n_d \) is the normal vector that points outward of the draw-side membrane, \( \rho_d \) [kg m\(^{-3}\)] is the draw-side fluid density, \( C_{m,d} \) [kg m\(^{-3}\)] is the sodium chloride concentration on the draw side and \( \Gamma_{m,d} \) is the surface of draw-side membrane. To incorporate the effect of temperature and concentration in the simulations, we calculate the thermophysical properties of the fluid as a function of temperature and concentration. Details can be found in Appendix A.

2.2. Numerical method implementation and validation

In this study, we solve the Navier-Stokes equation (equation 1) by implementing a solver in OpenFOAM [54] based on the low-Mach number flow approximation [55]. For the pressure-velocity coupling, the noniterative method, pressure-implicit algorithm with operators splitting (PISO) is adopted to satisfy mass conservation using predictor-corrector steps [56]. The governing equations are discretized with first-order backward Euler in time to avoid time-step constraints. Divergence terms are discretized with second-order accurate upwind schemes [57] while Laplacian terms are discretized with a second-order central difference scheme. The numerical solver used in this study is validated and verified through direct comparison with
Figure 1: (a) Calibration of vapor permeability $A$ based on experimental results and (b) validation and verification of present work with results by Lou et al.\cite{43}.

experiments by Vanneste et al.\cite{58} and two-dimensional simulations by Lou et al.\cite{13}. The inlet concentration of sodium chloride, $C_{in,f}$, is set to 1 kg m$^{-3}$ and the inlet velocities in both feed and draw sides, $u_{in,f}$ and $u_{in,d}$, are set as laminar parabolic profiles such that

$$u_{in,i}(y) = \frac{3u_{\text{max}}}{2} \left( 1 - \frac{y^2}{H^2} \right),$$

(17)

where $u_{\text{max}} = 0.124$ m s$^{-1}$ is the maximum velocity, and $H$ [m] is the height of the channel.

To determine vapor permeability $A$, we perform four simulations with $T_{in,d} = 20$°C, $T_{in,f} = 50$°C and $A = 2 \times 10^{-6}, 2.5 \times 10^{-6}, 3 \times 10^{-6}, 3.5 \times 10^{-6}$ m$^3$ s$^{-1}$. Figure 1(a) shows the permeate flux $J_w$ as a function of vapor permeability $A$. The optimal vapor permeability is given by the intersection between the experimental result (black) and the best-fit line (blue), which corresponds to
\[ A = 2.96 \times 10^{-6} \text{ m}^3\text{s}^{-1} \]. The remaining simulations use such value for \( A \).

To validate and verify our numerical results with the experimental and simulation results by Lou et al. [43], we set the inlet temperature on the draw side \( T_{in,d} \) to 20°C while the inlet temperature on the feed side \( T_{in,f} \) varies between 20°C and 60°C with an increment of 10°C. Figure 1(b) shows the permeate flux as a function of the inlet temperature on the feed side, \( T_{in,f} \). As demonstrated, the difference between our results and the experimental and simulation results by Lou et al. [43] is negligible, demonstrating the accuracy of the developed solver. Differently from [43, 44], the solver implemented in OpenFOAM can efficiently utilize high-performance computing clusters to perform three-dimensional simulations, as shown in the following analyses.

2.3. Three-dimensional simulations setup

Three-dimensional simulations are performed in rectangular channels with four representative designs to elucidate the effects of right-angled bends and inlet. Dimensions and sketches of each design are shown in Figure 2 and in Figure 3, respectively. The thermophysical properties of the fluid, such as viscosity, density, etc., are calculated with the models described in Appendix A. The grid spacing is uniform in the \( x \)-, \( y \)- and \( z \)-directions (\( \Delta x = \Delta y = \Delta z_{\text{max}} = 1.25 \times 10^{-4} \text{ m} \)) except in proximity of the membrane (details about grid convergence studies can be found in Section 2.4). To fully resolve the boundary layers near the membrane, a non-uniform grid spacing is used such that \( \Delta x = \Delta y = 1.25 \times 10^{-4} \text{ m} \) and \( \Delta z_{\text{min}} = 6.25 \times 10^{-6} \text{ m} \). In these simulations, we used adaptive time-step size such that the maximum
Courant number

\[
CFL_{\text{max}} = \max \left( \frac{u \Delta t}{\Delta x} + \frac{v \Delta t}{\Delta y} + \frac{w \Delta t}{\Delta z} \right)
\]  

(18)

is 0.8 and \( \Delta t \) [s] is the time step size. We simulate MD systems in counter-flow operation and the inlet velocity of the simulations ranges from 0.001 to 0.7 m s\(^{-1}\), with Reynolds number, \( Re_{\text{in}} \), ranging between 5.0 and 3500 where \( Re_{\text{in}} \) is defined as

\[
Re_{\text{in}} = \frac{u_{\text{in}} D_{h,\text{in}}}{\nu_0},
\]  

(19)

with \( D_{h,\text{in}} \) [m] the hydraulic diameter of the inlet and \( \nu_0 = 1 \times 10^{-6} \) [m\(^2\) s\(^{-1}\)] the kinematic viscosity of pure water. The inlet temperatures of the feed and draw sides are 313.15 K and 293.15 K, which provides a temperature difference of 20 K. The inlet concentration of sodium chloride on the feed side is 35 kg m\(^{-3}\) while that of the draw side is 0 kg m\(^{-3}\). All simulations are initiated with \( u(x, 0) = 0 \) m s\(^{-1}\), \( T(x_f, 0) = 313.15 \) K, \( T(x_d, 0) = 293.15 \) K, \( C(x_f, 0) = 35 \) kg m\(^{-3}\) and \( C(x_d, 0) = 0 \) kg m\(^{-3}\) where \( x_f \) and \( x_d \) refer to locations within the feed and draw chamber, respectively. Table I summarizes the geometry and simulation parameters. The total simulation time \( t_f \) is 100 \( \tau \) to ensure the flow is sufficiently developed where

\[
\tau = \frac{L_f}{u_{\text{in}} A_c},
\]  

(20)

represents the estimated water retention time from inlet to outlet, \( A_{\text{in}} \) [m\(^2\)] = \( L_I \times W_I \) is the area of the inlet, \( A_c \) [m\(^2\)] = \( W_C \times H_C \) is the cross-sectional area of the main channel, and \( L_f = 2H_I + 2H_S + L_C = 0.06 \) m is the approximate length of the systems.
Table 1: Summary of geometrical and simulation parameters.

