CFD SIMULATION OF POLARIZATION PHENOMENA
IN DIRECT CONTACT MEMBRANE DISTILLATION
SYSTEMS

by

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ABSTRACT

Direct contact membrane distillation (DCMD) is a thermal process in which warm feed and cool distilled water flow on opposite sides of a hydrophobic membrane. The temperature difference causes water to evaporate from the feed, travel through the membrane, and condense in the distillate. Because DCMD is insensitive to osmotic pressure, it has emerged as a promising means of concentrating brines to their saturation limit. Studies have shown that temperature and concentration polarization are the two crucial factors affecting DCMD performance in the treatment of hypersaline brines. Temperature polarization refers to a reduction in the transmembrane temperature difference due to heat transfer through the membrane. Concentration polarization describes the accumulation of solutes adjacent to the feed side of the membrane. To date, computational fluid dynamics (CFD) studies of DCMD focus primarily on the challenge of temperature polarization. For high concentration brines, however, concentration polarization is another major challenge that reduces system efficiency and leads to mineral scaling. Temperature and concentration polarization are further complicated by spacers, a mesh-like material that separates and supports tightly packed membrane sheets. These interactions are not well understood, because they are difficult to study experimentally and numerically, and the flow regimes are not fully charted. We consequently develop a tailored in-house CFD code that simulates unsteady two-dimensional heat and mass transport in plate-and-frame DCMD systems with cylindrical spacers. The code uses an efficient combination of finite-volume methods in space, projection methods in time, and recent advances in immersed boundary methods for the spacer surfaces.

For DCMD systems without spacers, we perform a comprehensive parametric study of polarization phenomena for a wide range of feed and distillate operating conditions, system length, and co-current versus counter-current operation. We also investigate the system-level performance by measuring the average permeate flux, single-pass water recovery, maximum
concentration polarization coefficient, and gained output ratio of DCMD systems with heat recovery. Though the transmembrane vapor flux is small, we observe dramatic increases in solute concentration at the membrane surface, exceeding 1.6 times the feed value. The temperatures, concentration, and vapor flux vary considerably in the downstream direction, and are poorly approximated by common Nusselt and Sherwood correlations.

For DCMD systems with spacers, we investigate the impact of the Reynolds number, spacer diameter, and spacer position on polarization and system performance. We show that the impact of spacers can be explained by examining the various steady and unsteady vortical flow structures generated in the bulk and near the bounding plates and membranes. Overall, we show that though unsteady vortex structures tend to mix temperature polarization layers with the bulk, they are not similarly able to mix the thin concentration layers. Rather, vortical structures tend to create regions of preferential salt accumulation. In the vortex shedding regime, the net result is that spacers often increase vapor production at the expense of increasing the risk of mineral scaling.
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Cartesian coordinates (m) ............................................. \( x, y \)

Gained Output Ratio .................................................. GOR

Intermediate variable used in projection method ................. \( \phi \)

Lewis number .............................................................. \( Le \)

\( \text{Lm}^{-2}\text{hr}^{-1} \) .................................................. \( \text{LMH} \)

NaCl molality (mol/kg) .................................................. \( b \)

Numerical time step (s) .................................................. \( dt \)

Provisional velocity vector in projection method (m/s) ........ \( \mathbf{u}^* \)

Reynolds number .......................................................... \( Re \)

Spatial error .............................................................. \( Err_N \)

Strouhal number .......................................................... \( St \)

Temporal error ............................................................ \( Err_t \)

Water Recovery (%) .................................................... \( WR \)

average transmembrane vapor flux (L/m\(^2\) h) ................. \( v_{m}^{ave} \)

channel height (m) ....................................................... \( H \)

channel length (m) ....................................................... \( L \)

concentration (g/L) ...................................................... \( c \)

concentration boundary layer thickness (m) ....................... \( \delta_c \)

concentration polarization coefficient ......................... \( \text{CPC} \)

convective heat transfer coefficient (W/m\(^2\) °C) .......... \( h_T \)
convective mass transfer coefficient (W/m^2 °C) \( h_c \)
critical Reynolds number \( Re_c \)
critical Strouhal number \( St_c \)
density (kg/m^3) \( \rho \)
density of feed and distillate fluid (kg/m^3) \( \rho^f, \rho^d \)
distillate inlet latent heat of water (J/kg) \( \lambda^d_{in} \)
dynamic viscosity (Pa s) \( \mu \)
effectiveness of heat exchangers \( \epsilon_{HX} \)
feed and distillate flow Reynolds number \( Re_f, Re_d \)
feed and distillate inlet temperature (°C) \( T_{in}^f, T_{in}^d \)
feed channel pressure drop (Pa/m) \( \Delta P/L \)
feed concentration (g/L) \( C_{in} \)
feed inlet latent heat of water (J/kg) \( \lambda_{in}^f \)
gas phase thermal conductivity (W/m °C) \( k_v \)
hydraulic Reynolds number \( Re_h \)
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For my parents, Lianlian Dai and Kangmei Lou, and my sister, Jing Lou, whose tremendous love and support make this work possible.
Population growth, climate change, and overdrawn freshwater sources have provoked a growing potable water deficit that threatens global energy, food, and economic security. Membrane separation processes offer promising solutions to this crisis through their applications to desalination, potable reuse, and treatment of agricultural and industrial waste streams [1–3]. Currently, the global capacity of reverse osmosis (RO) and nanofiltration water treatment systems exceeds 42 million m$^3$/day (equivalent to the volume of 40 Empire State Buildings per day)[1, 4, 5]. This growth is expected to occur primarily in the form of RO plants, as the cost and energy consumption of large RO plants have decreased to as little as US $0.50 and 2.0 kWhr per cubic meter of produced water. RO is a membrane filtration process in which water is driven through a semipermeable membrane by applying a large transmembrane pressure difference. Due to osmotic pressure across the membrane, water recovery from RO typically varies between 50% for seawater and up to 80% for brackish water. The remaining brine has a salt concentration around 70 g/l and contains residual pretreatment and cleaning chemicals, as well as heavy metals from corrosion. The rapid growth in RO brings the challenge of managing this waste brine and chemical discharge, particularly for inland applications [6, 7]. Membrane distillation (MD) has emerged as a promising means of concentrating waste brines to their saturation limit, after which they can be discharged to crystallizers or small evaporation ponds [8–19].

The energy efficiency, water recovery, and environmental sustainability of MD depend on coupled heat, mass, and momentum transport phenomena that are difficult to observe experimentally. MD is also quite challenging to simulate numerically. MD systems have complicated geometries in which the flow regime is poorly understood, and the separation process includes phase change effects and transmembrane heat and vapor transport that are
not straightforward to model. The current work overcomes these challenges by developing tailored numerical methods for simulating MD systems. The methods are then used to gain a more fundamental understanding of heat and mass transport in MD systems.

1.1 Motivation

MD is a membrane filtration process in which volatile compounds are driven across a hydrophobic membrane by an imposed temperature difference [20]. Though various modes of MD exist, we focus here on the most common arrangement, known as direct contact membrane distillation (DCMD). In this arrangement, warm feed and cool distillate water flow on opposite sides of a hydrophobic microporous membrane in a co-current or counter-current manner, as sketched in Figure 1.1. The hydrophobic membrane creates vapor-liquid interfaces on the feed and distillate sides of the membrane. The temperature difference across the membrane causes volatile components (i.e. H$_2$O) to evaporate from the feed side of the membrane, travel through the vapor-filled pores, and condense on the distillate side of the membrane. Non-volatile solutes remain in the feed. DCMD has several advantages over pressure-driven processes such as reverse osmosis. First, DCMD can treat hypersaline brines because it is not sensitive to osmotic pressure and rejects 99-100% of salts. While reverse osmosis can treat NaCl solutions up to approximately 70 g/L, the limit for DCMD
is approximately 300 g/L [21]. Second, DCMD systems do not require costly high-pressure pumps and stainless steel piping. However, the resulting cost savings can be offset by the need for heat exchangers that can withstand high salinity fluids. Third, DCMD operates at feed inlet temperatures below 90 °C that are readily produced by renewable energy and industrial waste heat.

A study by Bouchrit et al. [9] concluded that temperature and concentration polarization are the most crucial factors affecting DCMD performance in the treatment of hypersaline brines. Temperature polarization refers to a reduction in the transmembrane temperature difference due to heat transfer through the membrane, as illustrated by the temperature profile sketched in Figure 1.1. Concentration polarization describes the accumulation of solutes adjacent to the feed side of the membrane. Both polarization phenomena reduce the transmembrane vapor flux by reducing the transmembrane vapor pressure difference. Concentration polarization is also responsible for mineral scaling, which occurs when the concentration at the membrane surface exceeds the saturation limit. In addition to blocking the membrane, scaling can lead to pore wetting and permanent membrane damage.

Numerous studies have successfully modeled the system-level performance of DCMD systems using approximate Nusselt and Sherwood number correlations [22]. However, these correlations do not capture the downstream variation of polarization, permeate flux, and conductive heat loss along the membrane. In some cases, these correlations rely on fitting parameters or physical assumptions that are unclear. CFD offers a valuable complement to such studies because it predicts the full temperature, concentration, and velocity fields, and can identify performance bottlenecks that are difficult to diagnose experimentally [22].

Though numerous CFD studies have investigated DCMD systems, most solve the coupled heat, continuity, and Navier-Stokes equations without considering solute transport [23–45]. Of the studies that include salt transport [46–50], there is sometimes only limited discussion of concentration polarization. For example, studies by Hayer et al. [46], Lousiff [47], and Seo [48] include salt transport in their simulations, but focus their discussion on net permeate
Figure 1.2: (a) Sketch (not to scale) of the membrane spacer in between the membrane and the outer wall. (b) Autopsy of mineral scaling on membrane filtration system with spacer. Both pictures are provided by Courtesy of Desalitech

flux and heat transport. A study by Soukane [49] reports some results for turbulent salt transport in a 3D DCMD system with strong inlet and outlet effects.

Temperature and concentration polarization are further complicated by spacers, a meshlike material that separates and supports tightly packed membrane sheets, as illustrated in Figure 1.2(a). Thinner spacers increase the membrane surface area that can be packed in a system volume, but at the expense of increasing the channel pressure drop (and pumping costs) required to drive the feed and distillate flows. Spacers also generate three-dimensional flow structures that influence polarization and create regions of preferential solute accumulation and precipitation. Though this influence is documented for RO [51–57], there is less
work on scaling in DCMD systems. Literature suggests that solute accumulation tends to occur near what are referred to as “stagnant” or “dead” zones [58–62]. The same is also said of biofouling. The definitions of “stagnant” or “dead” are not always precise, but they tend to refer to locations on the membrane surface where the flow velocity is low or mixing is weak [59, 60, 62–64]. These zones often form near spacers, particularly the contact points where spacers meet the membrane surface [59, 60, 63]. This is demonstrated in Figure 1.2(b), which shows a membrane that experienced scaling in a high-recovery RO system operated by Desalitech. An autopsy indeed suggested that the scaling occurred near contact points (personal communication).

There is potential to increase the water recovery, energy efficiency, and membrane life of DCMD systems by designing spacers that strike a balance between maximizing membrane packing while minimizing the downstream pressure drop, polarization, and scaling. Designing such spacers is complicated by the coupled heat and mass transport in the feed, membrane, and distillate. These coupled processes are not fully understood, particularly when interactions between polarization and spacers are important.

CFD studies have made important contributions to understanding the effects of spacers on heat and mass transport in membrane processes. Reviews can be found in references [22, 65–67]. Our review finds three persistent challenges. The first is the simulation of near-membrane transport, which is difficult even in the absence of spacers. For pressure-driven processes such as RO, the dependence of the transmembrane flow on the pressure field causes traditional CFD methods to lose accuracy [68]. For DCMD, the accurate prediction of polarization requires the simultaneous simulation of the coupled feed channel, membrane, and distillate channel flows [69]. Due in part to these complications, studies of spacers sometimes neglect the membrane altogether [70–84]. Such studies focus on the effects of spacers on the downstream pressure drop and near-membrane shear stress, for which the small transmembrane flow likely has a minimal role. Nevertheless, one could argue that this assumption needs validation, because spacers generate hydrodynamic instabilities, and
instabilities can be surprisingly sensitive to small velocity components [85].

A second challenge arises because the flow regime in spacer-filled channels is not fully understood. Though spacers are often called “turbulence promoters,” it is not clear whether membrane systems actually operate in turbulent regimes. RO and DCMD systems typically operate with cross-flow Reynolds numbers in the range of $\text{Re} \leq 1000$, where $\text{Re} = \frac{U_{in} H}{\nu}$ is defined using the mean feed inlet velocity $U_{in}$ and feed channel height $H$ (see Figure 5.3). In this range, experiments [34, 67, 84, 86, 87] and simulations [34, 35, 67, 79–84, 86–94] suggest that the flow is steady at low Reynolds numbers, and transitions to unsteady laminar vortex shedding at higher Reynolds number. These studies show that the critical Reynolds number $Re_c$ for transition to vortex shedding varies between roughly $70 \leq Re_c \leq 500$, depending on the spacer geometry [34, 67, 79, 81, 82, 84, 86, 91–93]. Studies suggest that vortex shedding reduces polarization and scaling by increasing shear stress near the membrane and directing bulk fluid towards the membrane surface [34, 88–92]. Comparatively little work exists on the transition to turbulence [35, 77, 78, 84], and studies sometimes assume turbulent flow by incorporating Reynolds-averaged models [35, 77, 78].

A third challenge arises because CFD studies typically rely on software that simulate spacers using body-fitted grids. Such grids are time-consuming to generate and limit the number of simulations that can be reasonably performed. A similar situation is faced in the CFD community simulating porous media [95, 96]. In that case, the state-of-the-art has turned to immersed boundary methods (IBM) [97] that use a simple Cartesian grid, with grid points located in both the fluid and solid regions. Solid surfaces are then modeled by introducing a body force in the governing equations to force the fluid velocity to zero in the solid. Depending on the implementation, this achieves the same order-of-accuracy as body-fitted grids.