| Parameter                              | MD-5x10S | MD-5x10 | MD-5x5  | MD-3x3  |
|----------------------------------------|----------|---------|---------|---------|
| Inlet/Outlet (\(L_I \times W_I \times H_I\) \([10^{-3}m]\)) | 5x10x5   | 5x10x5  | 5x5x5   | 3x3x5   |
| Side chamber (\(L_S \times W_S \times H_S\) \([10^{-3}m]\)) | 10x10x5  |         | 5x10x10 |         |
| Main channel (\(L_C \times W_C \times H_C\) \([10^{-3}m]\)) | 30x10x5  | 30x10x5 |         |         |
| Bends                                  | No       |         | Yes     |         |
| Volumetric flow rate \([10^{-8}m^3 s^{-1}]\)     | 7.50 – 1500 | 7.50 – 1500 | 2.5 – 1750 | 3.0 – 600 |
| Inlet velocity (\(u_{in}\) \([m s^{-1}]\))     | 0.0015 – 0.3000 | 0.0015 – 0.3000 | 0.0010 – 0.7000 | 0.0033 – 0.6667 |
| Reynolds number (\(Re_{in}\))          | 10 – 2000 | 10 – 2000 | 5.0 – 3500 | 10 – 2000 |
| Feed inlet concentration (\(C_{in,f}\) \([kg m^{-3}]\)) |         |         | 35      |         |
| Draw inlet concentration (\(C_{in,d}\) \([kg m^{-3}]\)) |         |         | 0       |         |
| Feed inlet temperature (\(T_{in,f}\) \([K]\)) |         |         | 313.15  |         |
| Draw inlet temperature (\(T_{in,d}\) \([K]\)) |         |         | 293.15  |         |
| Maximum Courant number \(CFL_{max}\) |         |         | 0.8     |         |
| Number of simulations                   | 20       | 14      | 20      | 25      | 22      |
Figure 2: Illustration of geometry schematic diagram and dimensions.

Figure 3: Schematic diagrams of different geometries
2.4. Grid convergence studies

To understand the grid resolution required to obtain accurate simulation results, we perform grid convergence studies with geometry MD-5x5 of Figure 3(c). The simulation is set up according to Section 2.3 and the largest \( Re_{in} = 2000 \) is chosen as the inlet boundary condition. Table 2 summarizes the resolution of the grid (\( \Delta x \) [m]) and the total number of cells. We define two types of error for each quantity of interest \( QI \) on the membrane surface, \( err_{fro} \) and \( err_{\infty} \), as

\[
err_{fro} = \frac{\| QI_{\Delta x} - QI_{\Delta x=0.0625} \|_{fro}}{\langle QI_{\Delta x=0.0625} \rangle}, \tag{21a}
\]

\[
err_{\infty} = \frac{\| QI_{\Delta x} - QI_{\Delta x=0.0625} \|_{\infty}}{\langle QI_{\Delta x=0.0625} \rangle}, \tag{21b}
\]

where \( QI \) is the quantity of interest, i.e. \( T, C \) and \( J_w \), and \( \langle QI \rangle \) is defined as the time- and spatial-average \( QI \):

\[
\langle QI \rangle = \frac{1}{N_tN_xN_y} \sum_{n,i,j} QI_{i,j,n}^{n}, \tag{22}
\]

where \( QI_{i,j,n} = QI(x_i,y_j,t_n) \) is \( QI \) at locations \( x_i \) and \( y_j \) and time \( t_n \), \( i = \{1,2,\cdots N_x\}, \quad j = \{1,2,\cdots N_y\}, \quad n = \{51\tau,52\tau,\cdots100\tau\} \), \( N_x \) and \( N_y \) are the mesh resolutions in the \( x \) and \( y \) directions, and \( N_t = 50 \) is the number of time snapshots. The errors \( err_{fro} \) and \( err_{\infty} \) measure the total and maximum errors, respectively. Figures 4(a) and 4(b) show \( err_{fro} \) and \( err_{\infty} \) as functions of \( \Delta x \) for the feed-side membrane. Overall, convergence in both errors has been observed. We choose \( \Delta x = 0.125 \times 10^{-3} \) m as the grid resolution for the subsequent simulations because both errors for all three quantities of interest are less than 1%.
Table 2: Summary of grid resolutions and total number of cells used for grid convergence studies.

| $\Delta x$ [$10^{-3}$ m] | 0.5  | 0.25 | 0.125 | 0.0625 |
|--------------------------|------|------|-------|--------|
| No. of grid cells        | 53,600 | 454,400 | 3,686,400 | 29,491,200 |

Figure 4: Grid convergence studies for temperature, concentration and permeate flux of two types of errors, (a) $err_{fro}$ and (b) $err_{\infty}$, respectively.
3. Results

3.1. The effect of right-angled bend and inlets with sudden expansions on the formation of Dean vortices

To understand the flow dynamics in MD systems, the instantaneous fluid streamlines for three representative Reynolds numbers $Re_{in} = 10, 250$ and 2000 and all four geometries are calculated and plotted in Figure 5. For a low Reynolds number ($Re_{in} = 10$), the flow is laminar and no distortion or swirling is observed, as indicated by the smooth/straight streamlines in Figures 5(a) – (d). For a moderate Reynolds number ($Re_{in} = 250$) (Figures 5(e) – (h)), no swirling is observed for the straight channel systems (MD-5x10S). The extent of swirling gradually intensifies in the MD-5x10, MD-5x5 and MD-3x3 systems with the presence of right-angled bends and for inlets with sudden expansions. As the Reynolds number further increases ($Re_{in} = 2000$) (Figures 5(i) – (l)), the streamlines in the MD-5x10, MD-5x5 and MD-3x3 systems become more chaotic while those in the MD-5x10S geometry remain smooth. When comparing the moderate Reynolds number cases for designs MD-5x10 and MD-5x5 (Figures 5(f) vs (g)), the original/appearance of the swirls differs. In MD-5x10, the swirling originates in the main channel after the right-angled bend, while in MD-5x5 design the onset of the swirling motion is in the side chamber, i.e. after the inlet and before the right-angled bend. This suggests that two mechanisms may play a role in the formation of vortices.

To visualize the swirling of the fluid in MD systems, we calculate the
$Q$-criterion ($Q$) of the velocity field as

$$Q = \frac{1}{2} \left( \|\Omega\| + \|S\| \right),$$  \hspace{1cm} (23)

where

$$S = \frac{1}{2} \left( \nabla u + (\nabla u)^T \right),$$  \hspace{1cm} (24a)

$$\Omega = \frac{1}{2} \left( \nabla u - (\nabla u)^T \right),$$  \hspace{1cm} (24b)

are defined as the rate of strain and the vorticity tensor, respectively [59]. A positive $Q$-criterion ($Q > 0$) means that the magnitude of the vorticity is greater than the magnitude of the rate of strain, indicating the existence of vortices. Figure 6 shows the isosurfaces of the $Q$-criterion ($Q = 50$) for cases with different Reynolds numbers. For $Re_{in} = 10$ (not shown), no pair of (Dean) vortex tubes or vortices are observed. For $Re_{in} = 250$, the MD-5x10S design does not lead to the formation of visible Dean vortex tubes or vortex structures (Figure 6(a)). Fast-decaying Dean vortex tubes in the main channel can be observed for MD-5x10. No visible vortices were found in the side chamber below the inlet: this is consistent with the streamlines plot of Figure 5(a), which suggests that the formation of vortices occurs in the main channel after the right-angled bend. Stable Dean vortex tubes are observed for both MD-5x5 and MD-3x3. This is likely due to the diverging flow or impinging jets when the inlet has a smaller opening than the side chamber, in presence of a wall where the flow can rebound. Significant vortex structures are observed in the side chamber for both MD-5x5 (Figure 6(c)) and MD-3x3 (Figure 6(d)). Therefore, it is likely that the formation of stable Dean vortex tubes in MD-5x5 and MD-3x3 is due both to the effects of right-angled bends...
Figure 5: Instantaneous streamlines colored by the magnitude of vorticity for $Re_{in} = 10$ (first row) $Re_{in} = 250$ (second row) and $Re_{in} = 2000$ (third row) of MD-5x10S, MD-5x10, MD-5x5 and MD-3x3 (left to right).
and inlets with sudden expansions. For $Re_{in} = 2000$, the number of fine-scale vortex structures increases drastically for all cases except MD-5x10S due to the flow transition to chaotic regimes. Furthermore, Dean vortex tubes can only be observed for MD-5x5 and MD-3x3 with jet-like inlets. A possible explanation is that inlets with sudden expansions result in strong vortex structures that are less likely to be broken into smaller and irregular vortex structures by flow.

Figures 7 shows the instantaneous vorticity in the $x$-direction, $\omega_x$, at the center of the channel ($x = 0.02$ m for MD-5x10, MD-5x5 and MD-3x3, and $0.025$ m for MD-5x10S) with different Reynolds numbers where

$$\omega_x = \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}. \quad (25)$$

At low Reynolds number ($Re_{in} = 10$) (Figure 7(a) – (d)), no noticeable Dean vortices are observed, since the flow is laminar. The effects of right-angled bends and inlets with sudden expansions have no significant impact on flow characteristics. At moderate Reynolds number ($Re_{in} = 250$) (Figure 7(e) – (h)), the right-angled bends and inlets with sudden expansions result in the formation of Dean vortices for MD-5x10, MD-5x5 and MD-3x3. Additionally, inlets with sudden expansions (MD-5x5 and MD-3x3) lead to Dean vortices of greater intensities and with more regular shapes. As the Reynolds number increases ($Re_{in} = 2000$) (Figure 7(i) – (l)), the flow in MD-5x10 transitions into a chaotic flow with fine-scale vortex structures similar to those observed in turbulent flows. For MD-5x5 and MD-3x3, one can observe Dean-vortex-like structures with significant fluctuations.
Figure 6: Isosurface of vortex tubes ($Q = 50$) colored by the magnitude of vorticity at $Re_{in} = 250$ for (a) MD-5x10S, (b) MD-5x10, (c) MD-5x5 and (d) MD-3x3, and $Re_{in} = 2000$ for (e) MD-5x10S, (f) MD-5x10, (g) MD-5x5 and (h) MD-3x3.
Figure 7: The instantaneous $x$-direction vorticity $\omega_x$ for $Re_{in} = 10$ ((a) – (d)) $Re_{in} = 250$ ((e) – (h)) and $Re_{in} = 2000$ ((i) – (l)) of MD-5x10S, MD-5x10, MD-5x5 and MD-3x3.
To eliminate time fluctuations, we compute the time-average of $\omega_x$ as

$$\overline{\omega}_x = \frac{1}{N_t} \sum_{n} \omega^n_x,$$

(26)

where $\omega^n_x = \omega_x(t_n)$ refers to the vorticity in $x$-direction at time $t_n$. Figure 8 shows the time-average vorticity $\overline{\omega}_x$ for the respective cases at different Reynolds numbers. For low and moderate Reynolds numbers, no significant differences are observed between the instantaneous and time-averaged vorticity results: this is expected since the flow is in the laminar regime. At high Reynolds numbers ($Re_{in} = 2000$), one can clearly identify the pair of Dean vortices for MD-5x5 and MD-3x3 (Figures 8(k) and (l)) but not for MD-5x10 (Figures 8(j)): this suggests that the inlet can stabilize the Dean vortices at high Reynolds numbers. Overall, instantaneous vorticity can differentiate between stable and unstable Dean vortices while time-average vorticity can identify Dean vortices in chaotic flows.

3.2. The effect of right-angled bend and inlet with sudden expansions on the temperature and concentration polarization

One major concern in operating MD systems is temperature and concentration polarization, which will ultimately result in membrane fouling and an increase in the cost of operation. The ability to predict temperature and concentration polarization is critical to the development of efficient and low-cost MD systems. In this section, the effects of the right-angled bends and inlet design on temperature and concentration polarization are studied.

Figure 9 shows the instantaneous temperature distributions of the feed side membrane for three representative Reynolds numbers. At low Reynolds number ($Re_{in} = 10$) (Figure 9(a) – (d)), the temperature gradually decreases
Figure 8: The time-average x-direction vorticity $\langle \omega \rangle_x$ for $Re_{in} = 10$ ((a) – (d)), $Re_{in} = 250$ ((e) – (h)) and $Re_{in} = 2000$ ((i) – (l)) of MD-5x10S, MD-5x10, MD-5x5 and MD-3x3.
in the flow direction \((x\) direction) and is approximately homogeneous with insignificant boundary effects indicated by the lower temperature near the walls in the perpendicular direction \((y\) direction). The difference in the temperature distribution for cases with right-angled bends (i.e. Figure 9(b)) and inlets with sudden expansions (i.e. Figures 9(c) and (d)) is negligible because the flow is laminar. At moderate Reynolds numbers \((Re_{in} = 250)\) (Figure 9(e) – (h)), the temperature is approximately homogeneous in the perpendicular direction for MD-5x10S, while significant heterogeneity is observed for cases with right-angled bends and inlets with sudden expansions (MD-5x10, MD-5x5 and MD-3x3). For example, the temperature at the center in the flow direction is much higher than in the near-wall regions. As the Reynolds number further increases \((Re_{in} = 2000)\) (Figure 9(i) – (l)), so do temperature fluctuations. For MD-5x10 with only right-angled bends, the temperature distribution becomes more irregular. For MD-5x5 and MD-3x3, the high-temperature region appears to fluctuate. Figure 10 shows the \(y\)-direction centerline of instantaneous temperature profiles. At a low Reynolds number (Figure 10(a)), the temperature distributions are similar with a slight difference in magnitude between different designs. The magnitude difference between the low- and high-temperature regions at low Reynolds numbers is much smaller than that at moderate and high Reynolds numbers. At moderate Reynolds number (Figure 10(b)), we can clearly observe three regions with alternating low and high temperatures for MD-5x5 and MD-3x3. As the Reynolds number increases, the instantaneous temperature for all cases except MD-5x10S fluctuates.
Figure 9: The instantaneous temperature distribution for $Re_{in} = 10$ (first row) $Re_{in} = 250$ (second row) and $Re_{in} = 2000$ (third row) of MD-5x10S, MD-5x10, MD-5x5 and MD-3x3 (left to right).
Figure 10: The centerline instantaneous temperature in the $y$-direction on the feed-side membrane for (a) $Re_{in} = 10$, (b) $Re_{in} = 250$ and (c) $Re_{in} = 2000$. 
In MD systems, one of the challenges is to control membrane fouling due to both the temperature and concentration polarizations.