1.2 Objectives

To study the effects of operating conditions and spacers on polarization and system performance, we develop a 2D CFD code that solves the Navier-Stokes, continuity, advection-
diffusion, and heat equations using a finite-volume method in space and an efficient projection method in time. The spacer surfaces are simulated using a novel immersed boundary method developed in our group to apply no-slip and no-flux boundary conditions to second-order spatial and temporal accuracy. Note that the immersed boundary methods proposed in chapter 3 were developed by PhD student Jacob Johnston and implemented by the author of this thesis. All other numerical methods and codes were developed by the author. Using our methods, we perform two studies of transport in DCMD systems. The first performs a comprehensive parametric study of 2D DCMD systems without spacers. We systematically vary the feed and distillate inlet conditions (such as flow rate, temperature, and concentration), as well as the system length and co-current versus counter-current operation. We investigate the system-level performance by measuring the average permeate flux, single-pass water recovery, maximum concentration polarization coefficient, and gained output ratio of DCMD systems with heat recovery. In the process, we also compare the results of our simulations with the predictions of two popular Nusselt and Sherwood correlations. Our second study explores how transition from laminar flow to unsteady laminar vortex shedding affects polarization in DCMD systems with spacers. For that purpose, we consider an idealized 2D spacers filament placed in the feed and distillate channel of a plate-and-frame DCMD system, as sketched in Figure 2.1. Though spacers are inherently 3D, we focus on idealized 2D spacers because their hydrodynamic stability is much better understood in the fluid mechanics literature [98], and their simplicity allows us to perform a comprehensive parametric study and identify fundamental transport phenomena. It is our philosophy that elucidating such phenomena is prerequisite to intelligently designing 3-D spacers. Considering the various spacer geometries encountered in industry and literature [61], our geometry is closest to ladder-type spacers with filaments perpendicular to the downstream flow direction [61, 99, 100]. Finally, though beyond the scope of the current study, 2-D spacers are more amenable to quantitative experimental study, which is the topic of ongoing work in our group.
1.3 Organization of thesis

The remainder of this study is organized as follows. Chapter 2 presents the system geometry, governing equations, and boundary conditions. Chapter 3 presents and validates our numerical methods. The chapter is a manuscript that has been accepted for publication in Computers & Fluids, pending minor revisions. Chapter 4 presents our parametric study of DCMD systems without spacers. This chapter is an article published in the Journal of Membrane Science. Chapter 5 presents our parametric study of DCMD systems with spacers. This chapter is a manuscript to be submitted to the Journal of Membrane Science. Chapter 6 summarizes our conclusions.
CHAPTER 2
GEOMETRY AND MATHEMATICAL MODEL

This chapter presents the module geometry and mathematical model that are used throughout our study. Section 2.1 presents the plate-and-frame DCMD geometry. Sections 2.2 and 2.3 present our model of transmembrane heat and mass transport. Section 2.4 presents the governing equations and boundary conditions used to simulate transport in the feed and distillate channels.

2.1 Module geometry

We consider a 2D plate-and-frame DCMD system with feed and distillate channels of length $L$ and height $H$, as sketched in Figure 2.1. In both the feed and distillate channels, we consider idealized 2-D cylindrical spacers of diameter $D_{sp}$. The centers of both cylinders are situated at $x = L/2$, and a distance $y_c$ from the membrane. NaCl solution enters the feed channel with temperature $T_f$, concentration $C$, and mean velocity $U_f$. Pure water enters the distillate channel with temperature $T_d$ and mean velocity $U_d$. Note that throughout our study, the feed and distillate channels have identical inlet flow rates. We consider both co-current and counter-current operations. Though Figure 2.1 shows the membrane as a shaded region about $y = 0$, we model transmembrane heat and mass transport using effective interface conditions that couple the feed ($0 \leq y \leq H$) and the distillate ($-H \leq y \leq 0$) channels.

2.2 Transmembrane mass transport

As in most previous literature, we assume the transmembrane mass flux, $j_v$, is linearly proportional to the transmembrane vapor pressure difference [20],

$$j_v = -B(p_m^f - p_m^d),$$  \hspace{1cm} (2.1)
Figure 2.1: Sketch (not to scale) of the 2-D DCMD flow channels considered in this study. Each channel has a length $L$ and height $H$. The membrane is shaded gray. Both channels have a cylindrical spacer filament centered at $x = L/2$ and $y = \pm y_c$. NaCl solution enters the feed channel with temperature $T_{in}^f$, concentration $C_{in}$, and mean velocity $U_{in}$. Pure water enters the distillate channel with temperature $T_{in}^d$ and mean velocity $U_{in}$.

where $B$ is the vapor permeability and $p_m^f$ and $p_m^d$ are the water vapor pressures on the feed and distillate sides of the membrane, respectively, as illustrated in Figure 2.2. A fundamental difference between DCMD models is the evaluation of $B$ [22]. Though $B$ can depend on temperature and pressure [20], studies have shown that approximating $B$ as a constant membrane property matches experimental data well [39, 101]. We take this approach and determine $B$ by fitting to experimental measurements described in section 4.4.1.

The vapor pressures $p_m^f$ and $p_m^d$ are functions of the local temperature and concentration at the membrane surface [101]. We evaluate $p_m^f$ and $p_m^d$ as the product of the vapor saturation pressure $P^{sat}$ and water activity $a_w$,

$$p_m = a_w P^{sat}, \quad P^{sat} = \exp \left( 23.238 - \frac{3841}{T_m - 45} \right),$$

(2.2)

where $P^{sat}$ is determined using the Antoine equation [102] and $T_m$ is the local temperature on the membrane surface. The activity is determined from the expression $a_w = 1 - 0.03112b - 0.001482b^2$ [22], where $b$ is the NaCl molality (mol/kg). We assume complete salt rejection, such that $a_w = 1$ in the distillate.
2.3 Transmembrane heat transport

As in most previous literature, we model transmembrane heat conduction as

$$q_c = -\frac{k_m}{\delta}(T^f_m - T^d_m),$$  \hspace{0.5cm} (2.3)$$

where $\delta$ and $k_m$ are the membrane thickness and thermal conductivity, respectively, and $T^f_m$ and $T^d_m$ are the temperatures on the feed and distillate sides of the membrane, respectively.

In the literature, the membrane thermal conductivity is often approximated as $k_m = \epsilon k_v + (1-\epsilon)k_s$, where $\epsilon$ is the membrane porosity and $k_v$ and $k_s$ are the gas and solid conductivities, respectively [103]. However, in practice $k_m/\delta$ is often treated as an effective heat transfer coefficient. We take that approach by fitting $k_m/\delta$ to experiments.

Applying conservation of energy principles for liquid-vapor interfaces with phase change (see Leal [104]), one finds that on the membrane feed surface, conductive heat transport within the liquid phase must equal

$$-k \frac{\partial T^f_m}{\partial y} \bigg|_{y=0^+} = j_v \lambda - \frac{k_m}{\delta}(T^f_m - T^d_m),$$  \hspace{0.5cm} (2.4)$$

where $\lambda$ is the latent heat per unit mass, and the “$+$” superscript signifies that the derivative is evaluated from the feed side of the membrane. Detailed derivation of equation (2.4) can be found in section 3.8.4. Though not shown for brevity, similar conditions are applied on the distillate surface.
2.4 Transport in the feed and distillate channels

Fluid flows in the feed and distillate channels are governed by the incompressible continuity and Navier-Stokes equations for Newtonian fluids,

$$\nabla \cdot \mathbf{u} = 0, \quad (2.5)$$

$$\rho \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}), \quad (2.6)$$

where \( \mathbf{u} = [u \ v \ w], \ p, \ \rho \) and \( \mu \) are the fluid velocity vector, pressure, density, and dynamic viscosity, respectively. Within each channel, we neglect variations in density with temperature and concentration because the maximum variation of density is typically within 3%. In each channel, we set the density to the inlet value. Heat transport is governed by the thermal energy equation,

$$\rho c_p \left[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right] = \nabla \cdot (k \nabla T), \quad (2.7)$$

where \( c_p \) is the fluid heat capacity \([105]\). NaCl transport is modeled using the advection-diffusion equation

$$\frac{\partial c}{\partial t} + (\mathbf{u} \cdot \nabla)c = \nabla \cdot (D \nabla c), \quad (2.8)$$

where \( D \) is the effective mass diffusivity.

At the plates \( (y = \pm H) \) and spacer surfaces, we apply the no-slip, no-penetration, and no-flux conditions, \( u = v = \nabla c \cdot \mathbf{n} = \nabla T \cdot \mathbf{n} = 0, \) where \( \mathbf{n} \) is the normal vector. These conditions are applied on the spacers using direct-forcing immersed boundary methods developed in chapter 3. These allow us to simulate the spacers using simple Cartesian grids. On the membrane surfaces, we apply the no-slip condition, \( u = 0, \) and the following conditions determined from the models discussed in sections 2.2 and 2.3. The feed side conditions are,

$$v = \frac{j_v}{\rho^f}, \quad -k \left. \frac{\partial T}{\partial y} \right|_{y=0^+} + \frac{k_m T_f}{\delta} = j_v \lambda + \frac{k_m T_m}{\delta}, \quad v_m - D \frac{\partial c}{\partial y} = 0. \quad (2.9)$$
and the distillate side conditions are,

\[
v = \frac{j_v}{\rho \nu} - k \frac{\partial T}{\partial y} \bigg|_{y=0} - \frac{k m}{\delta} T_m^d = j_v \lambda - \frac{k m}{\delta} T_m^f.
\]  

(2.10)

At the channel inlets, we apply the desired temperatures and concentrations, and fully developed laminar velocity profiles with desired mean velocity \( U_{in} \),

\[
u = 6U_{in} \left[ \frac{y}{H} - \frac{y^2}{H^2} \right], \quad v = 0, \quad T = T_{in}, \quad c = C_{in}.
\]  

(2.11)

At the channel outlets, we consider two popular channel outlet conditions [106–108],

\[
\frac{\partial g}{\partial x} = 0, \quad \frac{\partial g}{\partial t} + U_{in} \frac{\partial g}{\partial x} = 0,
\]  

(2.12)

where \( g = [u, T, c] \), is the velocity, temperature and concentration field. The first condition is a Neumann condition, while the second is a convective condition.

At \( t = 0 \), we set the initial flow fields to the inlet conditions, and integrate in time until the flow fields reach a steady-state or transition to vortex shedding. In the latter case, the simulation is run sufficiently long to minimize any transient effects from the initial start-up. It is worth stressing that our governing equations do not assume laminar conditions. Nevertheless, for the Reynolds numbers considered, we find all simulations produce laminar flows.
CHAPTER 3

APPLICATION OF PROJECTION AND IMMERSED BOUNDARY METHODS TO SIMULATING HEAT AND MASS TRANSPORT IN MEMBRANE DISTILLATION

A manuscript submitted to Computers&Fluids

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3.1 Abstract

Membrane distillation is an emerging desalination process with important applications to the energy-water nexus. Its performance depends, however, on heat and mass transport phenomena that are uniquely challenging to simulate. Difficulties include two adjacent channel flows coupled by heat and mass transport across a semi-permeable membrane. Within the channels, heat and mass boundary layers interact with the membrane surface and vortical flow structures generated by complicated geometries. The presence of multiple inlets and outlets also complicates the application of mass-conserving outlet conditions. Moreover, even small amounts of outlet noise affect the resolution of important near-membrane fluid velocities. We show these phenomena can be simulated to second-order spatial and temporal accuracy using finite volume methods with immersed boundaries and projection methods. Our approach includes a projection method that staggers the coupled channel flows and applies Robin boundary conditions to facilitate mass conservation at the outlets. We also develop an immersed boundary method that applies Neumann boundary conditions to second-order spatial accuracy. The methods are verified and validated against manufactured solutions and theoretical predictions of vortex shedding. They are then applied to the simulation of steady and unsteady transport phenomena in membrane distillation. The

\textsuperscript{*}Corresponding author
methods have important applications to the broad field of chemical engineering and deal with long-standing issues in both theoretical and computational fluid dynamics.

*keyword*: Membrane Distillation, Immersed Boundary Methods, Projection Methods, Outlet Conditions

### 3.2 Introduction

Membrane distillation is an emerging method of desalinating wastewaters produced by industry, agriculture, and municipalities [8–10]. Though the method has attracted considerable attention as a means of addressing global water crises, its energy efficiency depends on heat and mass transport phenomena that are poorly understood because they are difficult to simulate or observe experimentally [69]. Challenges include simultaneous heat and mass boundary layers that interact with semi-permeable membranes and unsteady vortical flow structures generated by bluff bodies with complicated geometries. These phenomena occur in small flow channels with gap heights on the order of 1 mm. Membrane distillation systems are also open systems with multiple inlets and outlets that complicate the application of mass-conserving outlet conditions. Even small amounts of outlet noise can also affect the resolution of important near-membrane fluid velocities that are four to five orders-of-magnitude smaller than the largest velocity magnitudes. We show that these compounding phenomena can be successfully simulated to second-order spatial and temporal accuracy using finite volume methods with immersed boundaries and projection methods. Our approach includes the development of a direct-forcing immersed boundary method that applies Neumann conditions to second-order spatial accuracy. Though developed here for membrane distillation, the methods have important applications to the broad field of chemical engineering and deal with long-standing issues in computational fluid dynamics (CFD).

We consider the common arrangement of Direct Contact Membrane Distillation (DCMD) sketched in Figure 3.1(a). Warm feed solution and cool distilled water flow on opposite sides of a hydrophobic membrane. The temperature difference across the membrane creates a difference in partial vapor pressure that causes water to evaporate from the feed side of the
membrane, travel through the pores as vapor, and condense on the distillate side of the membrane. Non-volatile solutes remain in the feed. In comparison to reverse osmosis desalination, DCMD’s primary advantage is that it can treat higher concentration feed solutions because it is insensitive to osmotic pressure. While reverse osmosis can only treat NaCl solutions up to approximately 70 g/L, the limit for DCMD is around 300 g/L [21]. DCMD also operates at low feed temperatures between 40 to 90 °C readily produced by renewable energy and waste heat.

DCMD is strongly influenced by two phenomena called temperature and concentration polarization [9], sketched in Figure 3.1(a). Temperature polarization refers to a reduction in the transmembrane temperature difference due to heat transfer through the membrane. Concentration polarization is the accumulation of solutes adjacent to the feed side of the membrane. Both phenomena reduce the transmembrane vapor pressure difference and permeate production. Concentration polarization also causes mineral scaling, which is the precipitation of salts onto the membrane surface. This blocks the membrane surface and causes permanent membrane damage. Understanding polarization is further complicated by the presence of membrane spacers. Spacers are woven mesh-like materials that separate and support tightly packed membrane sheets in filtration systems, as sketched in Figure 3.1(b). Spacers are present in both the feed and distillate channels of DCMD systems, where they induce three-dimensional mixing and generate regions of preferential solute accumulation and precipitation.

Numerous studies have made important progress in simulating membrane distillation. Reviews can be found in references [67, 69, 109]. We nevertheless find three persistent challenges. First, the accurate prediction of polarization requires the simultaneous simulation of the coupled feed channel, transmembrane flow, and distillate channel. This coupling is complicated to simulate, particularly when the flow is unsteady. We find that few studies of DCMD demonstrate the spatial and temporal accuracies of their methods, though mesh-independence is sometimes discussed. Second, simulations currently rely on body-fitted grids.
that require considerable time to generate, and limit the number of spacer geometries that can be considered. Third, the flow regime within DCMD systems is not fully understood. Though studies show that with increasing Reynolds number, the flow transitions from steady flow to laminar vortex shedding and perhaps turbulence [34, 67, 81, 82, 84, 86, 91, 93, 110], these transitions are not well understood. In fact, though spacers are often called “turbulence promoters,” it is not clear whether DCMD systems typically operate in turbulent regimes.