We compute the time-average temperature polarization coefficient \( \overline{T_{PC}} \) as

\[
\overline{T_{PC}} = \frac{1}{N_t} \sum_{n} \frac{T_{m,f}^n - T_{m,d}^n}{T_{b,f}^n - T_{b,d}^n},
\]

where \( T_{m,i}^n = T_{m,i}(t_n) \) and \( T_{b,i} \) are the temperature on the membrane surface \((m)\) at \( t_n \) and in the bulk fluid \((b)\) for region \( i \) that is equivalent to \( T_{in,i} \), respectively, and \( i = \{f,d\} \) refers to the feed and draw sides of the MD systems. Based on the definition in equation (27), \( \overline{T_{PC}} = 1 \) indicates that there is no temperature polarization, while \( \overline{T_{PC}} < 1 \) indicates the existence of temperature polarization. The concentration polarization coefficient \( \overline{C_{PC}} \) is calculated as

\[
\overline{C_{PC}} = \frac{1}{N_t} \sum_{n} \frac{C_{m,f}^n}{C_{b,f}^n},
\]

where \( C_{m,i}^n = C_{m,i}(t_n) \) and \( C_{b,i} \) are the concentration on the membrane surface at \( t_n \) and in the bulk fluid for region \( i \) that is equivalent to \( C_{in,i} \), respectively, and \( \overline{C_{PC}} > 1 \) indicates concentration polarization.
Figure 11: The centerline time-average temperature polarization $\text{TPC}(a - c)$ and concentration polarization $\text{CPC}(d - f)$ in the $y$-direction on the feed-side membrane for (a, d) $Re_{in} = 10$, (b, e) $Re_{in} = 250$ and (c,f) $Re_{in} = 2000$. 

(a) \hspace{1cm} (b) \hspace{1cm} (c) 

(d) \hspace{1cm} (e) \hspace{1cm} (f)
Figure 11(a) – (c) show the centerline plots in the $y$-direction of the time average $\overline{TPC}$. At low Reynolds number (Figure 11(a)), all cases have similar distributions of $\overline{TPC}$ because the flow is approximately laminar. Interestingly, MD-5x10S has the least temperature polarization indicated by the largest $\overline{TPC}$. A possible explanation is that right-angled bends and inlets with sudden expansions result in more energy loss in the flow, but mixing enhancement mechanisms in presence of vortices are absent due to laminar flow. At moderate Reynolds number (Figure 11(b)), MD-5x10S has the most significant temperature polarization, indicated by small $\overline{TPC}$ while MD-5x5 and MD-3x3 have significantly less temperature polarization because of the enhanced mixing near the membrane surface due to strong Dean vortical structures. For MD-5x10, whose design includes only the effect of right-angled bends, temperature polarization is lower than in MD-5x10S design but higher than in MD-5x5 and MD-3x3 designs. For high Reynolds number (Figure 11(c)), the trends remain consistent while the difference in the extent of temperature polarization becomes more significant.

Figure 11(d) – (f) show the centerline plots in the $y$-direction of the time-average $\overline{CPC}$. Similar trends to time-average temperature polarization can be observed. At low Reynolds number (Figure 11(d)), all cases have a similar distribution, with MD-5x10S showing the lower concentration polarization. At a moderate Reynolds number (Figure 11(e)), a slight improvement is observed for MD-5x10 with right-angled bends. For MD-5x5 and MD-3x3 designs with both right-angled bends and inlets with sudden expansions, a significant reduction in concentration polarization can be observed, indicated by the lower $\overline{CPC}$ at the center. As Reynolds number further increases
(Figure 11(f)), the trends remain similar to those for $Re_{in} = 250$ with MD-3x3 showing the lowest polarization because of its strongest inlet effect.

4. Discussion

4.1. Impact of vortices on predicted temperature and concentration polarization from Nusselt and Sherwood correlations

An established approach to predict temperature and concentration polarization in MD is to use the Nusselt and Sherwood correlation to predict temperature and concentration on the surface of the membrane [11]. Dudchenko et al. [10] have investigated the accuracy of different Nusselt correlations to predict temperature polarization. Once the thermophysical properties of the fluid mixture are defined, membrane surface temperatures on both the feed and draw sides can be determined. However, as demonstrated in this work and other relevant studies [43], membrane temperature can be spatially highly heterogeneous. We first compute the time- and spatial-averaged temperature polarization coefficient $\langle\text{TPC}\rangle$ through equation (22). To compare the simulation results with predicted values, we follow the algorithm outlined in Hitsov et al. [11]. Two Nusselt correlations by Stephan et al. [60] and Gryta et al. [61] are defined as

$$Nu = 0.097Re_{c}^{0.73}Pr_{b}^{0.13} \left( \frac{Pr_{b}}{Pr_{m}} \right)^{0.25},$$  

$$Nu = 7.55 + \frac{0.024 (Pr_{m}Re_{c}d_{ch}/L_{C})}{1 + 0.0358Pr_{m}^{0.81} / (L_{C}/d_{ch}Re_{c})^{0.64}} \left( \frac{\mu_{b}}{\mu_{m}} \right)^{0.14},$$

where $d_{ch}$ [m] is the hydraulic diameter of the channel, $\mu_{b}$ [kg m$^{-1}$ s$^{-1}$] and $\mu_{m}$ [kg m$^{-1}$ s$^{-1}$] are the dynamic viscosity of the fluid in the bulk and on the
membrane, respectively, and $Pr$ is the Prandtl number defined as

$$Pr = \frac{cp\mu}{k}.$$  \hfill (31)

Furthermore, we compute the concentration on the membrane surface with Sherwood correlation [11] such that

$$C_m = C_b \exp \left( \frac{J_w}{\rho h_c} \right),$$  \hfill (32)

$$Sh = \frac{d_{ch} h_c}{D} = 1.86 \left( Re_c Sc d_{ch} L_C \right)^{0.33},$$  \hfill (33)

$$Sc = \frac{\mu}{\rho D},$$  \hfill (34)

where $L_C$ m is the length of the main channel, $C_m$ [kg m$^{-3}$] and $C_b$ [kg m$^{-3}$] are the salt concentration on the membrane surface and in the bulk fluid and $h_c$ [m s$^{-1}$] is the convective mass transfer coefficient.

Figure 12(a) shows the time- and spatial-averaged temperature polarization $\langle TPC \rangle$ as a function of Reynolds number $Re_{in}$. As $Re_{in}$ increases, $\langle TPC \rangle$ increases, indicating weaker temperature polarization. At low $Re_{in}$, all cases show similar values of $\langle TPC \rangle$ since the flow is laminar and no Dean vortices are present. As $Re_{in}$ increases, $\langle TPC \rangle$ for MD-5x10, MD-5x5 and MD-3x3 is always higher than that of MD-5x10S, indicating the significant impacts of right-angled bends and jet-inducing inlets on the reduction of temperature polarization. However, $\langle TPC \rangle$ for MD-3x3 with stronger impinging jets does not result in lower temperature polarization compared to MD-5x5. One possible explanation is that $Re_{in}$ does not account for the effect of the volumetric flow rate: the same $Re_{in}$ does not necessarily correspond to the same volumetric flow rate because $Re_{in}$ is calculated based on the hydraulic diameter of the inlet.
To understand the effect of the volumetric flow rate, we introduce the channel Reynolds number, $Re_c$ as

$$Re_c = \left( \frac{u_{in} H_C}{\nu_0} \right) \left( \frac{A_{in}}{A_c} \right),$$  

(35)

where $H_C$ [m] is the height of the main channel. Figure 12(b) shows $\langle TPC \rangle$ as a function of channel Reynolds number $Re_c$ that includes the effect of volumetric flow rate. At low $Re_c$, $\langle TPC \rangle$ for all cases are approximately the same, indicating negligible effects of right-angled bends and jet-inducing inlets. As $Re_c$ increases, we observe that $\langle TPC \rangle$ for MD-3x3 is always the largest, followed by MD-5x5 and MD-5x10. This result suggests that the inlet with the strongest impinging jets results in the largest $\langle TPC \rangle$ and the least temperature polarization for the same volumetric flow rate or $Re_c$. Comparing MD-5x10 with MD-5x10S, we have also demonstrated that right-angled
bends results in less significant temperature polarization. As shown in Figure 12(b), at low $Re_c$, the Nusselt correlation of Gryta et al. [61] successfully captures the behavior. For high $Re_c$, both models consistently overpredict the temperature polarization coefficient and underestimate the temperature polarization by more than 10% for MD-3x3 and 40% for MD-5x10S. Furthermore, current models do not capture the effects induced by right-angled bends and inlet.

4.2. Relationship between the Dean vortices and polarization

In previous sections, we discussed separately the effects of right-angled bends and inlet design on flow dynamics and temperature and concentration polarization. In this section, we focus on establishing the relationship between the formation of vortices and improvement in polarization effects. Figure 13 shows a 3D visual of the flow field with Dean vortices and the underlying temperature polarization on the membrane for MD-5x5 at $Re_{in} = 250$. In the plot, we overlay the flow with the vortices, where the magnitude of the flow is proportional to the length of the arrows. As shown, the lowest temperature polarization, indicated by the red region, is observed at the location where two counter-rotating vortices touch each other, resulting in a strong flow perpendicular to the membrane surface, which leads to a reduction of the temperature boundary layer. On the contrary, no significant flow nor vortices are observed near the wall corners, resulting in significant boundary layer effects and stronger temperature polarization. Overall, the formation of Dean vortices enhances the flow perpendicular to the membrane, therefore reducing boundary layer effects, and ultimately minimizing both temperature and concentration polarization.
Figure 13: The intersection between instantaneous $x$-direction vorticity $\omega_x$ and temperature polarization on the membrane for MD-5x5 with $Re_{in} = 250$: (a) standard and (b) zoomed-in.

Figure 14: The root mean square fluctuations of the temperature polarization $TPC_{rms}$ as a function of (a) time- and spatial average temperature polarization coefficient $\langle TPC \rangle$ and (b) Reynolds number $Re_{in}$. 
To quantify the relationship, we introduce a metric to relate the effects of Dean vortices on temperature polarization. Theoretically, if there is no chaos in the flow, the distribution of temperature polarization on the membrane should remain constant over time (that is, $\overline{TPC}$ at a location should not change over time). Therefore, quantifying the fluctuation of $\overline{TPC}$ in time would indicate how chaotic the flow is. As demonstrated in Figure 7 and 8, the chaos in the flow of MD-5x10, MD-5x5 and MD-3x3 is related to the formation of dean vortices, therefore, we could equate the fluctuation of $\overline{TPC}$ in time with the formation of dean vortices. The spatial average fluctuation $\overline{TPC}_{rms}$ is defined as

$$\overline{TPC}_{rms} = \left\langle \left( \overline{TPC}(x, t) - \overline{TPC}(x) \right)^2 \right\rangle.$$ (36)

Figure 14(a) shows the root mean square fluctuations of the temperature polarization $\overline{TPC}_{rms}$ as a function of $\left\langle \overline{TPC} \right\rangle$. For MD-5x10S, $\overline{TPC}_{rms}$ remains negligible as $\left\langle \overline{TPC} \right\rangle$ increases, indicating that the temperature polarization coefficient does not change in time. This shows that the improvement in temperature polarization is not due to the chaos in the flow. For other cases (MD-5x10, MD-5x5 and MD-3x3), two regimes are identified. Initially, $\left\langle \overline{TPC} \right\rangle$ increases when the fluctuations remain zero. As $\left\langle \overline{TPC} \right\rangle$ increases to a critical value, the fluctuations increase. This shows that the improvement in temperature polarization after the critical value is correlated with the chaos in the flow.

Figure 14(b) shows the root mean square fluctuations of the temperature polarization $\overline{TPC}_{rms}$ as a function of $Re_c$. For MD-5x10S, $\overline{TPC}_{rms}$ remains negligible for all $Re_c$ as expected: since the MD-5x10S design is a straight channel of constant cross-section, Dean vortices are absent and mixing is
negligible. For the other designs, at low Reynolds numbers, $TPC_{rms}$ is approximately zero, indicating the absence of Dean vortices and mixing. As $Re_c$ increases beyond a threshold, we observe an increase in $TPC_{rms}$. Combining the findings in Figure 14, at low Reynolds numbers, the improvement in temperature polarization is due to the increase in volumetric flow rate, which reduces the thickness of the boundary layers. For cases with right-angled bends and jet-inducing inlets, vortices are generated when Reynolds number overcomes a threshold value: this causes an increase in the temporal fluctuations of the flow field which ultimately reduce temperature polarization.

4.3. Implications on model development with lab-scale systems

In this study, we have demonstrated how inlet designs of lab-scale systems can induce the formation of vortical structures in the flow field, which can greatly affect temperature and concentration polarization. Currently, experimental Sherwood and Nusselt correlations, calibrated on data from lab-scale systems, are applied to predict the performance of full-scale systems. Yet, boundary effects related to the inlet design (both shape and bends) can have a large impact on momentum, heat and mass transfer in systems at the lab scale. As a result, concentration and temperature polarization estimated from models calibrated on bench scale systems may not be representative of the system performance at the full scale. Such models developed for lab-scale systems (with right-angled bends and jet-inducing inlets) would result in an underestimation of temperature and concentration polarization in full-scale systems, where boundary effects will likely be attenuated by the length of the systems and mixing mechanisms to reduce temperature and concentra-
tion polarization are absent. As a result, dynamic similarity between relevant momentum, mass and temperature transfer mechanisms needs to be assessed and established between lab-scale and full-scale systems, when Sherwood and Nusselt correlations are used for temperature and concentration polarization predictions larger scales.