We address these issues using a combination of finite volume, projection, and immersed boundary methods. We first show that unsteady flow in the coupled feed and distillate channels can be simulated using a projection method that solves the two channel flows sequentially, rather than simultaneously. The projection method is also derived for general Robin conditions on the numerical domain to improve the application of outlet conditions. Noise at the inlet and outlet is also attenuated using a Total Variation Diminishing (TVD) scheme and a set of “buffer cells” appended to the inlets and outlets of the two channels. We next develop an immersed boundary method that applies no-slip (Dirichlet) and no-flux (Neumann) boundary conditions on spacer surfaces to second-order spatial accuracy. Finally, we combine these methods to investigate polarization and transition to vortex shedding in DCMD systems. The remaining article is organized as follows. Section 3.3 presents the
geometry and governing equations. Sections 3.4 and 3.5 present the projection and immersed boundary methods, respectively. Section 3.6 simulates vortex shedding in a DCMD system. Section 3.7 presents our conclusions.

3.3 Geometry and governing equations

We consider a 2-D flat-sheet membrane system (called a “plate-and-frame” system) with feed and distillate channels of length $L$ and height $h$, as sketched in Figure 3.2. NaCl solution enters the feed channel with temperature $T_{in}^f$, concentration $C_{in}$, and mean velocity $U_{in}$. Pure water enters the distillate channel with temperature $T_{in}^d$ and the same mean velocity $U_{in}$ as in the feed channel. Though Figure 3.2 shows the membrane as a shaded region about $y = 0$, we model transmembrane heat and mass transport using effective interface conditions that couple the feed ($0 \leq y \leq h$) and distillate ($-h \leq y \leq 0$) channels. To investigate vortex shedding, we consider cylindrical spacer filaments of diameter $D_c$, placed a distance $y_c$ from the membrane. Though spacers are inherently 3D, we focus first on idealized spacers because their hydrodynamic stability is far better understood [98, 111]. Their simplicity also allows us to perform a parametric study and complementary experimental study, both ongoing in our group.

Figure 3.2: Sketch (not to scale) of the 2-D plate-and-frame DCMD system considered in this study. See description in text.
Fluid flow in the feed and distillate channels is governed by the incompressible continuity and Navier-Stokes equations for Newtonian fluids,

\[ \nabla \cdot \mathbf{u} = 0, \quad \rho \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}_u, \quad (3.1) \]

where \( \mathbf{u} = [u \ v] \), \( p \), \( \rho \) and \( \mu \) are the fluid velocity, pressure, density, and viscosity, respectively. The force \( \mathbf{f}_u \) is added for benchmarking in section 3.4.1. In each channel, we neglect density variations with temperature and concentration, because the maximum density variation is within 3%. In each channel, we set the density to that evaluated at the inlet temperature and concentration. Though buoyancy-driven convection can be included using the Boussinesq approximation, we leave that topic to a future dedicated study.

Heat and NaCl transport are governed by the energy and advection-diffusion equations,

\[ \rho c_p \left[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right] = k \nabla^2 T + f_T, \quad (3.2) \]
\[ \frac{\partial c}{\partial t} + (\mathbf{u} \cdot \nabla) c = D \nabla^2 c + f_c, \quad (3.3) \]

where \( T \) is the temperature, \( c \) is the concentration, \( c_p \) is the fluid heat capacity, and \( D \) is the effective mass diffusivity. The source terms \( f_T \) and \( f_c \) are again added for benchmarking. For the systems considered in the current study, we found that variations of \( \mu \), \( k \), \( D \), and \( c_p \) with temperature and concentration had an order 1% effect on our simulations. Though they can be included using the procedure in Lou et al. [69], we neglect them here to simplify our presentation.

Assuming the impermeable plates and spacers are insulated, we apply the following no-slip, no-penetration, and no-flux boundary conditions,

\[ \mathbf{u} = \mathbf{n} \cdot \nabla c = \mathbf{n} \cdot \nabla T = 0, \quad (3.4) \]

where \( \mathbf{n} \) is the unit normal to the surface. We also apply the no-slip condition \( (u = 0) \) to the membrane surface \( (y = 0) \). Though usually neglected, slip due to hydrophobicity can be modeled using the Navier slip condition [112]. At the channel inlets, we apply parabolic laminar velocity profiles \( u_{in}(y) \) with the desired uniform temperature \( T_{in} \), and concentration
\[ C_{in}, \]
\[ u = u_{in}(y), \quad v = 0, \quad T = T_{in}, \quad c = C_{in}. \]  

(3.5)

We consider two popular channel outlet conditions [113],
\[ \frac{\partial f}{\partial x} = 0, \quad \frac{\partial f}{\partial t} + U_{in} \frac{\partial f}{\partial x} = 0, \]  

(3.6)

where \( f \) denotes \( u, c, \) and \( T. \) The first condition is a Neumann condition, while the second is a convective condition.

The channel flows are coupled by heat and vapor transport through the membrane. We first note that mass conservation across the membrane requires
\[ \rho^f v \bigg|_{y=0^+} - \rho^d v \bigg|_{y=0^-} = j_v, \]  

(3.7)

where \( j_v \) is the transmembrane vapor mass flux, and \( \rho^f \) and \( \rho^d \) are the liquid densities in the feed and distillate channels, respectively. The superscripts “+” and “-” denote evaluation of \( v \) on the feed and distillate sides of the membrane, respectively. Assuming no solutes pass through the membrane, salt diffusion and advection normal to the feed membrane surface must sum to zero,
\[ v c \bigg|_{y=0^+} - D \frac{\partial c}{\partial y} \bigg|_{y=0^+} = 0. \]  

(3.8)

MD membranes are typically fibrous materials with pore-spaces on the order of 1-10 \( \mu \)m. Experiments [69, 114] show that transmembrane heat and vapor transport is well approximated on a macroscopic level using a popular model proposed by Schofield et al. [101]. The model begins by assuming the vapor mass flux \( j_v \) is linearly proportional to the transmembrane vapor pressure difference,
\[ j_v = -B(p^f_m - p^d_m), \]  

(3.9)

where \( p^f_m \) and \( p^d_m \) are the partial vapor pressures on the feed and distillate sides of the membrane, respectively, and \( B \) is the membrane’s vapor permeability, which is determined experimentally [39, 69, 101]. We evaluate \( p^f_m \) and \( p^d_m \) as the product of the vapor saturation
pressure $P^\text{sat}$ and water activity $a_w$,

$$p_m = a_w P^\text{sat}, \quad P^\text{sat} = \exp \left( 23.238 - \frac{3841}{T_m - 45} \right),$$

where $P^\text{sat}$ is determined using the Antoine equation [102] and $T_m$ is the local temperature on the membrane surface. The activity is determined from the expression $a_w = 1 - 0.03112b - 0.001482b^2$ [22], where $b$ is the NaCl molality (mol/kg). This expression is valid from zero salinity to saturation.

Heat transport through MD membranes occurs due to conduction through the membrane material and combined conduction and advection in the vapor. The Schofield model [101] approximates transmembrane heat transport due to conduction ($q_c$) and advection ($q_v$) as

$$q_c = -\frac{k_m}{\delta} (T^f_m - T^d_m), \quad q_v = j_v \lambda,$$

where $\delta$ and $k_m$ are the membrane thickness and thermal conductivity, respectively, $T^f_m$ and $T^d_m$ are the local temperatures on the feed and distillate sides of the membrane, respectively, and $\lambda$ is the latent heat per unit mass. Following common practice, we determine the ratio $k_m/\delta$ by fitting to experiments [69]. Conservation of energy principles for phase changes at the liquid-vapor interfaces [104] produce the temperature conditions,

$$-k \frac{\partial T}{\partial y} \bigg|_{y=0^{\pm}} = j_v \lambda - \frac{k_m}{\delta} \left( T \big|_{y=0^+} - T \big|_{y=0^-} \right).$$

Though well established in the membranes community, the subtleties of how conditions (3.12) account for phase-change are provided in Appendix 3.8.4. Following common practice, we set $\lambda$ to the average of the two inlet values. The thermal conductivity $k$ on the left-hand-side is set to the feed value when $y = 0^+$, and the distillate value when $y = 0^-$.

### 3.4 Simulation of the coupled channel flows

This section presents our simulation of the coupled channels without spacers. The primary challenge arises from the membrane and outlet conditions. We address these issues separately in sections 3.4.1 and 3.4.2, below. We discretize the governing equations spatially using standard second-order finite volume methods on a non-uniform staggered grid [115].
Details are presented in Appendix 3.8.1.

### 3.4.1 Application of membrane conditions

To delay our discussion of outlet conditions, suppose we simulate the coupled channel flows in Figure 3.2 with the velocity, temperature, and concentration prescribed at the outlets. To implement the membrane conditions, we develop a projection method that staggers the solution of momentum transport in the coupled channel flows. We first discretize all equations semi-implicitly in time using the Crank-Nicolson method for linear terms and Adams-Bashforth methods for nonlinear terms, as below for the Navier-Stokes equation,

\[
\frac{\rho \mathbf{u}^{n+1} - \mathbf{u}^n}{dt} + \frac{3}{2} \mathbf{NL}^n - \frac{1}{2} \mathbf{NL}^{n-1} = -\nabla p^{n+1/2} + \frac{\mu}{2} \nabla^2 \left( \mathbf{u}^{n+1} + \mathbf{u}^n \right),
\]

where \( dt \) is the time step, the superscript \( n \) denotes time \( t = n \, dt \), and \( \mathbf{NL}^n = \rho (\mathbf{u}^n \cdot \nabla) \mathbf{u}^n \).

We enforce incompressibility using the projection method of Bell et al [116]. We first compute a provisional velocity \( \mathbf{u}^* \) by solving equation (3.13) with the pressure from the previous time step,

\[
\frac{\mathbf{u}^* - \mathbf{u}^n}{dt} + \frac{3}{2} \mathbf{NL}^n - \frac{1}{2} \mathbf{NL}^{n-1} = -\nabla p^{n-1/2} + \frac{\mu}{2} \nabla^2 (\mathbf{u}^* + \mathbf{u}^n).
\]

Subtracting equation (3.14) from equation (3.13), produces the relation

\[
\mathbf{u}^{n+1} = \mathbf{u}^* - \frac{dt}{\rho} \nabla \phi,
\]

where \( \phi = p^{n+1/2} - p^{n-1/2} \) is sometimes called the “pseudopressure.” Relation (3.15) neglects the viscous term \( \mu (\nabla^2 \mathbf{u}^{n+1} - \nabla^2 \mathbf{u}^*)/2 \), which has a negligible impact [117]. Taking the divergence of equation (3.15) and applying incompressibility produces a Poisson equation for \( \phi \),

\[
\nabla^2 \phi = \frac{\rho}{dt} \nabla \cdot \mathbf{u}^*.
\]

Selecting boundary conditions for \( \mathbf{u}^* \) and \( \phi \) is a topic of considerable discussion [113, 117–120]. Suppose we wish to prescribe the velocity \( \mathbf{u}^{n+1} = \mathbf{g}(y) \) on the boundary \( x = 0 \). It now well established that at \( x = 0 \), one can set \( \mathbf{u}^* = \mathbf{g} \) and \( \partial \phi / \partial x = 0 \). These conditions arise
from equation (3.15), which requires
\[
\frac{\partial \phi}{\partial x} \bigg|_{x=0} = \frac{\rho}{dt} \left[ u^* - u^{n+1} \right]_{x=0}.
\] (3.17)

More generally, if one wishes to set the velocity \( u^{n+1} = g \) on some boundary with unit normal \( \hat{n} \), one applies the conditions
\[
u^* = g, \quad \hat{n} \cdot \nabla \phi = 0.
\] (3.18)

Note that to ensure mass conservation, the above Poisson equation and boundary conditions must be derived using the spatially discretized Navier-Stokes and continuity equations, as demonstrated in Appendix 3.8.1.

To apply the above projection method to our coupled channel flows, we discretize the membrane conditions semi-implicitly in time to solve the flow fields in each channel sequentially, rather than simultaneously. Each time step begins by solving the heat and advection-diffusion equations (3.2)–(3.3) in the channels by discretizing the membrane conditions (3.8) and (3.12) as
\[
D \frac{\partial c^{n+1}}{\partial y} \bigg|_{y=0^+} = \overline{\nu c} \big|_{y=0^+},
\] (3.19)
\[
-k \frac{\partial T^{n+1}}{\partial y} \bigg|_{y=0^\pm} = -\frac{k_m}{\delta} \left( T \big|_{y=0^+} - T \big|_{y=0^-} \right) + \overline{\nu \lambda},
\] (3.20)
where the overline denotes the Adams-Bashforth approximation \( \overline{\nu c} = 2v^n c^n - v^{n-1} c^{n-1} \). This allows us to solve for \( c^{n+1} \) and \( T^{n+1} \) in each channel sequentially. We then compute the vapor flux \( j_v^{n+1} \) using equations (3.9) and (3.10), and solve the Navier-Stokes equations in both channels sequentially.

We verify the spatial and temporal accuracy of our coupled channel flow solver with respect to the manufactured analytical solution
\[
\begin{bmatrix}
u_f \\
p_f \\
p_f \\
T_f \\
c_f
\end{bmatrix}
= 
\begin{bmatrix}
-S(x)C(\pi y_f/2)

\frac{2}{\pi} C(x)S(\pi y_f/2)

S(x)S(y_f)

\frac{3}{\pi} C(x) y_f^2

S(x) y_f^2
\end{bmatrix}
\begin{bmatrix}
u_d \\
p_d \\
p_d \\
T_d
\end{bmatrix}
C(\omega t),
\]
\[
\begin{bmatrix}
u_d \\
p_d \\
p_d \\
T_d
\end{bmatrix}
= 
\begin{bmatrix}
S(x)C(\pi y_d/2)

\frac{2}{\pi} C(x)S(\pi y_d/2)

S(x)S(y_d)

\frac{1}{\pi} C(x) y_d^2
\end{bmatrix}
C(\omega t),
\] (3.21)

23
where \( y_f = y - 1/2 \), \( y_d = y + 1/2 \), \( C = \cos \) and \( S = \sin \). The subscripts \( f \) and \( d \) denote the solutions used in the feed and distillate channels, respectively. The solution assumes \( h = 2 \), \( L = \pi \), \( \rho = \mu = c_p = k = k_m/\delta = B = \lambda = a_w = 1 \), and replaces the Antoine equation (3.10) with \( P_{sat} = T_m \). This produces the transmembrane temperature difference \( T_m^f - T_m^d = (2/\pi) \cos(x) \cos(\omega t) \), membrane concentration \( c_m = \sin(x) \cos(\omega t) \), and transmembrane velocity \( v_m = -(2/\pi) \cos(x) \cos(\omega t) \). The solution satisfies the governing equations with the addition of appropriate forcing terms to equations (3.1)–(3.3) and conditions (3.8) and (3.12). On the inlets, outlets, and plates, we set \( u \), \( T \), and \( c \) to the test solution. We use a uniform grid in the \( x \)-direction and a non-uniform grid in the \( y \)-direction, given by equation (3.59) of Appendix 3.8.2.