5. Conclusions

Understanding and predicting membrane fouling in MD systems due to temperature and concentration polarization is critical to designing low-cost and efficient systems. In this study, we studied the effects of right-angled bends and inlet in lab-scale MD systems on flow characteristics, temperature and concentration polarization. We conducted a total of 87 CFD simulations with OpenFOAM for four designs (MD-5x10S, MD-5x10, MD-5x5 and MD-3x3) with different volumetric flow rates. We discovered that both right-angled bends and inlet design are responsible for the formation of Dean vortices in the main channel of the MD systems. Designs with both right-angled bends and jet-forming inlets (MD-5x5 and MD-3x3) resulted in more stable Dean vortices at higher Reynolds numbers. In addition, at low Reynolds numbers, differences in temperature and concentration polarization are negligible across different designs. At moderate and high Reynolds numbers, MD systems with right-angled bends and inlets have more heterogeneous distributions of the temperature and concentration polarization coefficients. By calculating time- and spatial-average temperature and concentration polarization coefficients, we discovered that MD systems with right-angled bends and inlets of variable cross-sections present much lower temperature and concen-
tration polarization. To assess the impact of vortex presence on polarization, a new metric based on the spatial fluctuation of the temperature polarization was calculated. At low Reynolds numbers, fluctuations remain zero for all cases. At moderate Reynolds numbers, the fluctuations increase significantly for cases with right-angled bends and inlet with varying cross-sections, while remaining zero for MD-5x10S. This shows that the improvement in temperature and concentration polarizations at higher Reynolds numbers is due to the formation of vortical structures in the channel. Additionally, time- and spatial-average temperature polarization coefficients are compared with values predicted from Sherwood and Nusselt correlations available in the literature: the error between models and CFD simulation results can be as high as 40%. These results suggest that in order to develop models that can accurately predict temperature and concentration polarization, the flow dynamics in the lab-scale systems have to be comparable, i.e. dynamically similar, to those in full-scale systems.

Acknowledgments

This material is based upon work supported by the National Alliance for Water Innovation (grant number: 1242861-12-SDGBM), funded by the U.S. Department of Energy, Energy Efficiency and Renewable Energy Office, Advanced Manufacturing Office under Funding Opportunity Announcement DE-FOA-0001905.
Appendix A. Thermophysical properties of fluid

The density of the fluid is calculated with the correlation proposed by Naftz et al. \[62\] as

\[
\rho = \rho_0 + 184.01062 + 1.04708C - 1.21061T \\
+ 3.14712 \times 10^{-4}C^2 + 0.00199T^2 - 0.00112CT,
\]

\[
\rho_0 = \left[ 999.83952 + 16.952577T_c - 7.9905127 \times 10^{-3}T_c^2 \\
- 4.6241757 \times 10^{-5}T_c^3 + 1.0574601 \times 10^{-7}T_c^4 \\
- 2.8103006 \times 10^{-10}T_c^5 \right] / \left[ 1 + 0.016887236T_c \right].
\]

where $\rho_0 \text{ [kg m}^{-3}\text{]}$ is the density of pure water and $T_c \text{ [°C]} = T - T_{stp}$ is the temperature in celsius. According to Naftz et al. \[62\], the correlation is valid for fluid density with a temperature range of 5 °C to 50 °C and a concentration range of 23 kg m$^{-3}$ to 182 kg m$^{-3}$.

We follow the models by Lou et al. \[43\] for the dynamic viscosity, specific heat capacity and latent heat of vaporization. The dynamic viscosity of the sodium chloride solution is calculated as

\[
\mu(T, C) = (P_\mu T_\mu) \cdot C_\mu,
\]

where $T_\mu = \left( T_c^0 \ T_c^1 \ T_c^2 \ T_c^3 \ T_c^4 \right)^T$ and $C_\mu = \left( C^0 \ C^1 \ C^2 \ C^3 \ C^4 \right)^T$ and $P_\mu$ is the matrix of polynomial coefficients given by
\[
P_{c} = \begin{pmatrix}
3.3922 \times 10^{-11} & -8.6874 \times 10^{-9} & 9.0999 \times 10^{-7} & -5.1893 \times 10^{-5} & 1.7415 \times 10^{-3} \\
1.0124 \times 10^{-6} & 4.1167 \times 10^{-8} & -1.5232 \times 10^{-9} & 1.8820 \times 10^{-11} & -8.3450 \times 10^{-14} \\
1.0827 \times 10^{-8} & -6.9728 \times 10^{-10} & 1.5945 \times 10^{-11} & -1.6487 \times 10^{-13} & 6.6306 \times 10^{-16} \\
4.7647 \times 10^{-15} & 1.2275 \times 10^{-12} & -3.1776 \times 10^{-14} & 3.1028 \times 10^{-16} & -1.1551 \times 10^{-18} \\
2.5617 \times 10^{-14} & -3.3743 \times 10^{-15} & 8.9878 \times 10^{-17} & -9.8135 \times 10^{-19} & 4.0912 \times 10^{-21}
\end{pmatrix}
\]

(A.3)

The specific heat capacity of sodium chloride solution is modeled as

\[c_p(T, C) = (P_{c} T_{c}) \cdot C_{c},\] (A.4)

where \(T_{c} = \begin{pmatrix} T_0^c \\ T_1^c \\ T_2^c \end{pmatrix}, C_{c} = \begin{pmatrix} C^0 \\ C^1 \\ C^2 \end{pmatrix}^T\) and \(P_{c}\) is the matrix of polynomial coefficients given by

\[
P_{c} = \begin{pmatrix}
4129.8 & 0.75986 & -6.1128 \times 10^{-4} \\
-4.6391 & -2.2851 \times 10^{-3} & 2.2508 \times 10^{-5} \\
3.2167 \times 10^{-8} & -9.1455 \times 10^{-6} & 2.4487 \times 10^{-3}
\end{pmatrix}.
\] (A.5)

The thermal conductivity of sodium chloride solution is calculated with the model by Ramires et al. [63] as

\[k(T, C) = (P_{k} T_{k}) \cdot C_{k},\] (A.6)

where \(T_{k} = \begin{pmatrix} T_0^k \\ T_1^k \\ T_2^k \end{pmatrix}, C_{k} = 0.01716 \begin{pmatrix} C^0 \\ C^1 \\ C^2 \end{pmatrix}^T\) and \(P_{k}\) is the matrix of polynomial coefficients given by

\[
P_{k} = \begin{pmatrix}
0.5621 & 0.00199 & -8.6 \times 10^{-6} \\
-0.01394 & 0.000294 & -2.3 \times 10^{-6} \\
0.00177 & -6.3 \times 10^{-5} & 4.5 \times 10^{-7}
\end{pmatrix}.
\] (A.7)
The latent heat of water is evaluated as

$$\lambda(T) = -2438.18T_c + 2502800,$$  \hspace{1cm} (A.8)

while the mass diffusivity of sodium chloride solution is calculated using the correlation by Harned and Hildreth [64]

$$D(T) = 17.872 \times 10^{-14}T \frac{\lambda_{Na,25}\lambda_{Cl,25}(1 + \alpha(T_c - 25))^2}{(\lambda_{Na,25} + \lambda_{Cl,25})(1 + \alpha(T_c - 25))},$$  \hspace{1cm} (A.9)

where $\lambda_{Na,25} = 50.09$ and $\lambda_{Cl,25} = 76.23$.

References

[1] A. D. Khawaji, I. K. Kutubkhanah, J.-M. Wie, Advances in seawater desalination technologies, Desalination 221 (1) (2008) 47–69. doi:10.1016/j.desal.2007.01.067.

[2] J. Miller, Review of water resources and desalination technologies, Tech. Rep. SAND2003-0800, Sandia National Laboratories (SNL) (Mar. 2003). doi:10.2172/809106.

[3] A. Subramani, J. G. Jacangelo, Emerging desalination technologies for water treatment: a critical review, Water Res. 75 (2015) 164–187. doi:10.1016/j.watres.2015.02.032.