![Figure 3.3: Error results for \( u \) (squares), \( v \) (asterisks), \( T \) (triangles), \( c \) (circles). (a) \( Err_N \) vs \( N \). The dashed line shows \( 1/N^2 \). (b) \( Err_t \) vs. \( dt \) using Neumann outlet conditions for all fields. The dashed line shows \( dt^2 \).](image-url)

We test the spatial convergence by setting \( \omega = 0 \) and integrating from \( u^0 = p^0 = T^0 = c^0 = 0 \) to steady state using \( N^2 \) finite-volumes in each channel (\( N \) volumes in each direction). We then measure the relative error of each field as,

\[
Err_N = \frac{\| f_e - f_N \|_\infty}{\| f_e \|_\infty},
\]

where \( f_e \) and \( f_N \) are the exact and numerical solutions, respectively. We test the temporal convergence by setting \( \omega = 2\pi \) and integrating from \( t = 0 \) to \( t = 1 \) using exact initial
conditions. We then compute the error

$$Err_t = \|f_e - f_t\|_\infty / \|f_e\|_\infty,$$

(3.23)

where $f_t$ is the numerical solution using the time step $dt$. Figure 3.3 shows that we observe second-order spatial ($a$) and temporal ($b$) accuracy for $u$, $T$, and $c$. The solver satisfied incompressibility ($\nabla \cdot u = 0$) to machine precision.

### 3.4.2 Application of outlet conditions

The implementation of outlet conditions are not always fully detailed in literature. We find studies often discretize convective conditions explicitly as

$$\frac{f^{n+1} - f^n}{dt} + U_{in} \frac{\partial f^n}{\partial x} = 0,$$

(3.24)

where $\partial f/\partial x$ is approximated using first-order upwinding to add stabilizing diffusion. Though this produces an explicit $f^{n+1}$ that can be applied as a Dirichlet condition, the resulting outlet velocity does not conserve mass. This is addressed by rescaling the outlet velocity at each time step to ensure the outlet mass flow rates balances that entering the system. This simple approach is unfortunately not always possible for membrane processes, because the mass flow rate through the membrane may not be known until after the Navier-Stokes equation has been solved, as in reverse osmosis systems [68]. We consequently investigate whether we can apply the outlet conditions implicitly as

$$\frac{\partial f^{n+1}}{\partial x} = 0, \quad \frac{f^{n+1} - f^n}{dt} + U_{in} \frac{\partial f^{n+1}}{\partial x} = 0,$$

(3.25)

to automatically satisfy mass conservation.

We present two approaches of applying conditions (3.25). For that purpose, Figure 3.4(a) shows an outlet boundary at $x = L$. To simplify our presentation, we assume a uniform grid, and express the outlet velocity conditions as $au^{n+1} + b(\partial u^{n+1}/\partial x) = g$, where $b = 1$ and $a = g = 0$ for the Neumann condition, and $a = 1/dt$, $b = U_{in}$, and $g = u^n/dt$ for the
convective condition. These are discretized spatially as
\[ a u_e + b \left( \frac{u_e - u_w}{dx} \right) = g, \quad a \left( \frac{v_e + v_w}{2} \right) + b \left( \frac{v_e - v_w}{dx} \right) = g, \] (3.26)
where the subscripts denote the locations labeled in Figure 3.4(a).

Our first method applies the discrete equations (3.26) to \( u^*, \) and then modifies the outlet condition for \( \phi \) to ensure \( u^{n+1} \) also satisfies equations (3.26) exactly. We derive the required condition for \( \phi \) in an analogous manner to the Neumann condition (3.18) in section 3.4.1. We begin with equation (3.15), repeated below
\[ u^{n+1} = u^* - \frac{dt}{\rho} \nabla \phi. \] (3.27)
When deriving the Poisson equation (3.16) for \( \phi \), we take the divergence of equation (3.27). This requires
\[ \frac{\partial u^{n+1}}{\partial x} = \frac{\partial u^*}{\partial x} - \frac{dt}{\rho} \frac{\partial^2 \phi}{\partial x^2}. \] (3.28)
We now make the usual assumption that when solving a partial differential equation subject to boundary conditions, the differential equation and conditions are both satisfied at the boundary. This suggests we can combine equations (3.27) and (3.28) to express
\( a u^{n+1} + b (\partial u^{n+1} / \partial x) = g \)

\[
\left. a \frac{\partial \phi}{\partial x} + b \frac{\partial^2 \phi}{\partial x^2} \right|_{x=L} = \frac{\rho}{dt} \left[ g - au^* - b \frac{\partial u^*}{\partial x} \right]_{x=L}. \tag{3.29}
\]

If we apply the desired outlet condition to \( u^* \), this simplifies to

\[
\left. a \frac{\partial \phi}{\partial x} + b \frac{\partial^2 \phi}{\partial x^2} \right|_{x=L} = 0. \tag{3.30}
\]

For \( b = 0 \), this recovers the usual Neumann condition (3.18) from section 3.4.1. Repeating the derivation on a discrete level, one finds

\[
a \left( \frac{\phi_E - \phi_P}{dx} \right) + b \left( \frac{\phi_W - 2\phi_P + \phi_E}{dx^2} \right) = 0. \tag{3.31}
\]

Though condition (3.30) appears consistent with the underlying differential equations, one wonders if it is well-posed, as it contains a second-derivative in \( x \). To address this issue, consider the case \( a = 0 \) and \( b = 1 \), for which \( \partial u^{n+1} / \partial x = 0 \) and \( \partial^2 \phi / \partial x^2 = 0 \) on the outlet. To be well-posed, this requires

\[
\frac{\partial^2 \phi}{\partial y^2} \bigg|_{x=L} = \frac{\rho}{dt} \left[ \nabla \cdot u^* \right]_{x=L}. \tag{3.32}
\]

which is equivalent to the Dirichlet condition

\[
\phi \bigg|_{x=L} = \phi_L(y), \tag{3.33}
\]

where \( \phi_L(y) \) satisfies the ordinary differential equation,

\[
\frac{d^2 \phi_L}{dy^2} = \frac{\rho}{dt} \left[ \nabla \cdot u^* \right]_{x=L}. \tag{3.34}
\]

We have found that one can indeed solve equation (3.34) numerically at each time step to apply the outlet condition \( \partial^2 \phi / \partial x^2 = 0 \) as an equivalent Dirichlet condition. Either method produces the same answer, and satisfies incompressibility.

The above analysis suggests we could also apply conditions (3.25) by applying the desired outlet conditions to \( u^* \), and then fix the outlet pressure to some desired \( p_{out}(y) \) using the Dirichlet condition

\[
\phi \bigg|_{x=L} = p_{out}(y) - p^n \bigg|_{x=L}. \tag{3.35}
\]
which is easily discretized as

\[
\frac{\phi_P + \phi_E}{2} = p_{out}(y) - \frac{3p^n_P - p^n_W}{2}.
\]  

(3.36)

Note that we must extrapolate \( p^n \) from interior nodes, because on staggered grids, the pressure at the ghost nodes is unphysical [118]. With the above approach, \( u^{n+1} \) satisfies the desired outlet condition to within a small deviation comparable to that already observed for \( v^{n+1} \). The Poisson equation nevertheless ensures global mass conservation.

In summary, both approaches apply the desired outlet conditions (3.25) to \( \mathbf{u}^* \), but differ in their treatment of \( \phi \). The first applies condition (3.30) to enforce the outlet condition for \( u^{n+1} \) exactly. The second applies the simple Dirichlet condition (3.35) to apply an outlet pressure. To compare the results, we first apply them to the manufactured solution

\[
u_e = \sin(x) \cos(y), \quad v_e = -\cos(x) \sin(y), \quad p_e = \sin(x) \sin(y).
\]  

(3.37)

Figure 3.4(b) shows the spatial accuracy of both approaches when we solve the Navier-Stokes equations on the domain \( 0 \leq x \leq 2\pi, 0 \leq y \leq 2\pi \). The outlet conditions are applied at \( x = 2\pi \), with Dirichlet velocity conditions applied on all other boundaries. The solid lines show results for \( u \) (squares) and \( v \) (asterisks) when we enforce \( u^{n+1} \). The dash-dotted lines show results using the pressure condition. Surprisingly, the latter produces second-order accuracy, while enforcing \( u^{n+1} \) produces accuracy closer to first-order. Though not shown, we found the accuracy of the first approach can be brought to second-order using a formally second-order accurate, one-sided, discretization of \( \partial u/\partial x \) at the boundary. Typically, however, the actual spatial and temporal accuracy of outlet conditions is of little concern in the literature.

We next apply our outlet conditions to the simulation of flow perturbations in a planar channel flow with impermeable walls. We first perform a simulation with a fully-developed laminar velocity profile at the inlet, and the desired condition at the outlet. For cases where we fixed the outlet pressure, we set \( p_{out} = 0 \). The simulation is run to steady-state and the resulting flow fields, denoted \([\mathbf{U}, P]\), are used as the initial condition for a second simulation.
with a disturbance \( v_p(y, t) \) introduced to the wall-normal inlet velocity,

\[
v_p(y, t) = 0.1 U_{in} \sin \left( \frac{2\pi y}{h} \right) \exp \left[ -10^7 (t - 0.002)^2 \right].
\] (3.38)

This produces a perturbation near \( t = 0.002 \), with a peak amplitude of \( 0.1 U_{in} \). We run the simulation sufficiently long to allow the perturbation to interact with the outlet, and we plot the evolution of the perturbation velocity \( \hat{u} = u - U \).

Figure 3.5 shows results for a channel flow of aspect ratio \( L/h = 20 \) and Reynolds number \( Re = U_{in} h / \nu = 3000 \) using the convective outlet condition. The condition for \( \phi \) enforces the outlet value of \( u^{n+1} \) exactly. Panels (a) and (b) show three snapshots of the perturbation velocity components at mid-gap, \( \hat{u}_{mid} = u(x, 0.5h, t) \) and \( \hat{v}_{mid} = v(x, 0.5h, t) \), respectively.
Figure 3.6: Sketch of the inlet and outlet buffer cells. The membrane is shaded grey and the buffer cells are indicated using dashed lines.

Though the results for \( \hat{u}_{\text{mid}} \) are smooth, \( \hat{v}_{\text{mid}} \) has unphysical oscillations on the order of \( 10^{-5}U_{\text{in}} \) that originate at the outlet. Such noise has been observed previously by Pauley [121] for both Neumann and convective conditions. Though likely often ignored, we prefer to attenuate outlet noise by discretizing all advection terms with a second-order TVD scheme described in Appendix 3.8.1. Panel (c) shows that this removes the oscillations, and exposes rapid variations in the two cells upstream of the outlet. These are likely what triggered the oscillations in panel (b). Overall, our tests showed that both Neumann and convective conditions performed equally well, using either outlet condition for \( \phi \). Further investigation of our outlet conditions for cases of vortex shedding is presented in Appendix 3.8.3. Due to the chronological order in which our outlet conditions for \( \phi \) were developed, the remaining simulations in our study apply the method that enforces \( u^{n+1} \) at the outlet exactly.

To inhibit the spreading of outlet noise between adjacent channels, further testing motivated us to append “buffer cells” at the inlet and outlet of both channels. The membrane permeability and thermal conductivity are set to zero in the buffers, as sketched in Figure 3.6. All other governing equations are simulated within the buffer, exactly as they are for internal cells. We found a buffer length of only two cells sufficed. When presenting simulation results, we only plot results from \( 0 \leq x \leq L \). For plotting purposes, we determine outlet values of \( T \) and \( c \) using quadratic extrapolation from upstream data. In Figure 3.6, the temperature at the point marked as an open circle would be determined using \( T_1, T_2, \) and \( T_3 \).
3.4.3 Application to polarization phenomena

We demonstrate our projection and outlet methods by simulating steady-state polarization in a bench-scale DCMD system without spacers. We set the channel dimensions to $h = 2$ mm and $L = 10$ cm, the inlet temperatures to $T_{in}^f = 80$ °C and $T_{in}^d = 20$ °C, and the inlet feed concentration to 100 g/L. The inlet velocities of both channels are set to $U_{in} = 0.127$ m/s, producing the feed Reynolds number $Re_f = U_{in}h/\nu_f = 600$, and the distillate Reynolds number $Re_d = U_{in}h/\nu_d = 252$, where $\nu_f$ and $\nu_d$ are the feed and distillate kinematic viscosities, respectively. The membrane properties ($k_m/\delta = 577$ W/m$^2$ K and $B = 1.87 \times 10^{-6}$ kg/m$^2$ s Pa) were determined experimentally by Lou et al. [69]. The thermophysical properties of the feed and distillate are set using correlations in [69]. Details of the grid and mesh-independence studies are provided in Appendix 3.8.2. The simulations are initiated using the inlet conditions and integrated to steady state using the Neumann outlet condition.

Figure 3.7(a) shows the resulting steady-state temperature field. Different color scales are used for the feed and distillate channels to highlight the cooling of the feed and the heating of the distillate. Figure 3.7(b) shows the streamwise variation of the membrane surface temperatures in the feed ($T_{m}^f$) and distillate ($T_{m}^d$). We observe that $T_{m}^f$ decreases monotonically from 80 to 47.6 °C in its downstream direction (rightwards), while $T_{m}^d$ increases monotonically from 20 to 60.7 °C in its downstream direction (leftward). Figure 3.7(c) shows that the temperature difference across the membrane, $\Delta T_m = T_{m}^f - T_{m}^d$, varies non-monotonically from 19.3 °C at $x = 0$, to a minimum of 11 °C at $x/L = 6.8$, and a maximum of 27.6 °C at $x/L = 50$.

Figure 3.7(d) shows the variation of the transmembrane feed velocity, $v_m = j_v/\rho_f$, normalized with $U_{in}$. We observe that though $\Delta T_m$ is maximized at the outlet, $v_m$ is maximized at the inlet. This occurs for two reasons. First, the saturation pressure $P_{sat}$ varies non-linearly with temperature, such that $dP_{sat}/dT$ increases with temperature, see equation (3.10). Second, concentration polarization is strongest at the feed outlet, where it decreases...
Figure 3.7: (a) Temperature field. (b) Temperatures on the feed and distillate membrane surfaces. (c) Transmembrane temperature difference $\Delta T_m$. (d) Non-dimensional transmembrane velocity, $v_m/U_m$.

the partial vapor pressure. This is demonstrated in Figure 3.8(a), which shows the feed channel concentration field. Because the mass diffusivity $D$ is much smaller than the thermal diffusivity $\alpha$, the concentration boundary layer is much thinner than the thermal layer. Consequently, Figure 3.8(a) is cropped at $0 < y/h < 0.15$. Figure 3.8(b) shows that the membrane surface concentration, $c_m(x)$, increases significantly from 100 g/L at the inlet to 155.4 g/L at the outlet.

Figure 3.9(a) shows cross-sectional temperature profiles in the feed channel at $x = L/4$, $L/2$, $3L/4$, and $L$. To measure the downstream growth of the thermal boundary layer, we
Figure 3.8: (a) Concentration field for $0 < y/h < 0.15$. (b) Concentration on the membrane, $c_m$.

Figure 3.9: (a) Temperature profiles in the feed channel at $x = L/4$ (asterisks), $x = L/2$ (triangles), $x = 3L/4$ (squares), and $x = L$ (crosses). (b) Self-similar temperature distributions. (c) Numerical result (solid line) for $\delta_T$ vs $\hat{x}$. The dashed line shows the power law $\delta_T = 0.2 \hat{x}^{0.36}$

define the non-dimensional temperature

$$\tilde{T}(x, y) = \frac{T(x, y) - T_m^f(x)}{T_{in}^f - T_m^f(x)}, \quad (3.39)$$
so that \( \hat{T} \) varies from zero on the membrane to unity when \( T = T_{in}' \). We then define the boundary layer thickness \( \delta_T \) as the location where

\[
\hat{T}\big|_{y=\delta_T} = 0.95.
\] (3.40)

Figure 3.9(b) shows that the four curves in Figure 3.9(a) collapse to a self-similar curve when \( \hat{T} \) is plotted with the similarity variable \( \eta = y/\delta_T \). Panel (c) shows that outside of the near-inlet region, \( \delta_T \) grows with \( x \) as the power law \( \delta_T/h = 0.2(x/h)^{0.36} \). The exponent is close to 1/3, which often occurs in thermal boundary layers due to an approximate balance between downstream advection and transverse diffusion [see discussion in Probstein 122]. Though not shown here, the concentration layer satisfies a similar power law. We refer to Lou et al. [69] for a detailed analysis.

### 3.5 Simulating spacer surfaces

We simulate spacer surfaces using a direct forcing method that extends work by Fadlun [123] and others [124–129] to simulate Neumann conditions for the temperature and concentration fields to second-order spatial accuracy. We present the method in section 3.5.1 and verify its accuracy in section 3.5.2 by reproducing manufactured solutions and theoretical results for the linear stability of flow over a cylinder in a plane channel. We also stress here that during the preparation of the current manuscript, a similar approach was independently reported by Yousefzadeh and Battiato [130], to whom we defer credit.

#### 3.5.1 Immersed boundary method

To demonstrate our procedure, Figure 3.10(a) shows nine temperature grid points (solid circles) through which six grid lines are drawn. We begin by identifying all grid points in the solid (shaded grey) for which an adjacent point on the same grid line is in the fluid. These points, called “forcing points,” are labeled \( f_1, f_2, \) and \( f_3 \) in Figure 3.10(a). The point labeled \( nf \) is not a forcing point. Though it has a neighboring point in the fluid, the two points lie on different lines. Treating such points as forcing points does not improve accuracy.
Figure 3.10: Selection of forcing point and normal point. Solid regions are shaded grey. See discussion in text.

For each forcing point, we compute the shortest normal distance to the surface using a procedure similar to Majumdar et al. [124], though we use the approach of Qin et al. [131] that leverages the properties of signed distance functions. We refer to them for details, and only summarize the procedure here. Consider the point \( f_1 \) in Figure 3.10(a). In the four boxes surrounding \( f_1 \), we approximate the surface as dashed line segments joining points where the surface intersects grid lines, and then find the surface point \( s \) (square symbol) that produces the normal distance to \( f_1 \). If multiple normal distances exist, as in Figure 3.10(b), we choose the shortest. In cases where no normals exist, the surface point is set to the closest point, as in Figure 3.10(c).

Our application of Dirichlet conditions is similar to that of Pacheco-Vega et al. [126]. Suppose we wish to prescribe the temperature \( T_s \) at the surface point \( s \) in Figure 3.11(a). Though \( s \) does not lie on the grid, the temperature there can be approximated to second order using a bi-linear interpolation with the points labeled 1, 2, 3, and \( f \),

\[
T_s = a_f T_f + a_1 T_1 + a_2 T_2 + a_3 T_3 + \mathcal{O}(d^2),
\]

where \( d \) is the distance between \( f \) and \( s \), and \( a_f, a_1, a_2, a_3 \) are coefficients of the interpolation.

From this interpolation, we can solve for the temperature \( T_f \)

\[
T_f = \frac{T_s - a_1 T_1 - a_2 T_2 - a_3 T_3}{a_f},
\]
that must be applied at point $f$ to satisfy the boundary condition to second-order spatial accuracy.

\begin{align*}
\text{(a)} & \quad \text{(b)} & \quad \text{(c)}
\end{align*}

Figure 3.11: Application of (a) Dirichlet and (b) Neumann boundary conditions. The triangular regions shaded light grey in panels (b) and (c) denote the interpolation space.

Next, suppose we wish to apply the Neumann condition

$$\mathbf{n} \cdot \nabla T = g_s,$$  \hfill (3.43)

at point $s$ in Figure 3.11(b). For that purpose, we introduce the fictitious point labeled $n$ such that $s$ is mid-distance between points $n$ and $f$. We can then discretize the boundary condition using a centered difference,

$$\frac{T_n - T_f}{2d} = g_s + \mathcal{O}(d^2).$$  \hfill (3.44)

If we approximate $T_n$ using a bilinear interpolation, as in equation (3.41), the accuracy of the Neumann condition will be only first-order. The decreased accuracy is straightforward to show using a Taylor series, and occurs because bilinear interpolation produces a second-order spatial error in the numerator of equation (3.44). This is then divided by the denominator $2d$, which is the same order as $dx$ and $dy$. To obtain second-order accuracy, we approximate $T_n$ to third order accuracy using the interpolation

$$T_n = b_f T_f + b_1 T_1 + b_2 T_2 + b_3 T_3 + b_4 T_4 + b_5 T_5 + \mathcal{O}(d^3),$$  \hfill (3.45)
where $b_f$ and $b_i$ ($i = 1, \ldots, 5$) are interpolation coefficients. Using interpolation (3.45) with the centered difference (3.44) produces net second-order accuracy.

For the case sketched in Figure 3.11(b), the fictitious point $n$ lies in the triangular interpolation space shaded light grey. When the point lies outside this space, we interpolate as demonstrated in Figure 3.11(c) to avoid extrapolation. Another special case occurs when an immersed surface has a cusp, as in Figure 3.12(a). Cusps are also generated when an immersed surface intersects the external domain of the simulation. This would occur in Figure 3.12(a) if the line labeled $ab$ was the external boundary. Such cusps project the point $n$ back into the solid or outside the domain. Refining the grid tends to simply push the issue further into the cusp. We address this issue as suggested by Finn and Apte [132], by locally modifying the immersed surface as in Figure 3.12(b).

![Figure 3.12](image)

Figure 3.12: At locations where an immersed surface intersects an external boundary (panel a), or at a cusp (panel b), the surface is modified as in (panel c).

As earlier mentioned, our approach is similar to that of Yousefzadeh and Battiato [130]. There are some differences worth mentioning. We integrate the pressure field using a projection method, while Yousefzadeh and Battiato use the SIMPLE scheme [133]. Our grids are non-uniform, while those of Yousefzadeh and Battiato are uniform. While we focus on immersed Neumann and Dirichlet conditions, Yousefzadeh and Battiato consider more general immersed Robin conditions. Next, while we reconstruct the immersed surface using the
distance function method of Qin et al. [131], Yousefzadeh and Battiato use a ray-casting method. Finally, in contrast to our interpolation stencils sketched in Figure 3.11, Yousefzadeh and Battiato propose stencils that exclude the forcing point to increase the stability and convergence of their iterative SIMPLE scheme. In our case, we have not observed any stability issues to date.

### 3.5.2 Verification and validation

We verify the spatial and temporal accuracy of our direct forcing method using the forced analytical solution

\[
\begin{bmatrix}
  u_e \\
  v_e \\
  p_e \\
  T_e
\end{bmatrix} = \begin{bmatrix}
  \sin(x) \cos(y) \\
  -\cos(x) \sin(y) \\
  \sin(x) \sin(y) \\
  \sin(x) \sin(y)
\end{bmatrix} \cos(\omega t).
\]  

We set all thermophysical properties to unity, and solve the continuity, Navier-Stokes, and heat equations (3.1)-(3.2) in the domain \((x, y) \in [0, 2\pi] \times [0, 2\pi]\) with a circular cylinder of diameter \(D_c = 3\) centered at \((x, y) = (\pi, \pi)\), as illustrated in Figure 3.13(a). On the cylinder surface, we apply the Dirichlet condition \(u = u_e\), and the Neumann condition \(n \cdot \nabla T = n \cdot \nabla T_e\). On the external boundaries, we apply Dirichlet conditions to \(u\) and \(T\). We test the spatial accuracy by setting \(\omega = 0\) and integrating to steady-state from the initial condition \(u = p = T = 0\). Simulations were performed using a non-uniform grid with Gauss-Lobatto-Chebyshev distributions in the \(x\) and \(y\)-directions.

Figure 3.13(b) shows that our method produces second-order spatial accuracy for the velocity and temperature fields when using the third-order interpolation for the Neumann condition. The scatter arises due to the nonlinear distribution of the grid points. Repeating the analysis with a uniform grid produces much smoother results. The cross symbols show that using a bi-linear interpolation for the Neumann condition reduces the accuracy of \(T\) to first-order. Though not shown for brevity, we also confirmed second-order temporal accuracy, and repeated our analysis for several cylinder locations.
Figure 3.13: (a) Streamlines of the test solution. (b) $Err_N$ vs. $N$ for $u$ (squares), $v$ (asterisks), and $T$ (triangles) using the third-order interpolation for the Neumann condition. The crosses show $Err_N$ for $T$ when the bi-linear interpolation is used for the Neumann condition. The dashed and dash-dotted lines show slopes of $1/N^2$ and $1/N$, respectively. (c) Instantaneous vorticity contours in a channel with an immersed cylinder when $(Re, \beta) = (266.7, 0.5)$. This case is equivalent to that in figure 11 of Sahin and Owens [111].

We validate our ability to simulate vortex shedding by comparing to a linear stability analysis performed by Sahin and Owens [111] of fully-developed channel flow with a circular cylinder on the centerline. We place the cylinder at least 3 diameters from the inlet and at least seven diameters from the outlet. We define the blockage ratio $\beta = D_c/h$ and Reynolds number $Re = U_{in}h/\nu$. To compute the critical Reynolds number for transition to vortex shedding, we perform simulations to determine two Reynolds numbers $Re_1$ and $Re_2$, for which $Re_2 - Re_1 \leq 5$ and for which the flow is steady at $Re_1$ and unsteady at $Re_2$. The critical Reynolds number is then set to $Re_c = (Re_1 + Re_2)/2$. At the unsteady Reynolds number $Re_2$, we compute the dominant frequency $f_c$ of oscillation by recording the centerline
velocity at a location downstream of the cylinder. We define the critical Strouhal number as 
$St_c = f_c D_c / U_{in}$. Table 3.1 demonstrates excellent agreement between our results and 
those of Sahin and Owens [111]. As further validation, Figure 3.13(c) shows instantaneous 
vorticity contours when $(Re, \beta) = (266.7, 0.5)$. These show excellent agreement with those 
shown in an identical simulation reported in figure 11 of Sahin and Owens [111].

Table 3.1: For the blockage ratios $\beta = D/h$ in the first column, the remaining columns 
compare the critical Reynolds number and Strouhal numbers computed in the current study 
(columns 2-3) with those of Sahin and Owens (columns 4-5).

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>Current study $Re_c$</th>
<th>$St$</th>
<th>Sahin &amp; Owens $Re_c$</th>
<th>Sahin &amp; Owens $St$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>213 ±2</td>
<td>0.317</td>
<td>212</td>
<td>0.312</td>
</tr>
<tr>
<td>0.5</td>
<td>168 ±1</td>
<td>0.509</td>
<td>167</td>
<td>0.505</td>
</tr>
<tr>
<td>0.7</td>
<td>106 ±0.5</td>
<td>0.681</td>
<td>106</td>
<td>0.707</td>
</tr>
</tbody>
</table>

3.6 Application to unsteady transport in DCMD systems

We now use our methods to simulate polarization in a DCMD system with spacers. We 
consider a short system of dimensions $h = 2$ mm and $L = 20$ mm with cylinders of diameter 
$D_c = 1$ mm placed on the centerlines of both channels at $x = 10$ mm. The length ensures 
the spacers are a distance of 10 diameters from the inlet and outlet. As in section 3.4.3, we 
set the operating temperatures to $T_{in}^f = 80$ °C and $T_{in}^d = 20$ °C, and the feed concentration 
to $C_{in} = 100$ g/L. The simulations are run to steady state for subcritical cases, and run 
sufficiently long to attenuate any transient startup effect for supercritical cases. Simulations 
were repeated using both Neumann and convective outlet conditions. The difference in the 
results were negligible.

Figure 3.14 shows results when $U_{in} = 2.11 \times 10^{-2}$ m/s. This produces the Reynolds 
numbers $Re_f = 100$ and $Re_d = 42$, for which the flow is steady in both channels. The 
streamlines in panel (a) show a pair of counter-rotating vortices in the downstream wakes of 
each spacer. As expected, the wake is larger in the feed channel due to its larger Reynolds
Figure 3.14: Steady-state streamlines (a), temperature field (b), and feed concentration field (c) for the subcritical case $Re_f = 100$ and $Re_d = 42$. Different color scales are used for temperatures in the feed and distillate channels. The concentration field is shown for $0 < y/h < 0.2$. For convenience, we present the position as both $x/h$ and $x/D_c$.

number. Panels (b) and (c) show that as the feed and distillate flows accelerate around the spacers, the temperature and concentration boundary layer thicknesses decrease, due to the increase in downstream advection. Because the concentration layer is quite thin, panel (c) shows results for $0 \leq y/h \leq 0.2$.

The solid lines in Figure 3.15 show the transmembrane temperature difference $\Delta T_m$ (a), surface concentration $c_m$ (b), and transmembrane feed velocity $v_m/U_{in}$ (c). The dashed lines show results for a simulation performed without the cylinders. We see that the influence of the spacers is limited to a region extending roughly two cylinder diameters up and downstream from the cylinder center. In that region, the cylinders increase $\Delta T_m$, decrease $c_m$, and increase vapor production. Overall, the simulation with the spacers produces an average
transmembrane vapor flux of $9.4 \times 10^{-6}$ m/s, compared to $8.5 \times 10^{-6}$ m/s for the case without spacers, an increase of 10.6 %.

Figure 3.16 shows snapshots of the streamlines (a), temperature field (b), and concentration field (c) when we increase the inlet velocity to $U_{in} = 8.46 \times 10^{-2}$ m/s, producing the Reynolds numbers $Re_f = 267$ and $Re_d = 112$. Based on $Re_c = 168$ in table Table 3.1, the distillate flow is subcritical and the feed flow is strongly supercritical ($Re_f - Re_c = 99$). Note that we performed additional simulations to determine the critical Reynolds number of the fully coupled DCMD system, and found the presence of the membrane and transmembrane flow had a negligible effect on $Re_c$. Panel (a) shows that instability in the feed channel produces strong wake oscillations and a pair of staggered recirculation zones that periodi-
Figure 3.16: Snapshots of the unsteady streamlines (a), temperature field (b), and feed concentration field (c) for the supercritical case $Re_f = 267$ and $Re_d = 112$. Different color scales are used for temperatures in the feed and distillate channels. The concentration field is shown for $0 < y/h < 0.2$. For convenience, we present the position as both $x/h$ and $x/D_c$.

cally appear and travel downstream along the membrane and outer wall. The period for the formation of these recirculation regions is identical to that of the vortex shedding behind the cylinder. Snapshots showing the evolution of these wall-vortices are provided in Figure 3.17. The temperature plot in Figure 3.16(b) suggests that the leading edge of the recirculation zone traveling along the membrane tends to eject near-membrane cool fluid into the bulk flow. This in turn brings warmer bulk fluid towards the membrane. The influence of the spacer on concentration polarization is less straightforward to evaluate. Though panel (c) suggests the recirculation zone also ejects high concentration fluid into bulk, we also observe a local region of salt accumulation near $x/h = 6.3$. 43
Figure 3.17: Snapshots of the streamlines at four equispaced times $t_1 < t_2 < t_3 < t_4$ where $t_n - t_{n-1}$ is approximately $3/(13f_s)$, where $f_s$ is the shedding frequency.