[4] C. Shin, A. Szczuka, R. Jiang, W. A. Mitch, C. S. Criddle, Optimization of reverse osmosis operational conditions to maximize ammonia removal from the effluent of an anaerobic membrane bioreactor, Environmental Science: Water Research & Technology 7 (4) (2021) 739–747. doi:10.1039/D0EW01112F.
[5] L. F. Greenlee, D. F. Lawler, B. D. Freeman, B. Marrot, P. Moulin, Reverse osmosis desalination: water sources, technology, and today's challenges, Water Res. 43 (9) (2009) 2317–2348. doi:10.1016/j.watres.2009.03.010

[6] L. D. Tijing, Y. C. Woo, J.-S. Choi, S. Lee, S.-H. Kim, H. K. Shon, Fouling and its control in membrane distillation—A review, J. Memb. Sci. 475 (2015) 215–244.

[7] E. Curcio, X. Ji, G. Di Profio, E. Fontananova, E. Drioli, Others, Membrane distillation operated at high seawater concentration factors: Role of the membrane on CaCO3 scaling in presence of humic acid, J. Memb. Sci. 346 (2) (2010) 263–269.

[8] M. Gryta, Fouling in direct contact membrane distillation process, J. Memb. Sci. 325 (1) (2008) 383–394.

[9] A. V. Dudchenko, M. Hardikar, R. Xin, S. Joshi, R. Wang, N. Sharma, M. S. Mauter, Impact of module design on heat transfer in membrane distillation, J. Memb. Sci. 601 (2020) 117898. doi:10.1016/j.memsci.2020.117898

[10] A. V. Dudchenko, M. Hardikar, A. Anand, R. Xin, R. Wang, C. Gopu, M. S. Mauter, Guidance on Nusselt Number Correlation Selection in Membrane Distillation, ACS EST Eng. doi:10.1021/acsestengg.1c00496

[11] I. Hitsov, T. Maere, K. De Sitter, C. Dotremont, I. Nopens, Modelling
approaches in membrane distillation: A critical review, Sep. Purif. Technol. 142 (2015) 48–64. doi:10.1016/j.seppur.2014.12.026

[12] A. Ali, F. Macedonio, E. Drioli, S. Aljlil, O. A. Alharbi, Experimental and theoretical evaluation of temperature polarization phenomenon in direct contact membrane distillation, Chem. Eng. Res. Des. 91 (10) (2013) 1966–1977.

[13] J. Phattaranawik, R. Jiraratananon, A. G. Fane, Heat transport and membrane distillation coefficients in direct contact membrane distillation, J. Memb. Sci. 212 (1-2) (2003) 177–193.

[14] E. Curcio, E. Drioli, Membrane distillation and related operations—a review, Sep. Purif. Rev. 34 (1) (2005) 35–86.

[15] Q. L. Ve, R. Koirala, M. Bawahab, H. Faqeha, M. C. Do, Q. L. Nguyen, A. Date, A. Akbarzadeh, Experimental investigation of the effect of the spacer and operating conditions on mass transfer in direct contact membrane distillation, Desalination 500 (2021) 114839.

[16] O. R. Lokare, R. D. Vidic, Impact of operating conditions on measured and predicted concentration polarization in membrane distillation, Environ. Sci. Technol. 53 (20) (2019) 11869–11876.

[17] K. Ohta, K. Kikuchi, I. Hayano, T. Okabe, T. Goto, S. Kimura, H. Ohya, Experiments on sea water desalination by membrane distillation, Desalination 78 (2) (1990) 177–185.
[18] T.-C. Chen, C.-D. Ho, H.-M. Yeh, Theoretical modeling and experimental analysis of direct contact membrane distillation, J. Memb. Sci. 330 (1-2) (2009) 279–287.

[19] M. Qtaishat, T. Matsuura, B. Kruczek, M. Khayet, Heat and mass transfer analysis in direct contact membrane distillation, Desalination 219 (1-3) (2008) 272–292.

[20] J.-G. Lee, W.-S. Kim, J.-S. Choi, N. Ghaffour, Y.-D. Kim, A novel multi-stage direct contact membrane distillation module: design, experimental and theoretical approaches, Water Res. 107 (2016) 47–56.

[21] A. Chafidz, F. N. Rahma, S. Nurkhamidah, S. Al-Zahrani, Portable Solar-powered Membrane Distillation System to Solve Water and Energy Problems Simultaneously, in: Journal of Physics: Conference Series, Vol. 1304, 2019, p. 012018.

[22] L. Song, B. Li, K. K. Sirkar, J. L. Gilron, Direct contact membrane distillation-based desalination: novel membranes, devices, larger-scale studies, and a model, Ind. Eng. Chem. Res. 46 (8) (2007) 2307–2323.

[23] M. S. Salem, A. H. El-shazly, N. Nady, M. R. Elmarghany, M. A. Shouman, M. N. Sabry, 3-D numerical investigation on commercial PTFE membranes for membrane distillation: Effect of inlet conditions on heat and mass transfer, Case Studies in Thermal Engineering 13 (2019) 100396.

[24] N. Nivedita, P. Ligrani, I. Papautsky, Dean Flow Dynamics in Low-
Aspect Ratio Spiral Microchannels, Sci. Rep. 7 (2017) 44072. doi:10.1038/srep44072

[25] A. Bottaro, O. J. E. Matsson, P. H. Alfredsson, Numerical and experimental results for developing curved channel flow, Physics of Fluids A: Fluid Dynamics 3 (6) (1991) 1473–1476.

[26] W. H. Finlay, J. B. Keller, J. H. Ferziger, Instability and transition in curved channel flow, J. Fluid Mech. 194 (1988) 417–456.

[27] L. Helin, L. Thais, G. Mompean, Numerical simulation of viscoelastic Dean vortices in a curved duct, J. Non-Newtonian Fluid Mech. 156 (1-2) (2009) 84–94.

[28] P. Naphon, S. Wongwises, A review of flow and heat transfer characteristics in curved tubes, Renewable Sustainable Energy Rev. 10 (5) (2006) 463–490.

[29] R. Altay, A. A. Yetisgin, K. Erdem, A. Koşar, The effect of varying radius of curvature on mixing in elliptical spiral microchannels, Chemical Engineering and Processing-Process Intensification 164 (2021) 108401.

[30] X. Wang, Z. Liu, B. Wang, Y. Cai, Y. Wan, Vortices degradation and periodical variation in spiral micromixers with various spiral structures, Int. J. Heat Mass Transf. 183 (2022) 122168.

[31] P. Bayat, P. Rezai, Semi-empirical estimation of dean flow velocity in curved microchannels, Sci. Rep. 7 (1) (2017) 1–13.
[32] P. M. Ligrani, R. D. Niver, Flow visualization of Dean vortices in a curved channel with 40 to 1 aspect ratio, The Physics of fluids 31 (12) (1988) 3605–3617.

[33] H. Chen, B. Zhang, Fluid flow and mixed convection heat transfer in a rotating curved pipe, Int. J. Therm. Sci. 42 (11) (2003) 1047–1059.

[34] J. O. de Brito Lira, H. G. Riella, N. Padoin, C. Soares, Fluid Dynamics and Mass Transfer in Curved Reactors: A CFD Study on Dean Flow Effects, Journal of Environmental Chemical Engineering (2022) 108304.