The solid lines in Figure 3.18 show snapshots of $\Delta T_m$ (a), $c_m$ (b), and $v_m/U_{in}$ (c) for the simulation with spacers. The dashed lines show the results of a simulation performed without spacers. Though the feed channel is strongly unsteady, the results at the membrane for $\Delta T_m$, $c_m$, and $v_m$ are all essentially steady, showing only negligible variations in time. Panel (a) shows that the spacer increases $\Delta T_m$, not only near the spacer, but also in the far downstream region. Panel (b) shows that while concentration polarization is reduced below the spacer, there is a region of preferential salt accumulation near $x/h = 6.3$. Overall, the simulation with the spacers produces an average transmembrane vapor flux of $1.25 \times 10^{-5}$ m/s, compared to $1.10 \times 10^{-5}$ m/s without spacers, an increase of 14.3%. Though not shown here for brevity, we found that as we further increase $U_{in}$, and consequently the Reynolds numbers, the spacers continue to increase vapor production over what is observed without spacers. Unfortunately, the maximum concentration within the region of preferential salt accumulation also grows significantly, suggesting that the increase in vapor production comes with a risk of increasing salt precipitation.
Figure 3.18: The transmembrane temperature difference $\Delta T_m$ (a), membrane surface concentration $c_m$ (b), and transmembrane vapor flux $v_m/U_{in}$ for the supercritical case $Re_f = 267$ and $Re_d = 112$. The solid and dashed lines show results of simulations performed with and without spacers, respectively.

3.7 Conclusions

In addition to DCMD’s important industrial applications, the process touches on numerous long-standing issues in both theoretical and computational fluid mechanics. The numerical issues include (1) extending projection methods to more general Robin boundary conditions; (2) developing approximate outlet conditions that conserve mass in open systems with multiple inlets and outlets; and (3) simulating complex geometries in flows with heat and mass transport. The theoretical issues include (1) heat and mass boundary layers with complicated wall-interactions, as opposed to the classic case of a thermal boundary layer evolving over a wall maintained at a constant temperature or heat flux; (2) understanding transitions of flow regimes over bluff bodies; and (3) understanding how vortical flow
structures influence mixing and interact with adjacent surfaces. Though not discussed here, further issues include multi-species transport in complex feed solutions, and the physics of nucleation and precipitation.

We showed that transport in the coupled feed and distillate channels can be simulated using a projection method that applies membrane boundary conditions using Adams-Bashforth extrapolation to solve the two channels sequentially, instead of simultaneously. We also showed that mass can be automatically conserved in the open system using Neumann and convective outlet conditions that are applied implicitly within a projection method. Though outside the scope of the current study, this approach is crucial for our parallel work simulating pressure-driven membrane separation processes such as reverse-osmosis. In these systems, the mass flow rate through the membrane is only known after the solution of the Poisson problem for $\phi$, as discussed in Tilton et al. [68].

We also showed that Neumann conditions can be simulated to second order spatial and temporal accuracy using a direct forcing immersed boundary method. We validated the method against forced analytical solutions and theoretical predictions of a linear stability analysis of transition to vortex shedding. We again note that a similar approach was recently independently reported by Yousefzadeh and Battiato [130], to whom we defer credit. Future work should extend this method to three-dimensions. Future work may also wish to explore whether it is better to formally apply immersed Neumann conditions to second order accuracy, as in our study, or if one can achieve comparable accuracy using a simpler first-order approach with Adaptive Mesh Refinement (AMR) at the immersed surface. Our approach requires a larger stencil at the immersed surface, and consequently reduces the sparsity of matrices required for semi-implicit temporal discretizations. This may influence memory, parallelization, and CPU time. That issue deserves a dedicate study using optimized codes. In contrast, the current study uses preliminary, un-optimized, sequential codes.

Finally, we applied our methods to simulate heat and mass transport in DCMD systems with and without an idealized two-dimensional spacer filament on the channel centerlines.
We note that our results for the case without spacers were recently reported in much greater detail in a separate publication [69]. The results for cases with a spacer are the topic of an ongoing parametric study. Within the limits of the current study, we showed that in steady flow regimes, the spacer filaments had a net positive impact by decreasing both temperature and concentration polarization, and thereby increasing permeate production. In supercritical flow regimes, however, the spacers improved permeate production at the expense of generating regions of preferential solute accumulation. That increases the risk of precipitation when treating high-concentration feed solutions, which is a major application of interest for DCMD systems.

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3.8 Appendices

The appendices present supplemental materials for this paper.

3.8.1 Spatial Discretization

Figure 3.19 demonstrates our staggered grid. As sketched in panel \((a)\), the variables \( p \), \( T \), and \( c \) are stored at the cell centroids, while \( u \) and \( v \) are stored at cell faces. To discretize the \( x \)-component of the Navier-Stokes equation, we consider the control volume shaded grey in Figure 3.19\((b)\). We write the equation in control volume form as

\[
\int_{CV} \rho \frac{\partial u}{\partial t} dV + \int_{S} \rho u (u \cdot n) dA = - \int_{S} p (i \cdot n) dS + \int_{S} \mu (\nabla u \cdot n) dA, \quad (3.47)
\]
where \( \mathbf{i} \) is the unit vector in the \( x \)-direction, \( \mathbf{n} \) is the unit normal vector pointing away from the control surface \( S \) of the control volume \( CV \). We approximate the volume integral and pressure term in equation (3.47) as

\[
\int_V \rho \frac{\partial u}{\partial t} dV \approx \rho \frac{\partial u P}{\partial t} dxdy, \quad \int_S (\mathbf{i} \cdot \mathbf{n}) dS \approx P_e dy - P_w dy, \tag{3.48}
\]

where \( dx \) and \( dy \) are the distances labeled in Figure 3.19(b).

\[
\int_S \mathbf{u} \cdot \mathbf{n} \ dA \approx \hat{m}_e u_e + \hat{m}_n u_n - \hat{m}_w u_w - \hat{m}_s u_s, \tag{3.49}
\]

where \( \hat{m}_e = \rho u_e dy, \hat{m}_n = \rho v_n dx, \hat{m}_w = \rho u_w dy, \) and \( \hat{m}_s = \rho v_s dx \) denote the mass flow rates through the four faces of the volume. The subscripts \( n \) and \( s \) denote the face locations marked with crosses in Figure 3.19(b). The velocities within the mass flow rates are approximated using linear interpolation. For example, we compute the velocity within \( \hat{m}_n \) as

\[
v_n \approx (1 - \alpha)v_{nw} + \alpha v_{ne}, \quad \alpha = \frac{x_n - x_{nw}}{dx}. \tag{3.50}
\]

We considered two methods of approximating the four face values of \( u \) that multiply the mass flow rates in equation (3.49). The first, commonly called “centered differencing,”
approximated the velocities using the same linear interpolation procedure above. The second
used a TVD scheme, which improved the outlet conditions. We compared the performance
of several TVD schemes, and the scheme commonly called “minmod” worked well. We refer
readers to reference [134] for details. For demonstration, the scheme approximates $u_e$ as
\[ u_e = u_{e \text{low}} - \phi_e(r_e)(u_{e \text{low}} - u_{e \text{high}}), \]
where $u_{e \text{low}}$ and $u_{e \text{high}}$ are evaluated using first-order upwinding and centered differencing,
respectively, and $\phi = \max[0, \min(r, 1)]$, where $r$ is the ratio of successive gradient in the flow
direction.

Finally, we approximate the viscous term in equation (3.47) as
\[ \int_S \mu (\nabla u \cdot n) \, dA \approx \mu \frac{\partial u_e}{\partial x} dy + \mu \frac{\partial u_n}{\partial y} dx - \mu \frac{\partial u_w}{\partial x} dy - \mu \frac{\partial u_s}{\partial y} dx, \]
where the gradients are approximated using centered differences, such as
\[ \frac{\partial u_e}{\partial x} \approx \frac{u_E - u_P}{x_E - x_P}. \]

![Figure 3.20: A corner pressure cell (shaded grey) with ghost nodes.](image)

The above approach is repeating to discretize the $y$-momentum equation using the control
volume sketched in Figure 3.19(c). We then find that equation (3.15) is expressed in discrete
form as
\[
\frac{u_{n+1}^e - u_{n}^e}{dx} = -\frac{dt}{\rho} \left( \frac{\phi_e - \phi_w}{dx} \right), \quad \frac{v_{n+1}^e - v_{n}^e}{dy} = -\frac{dt}{\rho} \left( \frac{\phi_n - \phi_s}{dy} \right),
\]
where the subscripts are explained in figures Figure 3.19(b) and Figure 3.19(c). Using the pressure cell in figure Figure 3.19(a), we then discretize the conservation of mass equation as
\[
\frac{u_{n+1}^e - u_{n}^e}{dx} + \frac{v_{n+1}^n - v_{n}^n}{dy} = 0.
\]
Substituting relations (3.54) into the above, we find the discrete Poisson equation
\[
\frac{1}{dx} \left( \frac{\phi_e - \phi_P}{x_E - x_P} \frac{\phi_P - \phi_W}{x_P - x_W} \right) + \frac{1}{dy} \left( \frac{\phi_N - \phi_P}{y_N - y_P} \frac{\phi_P - \phi_S}{y_P - y_S} \right) = \frac{\rho}{dt} \left( \frac{u_{n+1}^e - u_{w}^e}{dx} + \frac{v_{n+1}^n - v_{s}^n}{dy} \right).
\]
Using ghost nodes, we apply the discrete Poisson equation on boundary cells, such as that sketched in Figure 3.20. The Neumann conditions for the two boundaries of this corner cell are then applied as
\[
\frac{\phi_P - \phi_W}{dx} = 0, \quad \frac{\phi_P - \phi_S}{dy} = 0.
\]
Note that with all Neumann conditions, \(\phi\) is only defined up to a constant. To produce a non-singular matrix equation, we fix the constant using a scalar Lagrange multiplier \(\lambda\). Specifically, if \(A\phi = b\) represents the matrix problem generated by the Poisson equation and Neumann boundary conditions, we augment the matrix as
\[
\begin{bmatrix}
A & 1 \\
q & 0
\end{bmatrix}
\begin{bmatrix}
\phi \\
\lambda
\end{bmatrix} =
\begin{bmatrix}
b \\
0
\end{bmatrix},
\]
where \(q\) is a row of length \((N_x + 2)(N_y + 2)\) zeros, except for one entry set to unity. This sets \(\phi\) equal to unity at one of the grid points. After solving, we confirm that \(\lambda = 0\) to machine precision. In all cases, we find that mass conservation is indeed satisfied to machine precision.
3.8.2 Grid independence studies

The simulations of section 3.4.3 are performed using $N_x$ equispaced cells in the $x$-direction. The cells are concentrated in the $y$-direction near the membrane and outer walls by setting the $y$-coordinates of the horizontal faces to

$$y_i = \pm(h/2)(1 + \cos(\pi i/N)), \quad i = 0, 1, \ldots, N_y,$$

where the positive sign is used in the feed, and the negative is used in the distillate. These are simply the Gauss-Lobatto-Chebyshev points mapped to the interval $y \in [0, h]$ and $y \in [-h, 0]$. For the simulations of Section 3.6, we refine the grid near the cylinder by decomposing the $x$-direction into three sections, as demonstrated in Figure 3.21(a). A core section of length $L_1 = H$ is centered about the cylinder, and has $N_1$ equispaced cells in the $x$-direction. The inlet and outlet sections each have a length $L_2 = (L - L_1)/2$ and $N_2$ equispaced cells.

![Diagram of grid independence studies](image1)

Figure 3.21: (a) Demonstration of a channel grid for which $N_1 = 32$, $N_2 = 24$, and $N_y = 30$. (b) Variation of $Err_N$ with $N_x$ for $u$ (squares), $v$ (asterisks), $c$ (circles) and $T$ (triangles). The dashed line shows $1/N^2$. 

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To demonstrate our mesh independence studies, we consider here the simulation of a DCMD system with a spacer on the centerline of each channel. We set the system dimensions to $H = 2$ mm, $L = 20$ mm, and $D_c = 0.6$ mm, producing the blockage ratio $\beta = 0.3$. The operating conditions are set to $T_{in}^f = 80^\circ C$, $T_{in}^d = 20^\circ C$, $C_{in} = 100$ g/L, and $U_{in} = 0.021$ m/s. This produced a subcritical case for which the flow fields can be integrated to steady state. We fix the ratio $N_x/N_y = 3$ and varied $N_x$ and $N_y$ between $90 \leq N_x \leq 600$ and $30 \leq N_y \leq 200$, respectively. We also fix the ratio $N/1/4$, to force 20 % of the $N_x$ cells in the core region $L_1$. Simulations were run to steady-state, after which the spatial error was evaluated using the result at $(N_x, N_y) = (600, 200)$ as the exact solution. Figure 3.21(b) shows the error is below 1% when $N_x > 400$.

For cases with unsteady vortex shedding, we leverage the fact that $v$, $T$, and $c$ are remarkably steady on the membrane surface. We consequently repeat the above procedure measuring the error with respect to these fields on the membrane surface. To determine the time step $dt$ for unsteady cases, we first set $dt$ to the maximum allowable value for which the code is numerical stable. We then compare $dt$ to the computed period of oscillation $t_p = 1/f$ and ensure that $t_p/dt > 1000$.

### 3.8.3 Outlet performance studies

To explore the outlet conditions in the context of large-scale vortical flow structures, we considered flow over a cylinder in a planar channel flow. Varying the blockage ratio and cylinder position relative to the channel centerline allows us to generate a wide range of steady and unsteady vortical structures. Figure 3.22 shows two simulations performed of a channel flow with $Re = 320$ and blockage ratio $\beta = 0.5$. The cylinder has been placed closer to the upper wall. In this case, Zovatto and Pedrizzetti [135] have shown that the asymmetry stabilizes vortex shedding and produces elongated vortical structures behind the cylinder and along the upper wall. Figure 3.22 shows the results of two simulations in which the cylinder was placed three diameters from the channel inlet. The simulation in panel (a) uses a short downstream length that cuts through the vortex attached to the upper wall.
Figure 3.22: Comparison of two simulations of a channel flow with $Re = 320$ and blockage ratio $\beta = 0.5$ using a short (a) and long (b) domain. See discussion in text.

The simulation in panel (b) shows a second simulation using a longer domain that allows the near-wall vortex to close well upstream from the outlet. Comparing the streamlines of the two simulations shows excellent agreement.

3.8.4 Transmembrane heat transport

Here we provide a brief derivation of the Schofield model [101] of heat transport through MD membranes. Instead of simply repeating the original derivation, we provide an alternate approach that highlights heat transport at the liquid-vapor interfaces. Figure 3.23(a) depicts an idealized membrane whose surface is the plane $y = 0$. Liquid occupies the region $y > 0$. The membrane, composed of a solid phase and vapor-filled pores, occupies the region $y < 0$. To simplify our analysis, we neglect surface tension and assume all liquid-vapor and liquid-solid interfaces lie in the plane $y = 0$, as in Figure 3.23(a). More detailed discussion of surface tension effects can be found in the work of Lawson and Lloyd [20]. We assume the liquid-solid and liquid-vapor interfaces are in thermal equilibrium, such that the temperature is continuous at $y = 0$. The temperature gradient $\partial T/\partial y$ is generally discontinuous. For
Figure 3.23: (a) Idealized cross-section of a membrane pore showing the liquid (L), solid (S), and vapor (V) regions. The dashed line represents the liquid-vapor interface, in which curvature due to surface tension is neglected. (b) Sketch of the averaging area $\mathcal{A}$.

discussion of these common assumptions, we refer to the classic works of Leal [104] and Prosperetti [136]. In the following, we consider heat transport across the plane $y = 0$ on the pore-scale. This is then upscaled to produce a practical macroscopic model.

At liquid-solid interfaces, heat is transported by conduction only,

$$-k_l \frac{\partial T}{\partial y} \bigg|_{y=0^+} = -k_s \frac{\partial T}{\partial y} \bigg|_{y=0^-}$$  \hspace{1cm} (3.60)

where $k_l$ and $k_s$ are the thermal conductivities of the liquid and solid, respectively. For this Appendix, the subscripts $y = 0^+$ and $y = 0^-$ denote the evaluation of the gradient as $y$ approaches zero from above and below, respectively. At liquid-vapor interfaces, heat is transported by conduction and advection. Conservation of thermal energy at the liquid-vapor interfaces [104, 136] requires

$$-k_l \frac{\partial T}{\partial y} \bigg|_{y=0^+} + \rho_l v_l h_l \bigg|_{y=0^+} = -k_s \frac{\partial T}{\partial y} \bigg|_{y=0^-} + \rho_v v_v h_v \bigg|_{y=0^-} \hspace{1cm}, \hspace{1cm} (3.61)$$
where $h$ is the enthalpy per unit mass, and the subscripts $l$ and $v$ distinguish between properties of the liquid and vapor, respectively. The left-hand-side of equation (3.61) represents heat conduction and advection crossing the interface from the liquid side of the interface, while the right-hand-side represents conduction and advection from the vapor side. Using conservation of mass ($\rho_l v_l = \rho_v v_v$), equation (3.61) can be rewritten as

$$-k_l \frac{\partial T}{\partial y} \bigg|_{y=0^+} + k_s \frac{\partial T}{\partial y} \bigg|_{y=0^-} = \rho_l v_l \left( h_v \big|_{y=0^-} - h_l \big|_{y=0^+} \right) = \rho_l v_l \lambda. \quad (3.62)$$

To upscale the pore-scale heat transport represented by equations (3.60) and (3.62), we introduce the circular averaging area $A$ sketched in figure Figure 3.23(b). We assume the diameter of the averaging area is much larger than a typical pore diameter ($D_A \gg D_p$) but also much smaller than the channel height ($D_A \ll h$), which is naturally satisfied in MD systems. At every point $(x, z)$ on the membrane surface, we define area-averaged fields of the form

$$\langle v \rangle (x, z, t) = \frac{1}{A} \int_A v \big|_{y=0} dA, \quad \langle \frac{\partial T}{\partial y} \rangle (x, z, t) = \frac{1}{A} \int_A \frac{\partial T}{\partial y} \bigg|_{y=0} dA. \quad (3.63)$$

To reproduce the Schofield model, we approximate the average heat transport crossing the plane $y = 0$ from the liquid side as

$$q_m = -\left(1 - \phi\right) k_l \left\langle \frac{\partial T}{\partial y} \right\rangle_{0^+} \quad \phi k_l \left\langle \frac{\partial T}{\partial y} \right\rangle_{0^+} + \left\langle v_l \right\rangle \left\langle h_l \right\rangle_{0^+}, \quad (3.64)$$

where $\phi$ is the area porosity of the membrane surface. The first term in equation (3.64) represents heat conduction across liquid-solid interfaces. The second and third terms represent heat conduction and advection across the liquid-vapor interfaces, respectively. The approximation (3.64) assumes one effective temperature gradient for both the liquid-solid and liquid-vapor interfaces. Similarly, we approximate the average heat transport crossing the plane $y = 0$ from the membrane side as

$$q_m = -\left(1 - \phi\right) k_v \left\langle \frac{\partial T}{\partial y} \right\rangle_{0^-} \quad \phi k_v \left\langle \frac{\partial T}{\partial y} \right\rangle_{0^-} + \left\langle v_v \right\rangle \left\langle h_v \right\rangle_{0^-}. \quad (3.65)$$
Though approximations (3.64) and (3.65) are intuitive, a more formal derivation could consider the method of volume-averaging [137], which has been used extensively to model heat, mass, and momentum transport across porous surfaces [138]. Such analysis is beyond the scope of this study.

Equating expressions (3.64) and (3.65), and applying conservation of mass produces

\[-k_l \left. \frac{\partial T}{\partial y} \right|_{0^+} = -k_m \left. \frac{\partial T}{\partial y} \right|_{0^-} + j_v \langle \lambda \rangle, \tag{3.66}\]

where \( k_m = (1 - \phi)k_s + \phi k_v \) is the membrane thermal conductivity [101]. If we assume a linear temperature gradient within the membrane, the area-averaged temperature gradient on the membrane side of the interface \((y = 0^-)\) can be approximated as \((T_d^m - T_f^m)/\delta\). Furthermore, if the averaging area is small compared to the channel \((D_A \ll h)\), the brackets can be removed from the left-hand-side of equation (3.66) and the latent heat term so that equation (3.66) becomes

\[-k_l \left. \frac{\partial T}{\partial y} \right|_{0^+} = -\frac{k_m}{\delta} (T_f^m - T_d^m) + j_v \lambda, \tag{3.67}\]

which recovers the thermal boundary condition (3.12).
CHAPTER 4

COMPUTATIONAL FLUID DYNAMICS SIMULATIONS OF POLARIZATION PHENOMENA IN DIRECT CONTACT MEMBRANE DISTILLATION

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4.1 Abstract

Direct Contact Membrane Distillation (DCMD) has emerged as a promising means of concentrating brines to their saturation limit. To date, computational fluid dynamics (CFD) studies of DCMD focus primarily on temperature polarization. However, when treating hypersaline brines, concentration polarization is an additional challenge that reduces system efficiency and leads to mineral scaling. To study coupled temperature and concentration polarization in the DCMD treatment of hypersaline brines, we develop an experimentally validated two-dimensional CFD code that simulates heat and mass transport in plate-and-frame DCMD systems. We then perform a comprehensive parametric study of polarization phenomena for a wide range of feed and distillate operating conditions, system length, and co-current versus counter-current operation. We also investigate the system-level performance by measuring the average permeate flux, single-pass water recovery, maximum concentration polarization coefficient, and gained output ratio of DCMD systems with heat recovery. Though the transmembrane vapor flux is small, we observe dramatic increases in solute concentration at the membrane surface, exceeding 1.6 times the feed value. The temperatures,

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concentration, and vapor flux vary considerably in the downstream direction, and are poorly approximated by common Nusselt and Sherwood correlations.

**keyword**: Membrane Distillation, temperature polarization, concentration polarization, computational fluid dynamics

### 4.2 Introduction

The global capacity of reverse osmosis and nanofiltration water treatment systems exceeds 42 million m$^3$/day [1, 4, 5]. This brings the challenge of managing waste brine, particularly for inland applications [6, 7]. Direct contact membrane distillation (DCMD) has emerged as a promising means of concentrating waste brines to their saturation limit, after which they can be discharged to evaporation ponds or crystallizers [8–19]. The energy efficiency and water recovery of DCMD systems are governed by coupled heat and mass transport in the feed stream, membrane, and distillate stream. These processes and the coupling between them are not fully understood, particularly for hypersaline brines in which interactions between simultaneous temperature and concentration polarization are important. Understanding these interactions is necessary to maximize water recovery while minimizing mineral scaling. To that end, we perform a comprehensive set of numerical simulations of heat and mass transport for DCMD. The simulations are performed using an experimentally validated computational fluid dynamics (CFD) code and used to explore the underlying physics of temperature and concentration polarization in DCMD.

We focus on a DCMD arrangement in which hot feed and cool distillate water flow on opposite sides of a hydrophobic microporous membrane in a co-current or counter-current manner, as sketched in Figure 4.1. The hydrophobic membrane creates vapor-liquid interfaces on the feed and distillate sides of the membrane. The temperature difference across the membrane causes volatile components (i.e. H$_2$O) to evaporate from the feed side of the membrane, travel through the vapor-filled pores, and condense on the distillate side of the membrane. Non-volatile solutes remain in the feed. DCMD has several advantages over pressure-driven processes such as reverse osmosis. First, DCMD can treat hypersaline brines
because it is not sensitive to osmotic pressure and rejects 99-100% of salts. While reverse osmosis can treat NaCl solutions up to approximately 70 g/L, the limit for DCMD is approximately 300 g/L [21]. Second, DCMD systems do not require high-pressure pumps, and can be built with inexpensive plastics. Third, DCMD operates at feed inlet temperatures below 90 °C that are readily produced by renewable energy and industrial waste heat.

A study by Bouchrit et al. [9] concluded that temperature and concentration polarization are the most crucial factors affecting DCMD performance in the treatment of hypersaline brines. Temperature polarization refers to a reduction in the transmembrane temperature difference due to heat transfer through the membrane, as illustrated by the temperature profile sketched in Figure 4.1. Concentration polarization describes the accumulation of solutes adjacent to the feed side of the membrane. Both polarization phenomena reduce the transmembrane vapor flux by reducing the transmembrane vapor pressure difference. Concentration polarization can lead to mineral scaling, which occurs when the concentration at the membrane surface exceeds the saturation limit. Mineral scaling blocks pores, can damage the membrane, and can lead to pore wetting.

Numerous studies have successfully modeled the system-level performance of DCMD systems using approximate Nusselt and Sherwood number correlations [22]. However, these
correlations do not capture the downstream variation of polarization, permeate flux, and conductive heat loss along the membrane. In some cases, these correlations rely on fitting parameters or physical assumptions that are unclear. CFD offers a valuable complement to such studies because it predicts the full temperature, concentration, and velocity fields, and can identify performance bottlenecks that are difficult to diagnose experimentally [22].

Though numerous CFD studies have investigated DCMD systems, most solve the coupled heat, continuity, and Navier-Stokes equations without considering solute transport [23–45]. Of the studies that include salt transport [46–50], there is sometimes only limited discussion of concentration polarization. For example, studies by Hayer et al. [46], Lousi ff [47], and Seo [48] include salt transport in their simulations, but focus their discussion on net permeate flux and heat transport. A study by Soukane [49] reports some results for turbulent salt transport in a 3-D DCMD system with strong inlet and outlet effects. More recently, two promising studies by Amigo et al. [139] and Park et al. [50] investigate the effects of membrane spacers on salt transport. Amigo et al. shows that spacer geometry strongly influences where salts tend to accumulate, and consequently potentially precipitate.

To study the coupled effects of temperature and concentration polarization in the DCMD treatment of hypersaline brines (NaCl solution), we develop here a 2-D CFD code that solves the Navier-Stokes, continuity, advection-di ffusion, and heat equations using a finite-volume method in space and an efficient projection method in time. The 2-D code allows us to conduct a comprehensive parametric study of the effects of operating conditions such as feed and distillate flow rate and temperature, feed concentration, system length, and co-current versus counter-current operation. In the process, we also compare the results of our simulations with the predictions of two popular Nusselt and Sherwood correlations. The 2-D results presented here serve as a guide for developing computationally efficient 3-D analyses, currently underway in our group. The remainder of this study is organized as follows. Section 4.3 presents the system geometry and governing equations. Section 4.4 presents our numerical methods, experimental measurements, and the considered Nusselt and Sherwood
correlations. In section 4.5, we discuss the structure of temperature and concentration polarization layers and the dependence of the DCMD performance on operating conditions. Section 4.6 presents our conclusions.

4.3 Geometry and governing equations

We consider a 2-D flat-sheet membrane system with feed and distillate channels of length $L$ and height $H$, as sketched in Figure 4.1. NaCl solution enters the feed channel with temperature $T^f_{in}$, concentration $C_{in}$, and mean velocity $U_{in}$. Pure water enters the distillate channel with temperature $T^d_{in}$ and mean velocity $U_{in}$. We consider both co-current and counter-current operations. Though Figure 4.1 shows the membrane as a shaded region about $y = 0$, we model transmembrane heat and mass transport using effective interface conditions that couple the feed ($0 \leq y \leq H$) and the distillate ($-H \leq y \leq 0$) channels.

4.3.1 Transmembrane mass transport

Figure 4.2: Sketch (not to scale) demonstrating mass transport through a hydrophobic membrane with idealized pores. The vapor-liquid interfaces are shown as dashed black curves.
As in most previous literature, we assume the vapor mass flux, \( j_v \), is linearly proportional to the transmembrane vapor pressure difference [20],
\[
  j_v = -B(p_{fm}^f - p_{dm}^d), \tag{4.1}
\]
where \( B \) is the vapor permeability and \( p_{fm}^f \) and \( p_{dm}^d \) are the water vapor pressures on the feed and distillate sides of the membrane, respectively, as illustrated in Figure 4.2. A fundamental difference between DCMD models is the evaluation of \( B \) [22]. Though \( B \) can depend on temperature and pressure [20], studies have shown that approximating \( B \) as a constant membrane property matches experimental data well [39, 101]. We take this approach and determine \( B \) by fitting to experimental measurements described in section 4.4.

The vapor pressures \( p_{fm}^f \) and \( p_{dm}^d \) are functions of the local temperature and concentration at the membrane surface [101]. We evaluate \( p_{fm}^f \) and \( p_{dm}^d \) as the product of the vapor saturation pressure \( P_{sat} \) and water activity \( a_w \),
\[
  p_m = a_w P_{sat}, \quad P_{sat} = \exp \left( 23.238 - \frac{3841}{T_m - 45} \right), \tag{4.2}
\]
where \( P_{sat} \) is determined using the Antoine equation [102] and \( T_m \) is the local temperature on the membrane surface. The activity is determined from the expression
\[
  a_w = 1 - 0.03112b - 0.001482b^2 \tag{22},
\]
where \( b \) is the NaCl molality (mol/kg). This expression is valid from zero salinity to saturation. We assume complete salt rejection, such that \( a_w = 1 \) in the distillate.