[35] R. Gardon, J. C. Akfirat, The role of turbulence in determining the heat-transfer characteristics of impinging jets, Int. J. Heat Mass Transf. 8 (10) (1965) 1261–1272.

[36] D. Lytle, B. W. Webb, Air jet impingement heat transfer at low nozzle-plate spacings, Int. J. Heat Mass Transf. 37 (12) (1994) 1687–1697.

[37] E. M. Sparrow, T. C. Wong, Impingement transfer coefficients due to initially laminar slot jets, Int. J. Heat Mass Transf. 18 (5) (1975) 597–605.

[38] S. Feroz, Mass Transfer Coefficients at the Stagnation Point with Submerged Impinging Multi-Jet Flow of Fluid Electrolyte, Turk. J. Eng. Environ. Sci. 30 (4) (2006) 221–229.

[39] M. D. Fox, M. Kurosaka, L. Hedges, K. Hirano, The influence of vortical structures on the thermal fields of jets, J. Fluid Mech. 255 (1993) 447–472.
[40] V. Tesař, J. Barker, Dominant vortices in impinging jet flows, Journal of visualization 5 (2) (2002) 121–128.

[41] G. Le Song, M. Prud’homme, Prediction of coherent vortices in an impinging jet with unsteady averaging and a simple turbulent model, Int. J. Heat Fluid Flow 28 (5) (2007) 1125–1135.

[42] Y. Yao, C. S. Criddle, O. B. Fringer, The effects of particle clustering on hindered settling in high-concentration particle suspensions, J. Fluid Mech. 920 (2021) A40. doi:10.1017/jfm.2021.470.

[43] J. Lou, J. Vanneste, S. C. DeCaluwe, T. Y. Cath, N. Tilton, Computational fluid dynamics simulations of polarization phenomena in direct contact membrane distillation, J. Memb. Sci. 591 (2019) 117150. doi:10.1016/j.memsci.2019.05.074.

[44] J. Lou, J. Johnston, T. Y. Cath, D. Martinand, N. Tilton, Computational fluid dynamics simulations of unsteady mixing in spacer-filled direct contact membrane distillation channels, J. Memb. Sci. 622 (2021) 118931. doi:10.1016/j.memsci.2020.118931.

[45] Y. Yao, O. B. Fringer, C. S. Criddle, CFD-accelerated bioreactor optimization: reducing the hydrodynamic parameter space, Environ. Sci.: Water Res. Technol. 8 (3) (2022) 456–464. doi:10.1039/D1EW00666E.

[46] Y. Yao, C. S. Criddle, O. B. Fringer, Comparison of the properties of segregated layers in a bidispersed fluidized bed to those of a monodispersed fluidized bed, Phys. Rev. Fluids 6 (8) (2021) 084306. doi:10.1103/PhysRevFluids.6.084306.
[47] Y. Yao, C. S. Criddle, O. B. Fringer, Competing flow and collision effects in a monodispersed liquid–solid fluidized bed at a moderate Archimedes number, J. Fluid Mech. 927 (2021) A28. doi:10.1017/jfm.2021.780.

[48] B. Ling, I. Battiato, Rough or wiggly? Membrane topology and morphology for fouling control, J. Fluid Mech. 862 (2019) 753–780. doi:10.1017/jfm.2018.965.

[49] B. Ling, P. Xie, D. Ladner, I. Battiato, Dynamic Modeling of Fouling in Reverse Osmosis Membranes, Membranes 11 (5). doi:10.3390/membranes11050349.

[50] Z. Zhou, B. Ling, I. Battiato, S. M. Husson, D. A. Ladner, Concentration polarization over reverse osmosis membranes with engineered surface features, J. Memb. Sci. 617 (2021) 118199. doi:10.1016/j.memsci.2020.118199.

[51] J. M. Smith, Introduction to chemical engineering thermodynamics, J. Chem. Educ. 27 (10) (1950) 584. doi:10.1021/ed027p584.3.

[52] G. C. Sarti, C. Gostoli, S. Matulli, Low energy cost desalination processes using hydrophobic membranes, Desalination 56 (1985) 277–286. doi:10.1016/0011-9164(85)85031-1.

[53] M. Martín, F. J. Montes, M. A. Galán, Mass transfer rates from bubbles in stirred tanks operating with viscous fluids, Chem. Eng. Sci. 65 (12) (2010) 3814–3824. doi:10.1016/j.ces.2010.03.015.

[54] H. G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to
computational continuum mechanics using object-oriented techniques, Computers in Physics 12 (6) (1998) 620–631. doi:10.1063/1.168744.

[55] B. Lessani, M. V. Papalexandris, Time-accurate calculation of variable density flows with strong temperature gradients and combustion, J. Comput. Phys. 212 (1) (2006) 218–246. doi:10.1016/j.jcp.2005.07.001.

[56] R. I. Issa, Solution of the implicitly discretised fluid flow equations by operator-splitting, J. Comput. Phys. 62 (1) (1986) 40–65. doi:10.1016/0021-9991(86)90099-9.

[57] R. F. Warming, R. M. Beam, Upwind Second-Order Difference Schemes and Applications in Aerodynamic Flows, AIAA Journal 14 (9) (1976) 1241–1249. doi:10.2514/3.61457.

[58] J. Vanneste, J. A. Bush, K. L. Hickenbottom, C. A. Marks, D. Jassby, C. S. Turchi, T. Y. Cath, Novel thermal efficiency-based model for determination of thermal conductivity of membrane distillation membranes, J. Memb. Sci. 548 (2018) 298–308. doi:10.1016/j.memsci.2017.11.028.

[59] J. Jeong, F. Hussain, On the identification of a vortex, J. Fluid Mech. 285 (1995) 69–94. doi:10.1017/S0022112095000462.

[60] K. Stephan, Wärmeübergang und Druckabfall bei nicht ausgebildeter Laminarströmung in Rohren und in ebenen Spalten, Chem. Ing. Tech. 31 (12) (1959) 773–778. doi:10.1002/cite.330311204.
[61] M. Gryta, M. Tomaszewska, A. W. Morawski, Membrane distillation with laminar flow, Sep. Purif. Technol. 11 (2) (1997) 93–101. doi:10.1016/S1383-5866(97)00002-6

[62] D. L. Naftz, F. J. Millero, B. F. Jones, W. Reed Green, An Equation of State for Hypersaline Water in Great Salt Lake, Utah, USA, Aquat. Geochem. 17 (6) (2011) 809–820. doi:10.1007/s10498-011-9138-z

[63] M. L. V. Ramires, C. A. Nieto de Castro, J. M. N. A. Fareleira, W. A. Wakeham, Thermal conductivity of aqueous sodium chloride solutions, J. Chem. Eng. Data 39 (1) (1994) 186–190. doi:10.1021/je00013a053

[64] H. S. Harned, C. L. Hildreth, The Differential Diffusion Coefficients of Lithium and Sodium Chlorides in Dilute Aqueous Solution at 25°, J. Am. Chem. Soc. 73 (2) (1951) 650–652. doi:10.1021/ja01146a043