### 4.3.2 Transmembrane heat transport

As in most previous literature, we model transmembrane heat conduction as
\[
  q_c = -\frac{k_m}{\delta} (T_{fm}^f - T_{dm}^d), \tag{4.3}
\]
where \( \delta \) and \( k_m \) are the membrane thickness and thermal conductivity, respectively, and \( T_{fm}^f \) and \( T_{dm}^d \) are the temperatures on the feed and distillate sides of the membrane, respectively. In the literature, the membrane thermal conductivity is often approximated as \( k_m = \epsilon k_v + (1 - \epsilon)k_s \), where \( \epsilon \) is the membrane porosity and \( k_v \) and \( k_s \) are the gas and solid conductivities, respectively [103]. However, in practice \( k_m/\delta \) is often treated as an effective heat transfer
coefficient. We take that approach by fitting $k_m/\delta$ to experiments.

Applying conservation of energy principles for liquid-vapor interfaces with phase change (see Leal [104]), one finds that on the membrane feed surface, conductive heat transport within the liquid phase must equal

$$-k \frac{\partial T_f}{\partial y} \bigg|_{y=0^+} = j_v \lambda \frac{k_m}{\delta} (T_f - T_d),$$

(4.4)

where $\lambda$ is the latent heat per unit mass, and the “+” superscript signifies that the derivative is evaluated from the feed side of the membrane. Though not shown, for brevity, similar conditions are applied on the distillate surface.

### 4.3.3 Governing equations for the channel flows

Fluid flow in the feed and distillate channels is governed by the incompressible continuity and Navier-Stokes equations for Newtonian fluids,

$$\nabla \cdot \mathbf{u} = 0,$$

(4.5)

$$\rho \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \nabla \cdot \tau, \quad \tau = \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right],$$

(4.6)

where $\tau$ is the viscous stress tensor, $\mathbf{u} = [u \ v]$, $p$, $\rho$ and $\mu$ are the fluid velocity vector, pressure, density, and dynamic viscosity, respectively. Within each channel, we neglect variations in density with temperature and concentration because the maximum variation of density is typically within 3%. In each channel, we set the density to the inlet value. Heat transport is governed by the thermal energy equation,

$$\rho c_p \left[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right] = \nabla \cdot (k \nabla T),$$

(4.7)

where $c_p$ is the fluid heat capacity [105]. NaCl transport is modeled using the advection-diffusion equation

$$\frac{\partial c}{\partial t} + (\mathbf{u} \cdot \nabla) c = \nabla \cdot (D \nabla c),$$

(4.8)
where $D$ is the effective mass diffusivity. Though we approximate the flows as incompressible, we include the variations of all other thermo-physical properties with temperature and salt concentration. We derived correlations for $\mu(T, c)$, $c_p(T, c)$, and $\lambda(T)$ using the OLI Stream Analyzer database (OLI Systems, Morris Plains, NJ). We obtained correlations for $k(T, c)$ and $D(T)$ from the literature [140, 141]. The correlations are provided in appendix 4.8.1.

At the plates ($y = \pm H$), we apply the no-slip, no-penetration, and no-flux conditions, $u = v = \partial c / \partial y = \partial T / \partial y = 0$. On the membrane surfaces, we apply the no-slip condition, $u = 0$, and the following conditions determined from the models discussed in sections 4.3.1 and 4.3.2. The feed side conditions are,

$$v = \frac{j_v}{\rho^f}, \quad -k \frac{\partial T}{\partial y}_{|y=0^+} + \frac{k_m}{\delta} T_m^f = j_v \lambda + \frac{k_m}{\delta} T_m^d, \quad v c_m - D \frac{\partial c}{\partial y} = 0. \quad (4.9)$$

and the distillate side conditions are,

$$v = \frac{j_v}{\rho^d}, \quad -k \frac{\partial T}{\partial y}_{|y=0^-} - \frac{k_m}{\delta} T_m^d = j_v \lambda - \frac{k_m}{\delta} T_m^f. \quad (4.10)$$

At the channel inlets, we apply the desired temperatures and concentrations, and fully developed laminar velocity profiles with desired mean velocity $U_{in}$,

$$u = \frac{3U_{in}}{2} (1 - \frac{y^2}{H^2}), \quad v = 0, \quad T = T_{in}, \quad c = C_{in}. \quad (4.11)$$

For all cases, we assume that the feed and distillate channels have identical mean inlet velocities, $U_{in}$. At the channel outlets, we apply convective conditions [106] to the velocity, and Neumann conditions to the concentration and temperature,

$$\frac{\partial \mathbf{u}}{\partial t} + U_{in} \frac{\partial \mathbf{u}}{\partial x} = 0, \quad \frac{\partial T}{\partial x} = \frac{\partial c}{\partial x} = 0, \quad \text{at } x = L. \quad (4.12)$$

These conditions are required because our code is designed to operate in unsteady conditions for which it is important to allow flow perturbations to exit the channels without reflecting and polluting the simulation upstreams.

At $t = 0$, we set the initial flow fields to the inlet conditions (4.11)

$$u^0 = \frac{3U_{in}}{2} (1 - \frac{y^2}{H^2}), \quad v^0 = 0, \quad p^0 = 0, \quad T^0 = T_{in}, \quad c^0 = C_{in}. \quad (4.13)$$
and integrate in time to steady state. It is worth stressing that our governing equations do not assume laminar conditions. Nevertheless, for the Reynolds numbers considered, we find that all simulations converge to laminar steady-state conditions.

4.4 Numerical and experimental methodologies

We discretize Equations (4.5)–(4.12) spatially using second-order finite-volume methods on a staggered grid [115]. The grid is uniform in the $x$-direction, but is non-uniform in the $y$-direction to concentrate grid points near the membrane. The governing equations are discretized in time using second-order Adams-Bashforth and Crank-Nicolson methods for nonlinear and linear terms, respectively. The pressure is evaluated using an efficient, non-iterative, projection method [142]. Further details, benchmarking, and mesh-independence studies are provided in appendix 4.8.3.

Our methods produce an efficient code tailored to simulating unsteady heat and mass transport in DCMD systems. Our numerical implementation is motivated by ongoing work focused on unsteady mixing generated by feed spacers. The current manuscript focuses, however, on steady cases. In this case, our time-resolved method likely requires more CPU time than a method tailored to steady flows. Furthermore, because the code used for the current manuscript was written in MATLAB, little effort was dedicated to optimization. For that purpose, we are currently developing a fully 3D FORTRAN code optimized to run on multiple computer cores. Nevertheless, we report that the simulations presented in Figure 4.3(b) required roughly 11 hours each when running on a single core of an Intel Core i5-4590 CPU processor.

4.4.1 Experimental measurement of membrane properties

To measure the heat transfer coefficient $k_m/\delta$ and vapor permeability $B$ experimentally, we developed an acrylic flow cell with 10 feed and distillate channels machined into acrylic plates. Additional description is given in Bush et al. [143]. The 10 channels have identical length $L = 17.78$ cm, height $H = 3.175$ mm, and width $W = 6.35$ mm. The small
width reduces membrane warping that arises from shear and pressure forces. To minimize this warping, we operated the system in co-current mode. The system can operate with a minimum distillate temperature of 20 °C and maximum feed temperature of 70 °C.

Our experiments considered a 0.2 µm pore size polypropylene 3M membrane previously studied by [114]. This membrane was chosen for the high reproducibility of its vapor flux, with a standard deviation of 0.6%, see discussion in [114]. To determine the heat transfer coefficient $k_m/\delta$ and permeability $B$ of the membrane, we measured the average transmembrane flux $v_{m}^{\text{ave}}$ when the distillate inlet temperature was fixed to $T_{in}^d = 20$ °C and the feed inlet temperature was varied between $30 \leq T_{in}^f \leq 60$ °C in increments of 10 °C, producing the data shown as open circles in Figure 4.3(a). From these measurements, we determined the effective heat transfer coefficient $k_m/\delta$ as 576.72 W/m² K using the thermal model developed by Schofield [101] and extended by Vanneste [114]. Using the obtained $k_m/\delta$, we then
performed equivalent 2-D CFD simulations for the same channel dimensions and operating parameters to determine the permeability $B$ that best fit the experimental results. The CFD data is shown as the solid line in Figure 4.3(a). In this manner, we set the permeability to $B = 1.8676 \times 10^{-6}$ kg/m$^2$ s Pa.

After setting the membrane properties as discussed above, we performed a second set of experiments in which we fixed the distillate inlet temperature to $T_{d in}^d = 30$ °C and we varied the feed inlet temperature between $40 \leq T_{f in}^f \leq 70$ °C in increments of 10 °C. The resulting vapor flux measurements are shown in Figure 4.3(a) as open triangles. We then repeated our simulations for the same conditions, producing the CFD data shown as a dashed line. For the seven experiments performed using feed temperatures $T_{f in}^f \leq 60$ °C, our CFD agrees with experimental results with a relative error on the order of 3%. For the case $T_{f in}^f = 70$ °C, however, our CFD underpredicts the experimentally measured flux by 7%. This likely occurs because our measured thermal conductivity found using the method of Vanneste is an effective constant conductivity for temperature ranges between 20 to 60°C. Moreover, the method of Vanneste neglects downstream variations of the membrane temperature and vapor flux. Our CFD shows that these variations are in fact significant. Finally, because the channel aspect ratio $W/H = 2$ does not minimize 3-D effects, these are also likely lumped into the effective permeability.

To further validate our numerical model, we compare the simulated average feed outlet temperature $T_{f out}^f$ with experimental measurements, as shown in Figure 4.3(b). We find that our CFD results agree well with the experimental measurements, producing a relative error below 2.5%.

### 4.4.2 Correlations and system performance criteria

We compare the results of our simulations with two popular Nusselt and Sherwood number correlations. For this purpose, we mimic the manner in which these correlations are typically applied in theoretical and experimental studies for which CFD is not available, as there is otherwise no need for such correlations when corresponding CFD data is available.
For example, in the absence of CFD or direct experimental measurement, Nusselt number correlations are often used to estimate the feed and distillate membrane surface temperatures. We consider the popular correlation of Hausen [22, 144–147],

\[
Nu = \frac{h_T D_h}{k} = 4.36 + \frac{0.036 Re_h Pr D_h/L}{1 + 0.0011(Re_h Pr D_h/L)^{0.8}}, \quad Re_h = \frac{U_{in} D_h}{\nu},
\]  

(4.14)

where \( h_T \) is the convective heat transfer coefficient, \( Pr = c_p \mu / k \) is the Prandlt number, and \( D_h = 2H \) is the hydraulic diameter. Using the standard Nusselt number-based approach [22], we first compute \( h_T \) for each channel using Equation 4.14. We then follow the procedure outlined in detail by Khayet et al. [146] and Hitsov et al. [22] to compute the membrane surface temperature \( T_{fm} \) and \( T_{dm} \). The only CFD data used in this process is the average permeate flux.

Sherwood number correlations are commonly used to estimate the solute concentration at the membrane surface. We consider the popular Sherwood correlation of De and Bhattacharya [148],

\[
Sh = \frac{h_c D_h}{D} = 2.381 \left( \frac{Re_h Sc D_h/L}{I} \right)^{1/3}, \quad I = \int_0^\infty \exp(-\eta^3/3 - 0.42 \lambda_I \eta) d\eta,
\]  

(4.15)

where \( h_c \) is the convective mass transfer coefficient, \( Sc = \mu / (\rho D) \) is the Schmidt number, and \( \lambda_I = Re_h Sc / (Re Sc D_h/L)^{1/3} \) is a constant. Using the standard approach [22], we first compute \( h_c \) using Equation4.15. We then compute the membrane surface concentration \( c_m \) using the film model outlined in references [149] and [22]. Again, the only CFD data used in this process is the average permeate flux.

We characterize temperature polarization using a temperature polarization coefficient (TPC), which is defined as the ratio of the temperature difference across the membrane surfaces to the temperature difference between the feed and the permeate inlet streams,

\[
TPC = \frac{T_{fm}(x) - T_{dm}(x)}{T_{in} - T_{in}^d},
\]  

(4.16)
where $T_{m}^{f}(x)$ and $T_{m}^{d}(x)$ are the membrane surface temperatures on feed and distillate sides, respectively. Note that TPC = 1 denotes no temperature polarization, while TPC $\ll$ 1 indicates strong polarization.

We characterize concentration polarization using a concentration polarization coefficient (CPC), which is defined as the ratio of the membrane surface concentration to the feed inlet concentration,

$$CPC = \frac{c_{m}(x)}{C_{in}}, \quad (4.17)$$

Note that CPC = 1 denotes no concentration polarization, while CPC $\gg$ 1 indicates strong polarization.

To investigate the influence of operating temperatures on DCMD performance, we define the gained output ratio (GOR) as

$$GOR = \frac{Q_{v}}{Q_{in}}, \quad Q_{v} = \int_{0}^{L} j_{v} \lambda dx, \quad (4.18)$$

where $Q_{in}$ is the energy required to heat the feed. For practical applications, DCMD systems recover heat from the outlets to preheat the feed. For our computation of the GOR, we consider a system in which two heat exchangers preheat the feed using waste heat from the outlet flows, as sketched in Figure 4.4. After preheating, a heater supplies $Q_{in}$ to bring
the feed to the desired inlet temperature. To estimate the GOR, we consider plate heat ex-
changers manufactured by WCR Incorporated (Model: WCR-A102). Using the manufacturer
provided heat transfer coefficient, we use the Effectiveness-NTU method [150] to determine
$Q_m$.

4.5 Results and discussion

This section presents a parametric study of heat and mass transport in a bench-scale
DCMD system. We begin in section 4.5.1 by demonstrating temperature and concentration
polarization in a co-current operation. We repeat the analysis for counter-current operation
in section 4.5.2. We then systematically explore the influence of feed and distillate inlet
temperature, velocity, feed concentration, and system length in sections 4.5.3–4.5.6. Section
4.5.7 presents a case-study that investigates the combined effects of feed inlet temperature
and inlet velocity on a DCMD system treating hypersaline brines.

4.5.1 Co-current operation

Figure 4.5(a) shows the steady-state temperature field in a co-current system when $T_{in}^f$
= 60 °C, $T_{in}^d$ = 20 °C, $C_{in} = 100$ g/L, and $U_{in} = 0.124$ m/s. The dimensions are those
of our experimental system. The operating temperatures are typical of DCMD systems.
Throughout our study, we limit $U_{in}$ to ensure laminar flows. For the case illustrated in
Figure 4.5(a), the inlet conditions produce the feed and distillate Reynolds numbers $Re_f =$
528 and $Re_d = 393$, respectively. Note that though the feed and distillate channels have
identical inlet flow rates, they have different Reynolds numbers because their thermo-physical
properties differ.

Figure 4.5(a) shows distances as $y/H$ and $x/H$ and uses different color scales for the
distillate and feed channels to highlight cooling of the feed and heating of the distillate.
The solid lines in Figure 4.5(b) show the downstream variation of the membrane surface
temperatures, $T_{mf}(x)$ and $T_{md}(x)$. As expected for co-current operation, the transmembrane
temperature difference, $\Delta T_m(x)$, decreases monotonically. We also observe that $T_{mf}$ and $T_{md}$
Figure 4.5: (a) Temperature field for co-current operation. Different color scales are used in the distillate and feed channels. (b) The solid lines show $T_m^f(x)$ and $T_m^d(x)$. The dashed lines show $T_{m,Nu}^f$ and $T_{m,Nu}^d$. (c) The solid line shows the TPC. The dashed line shows $TPC_{Nu}$.

vary most rapidly near the inlet where the transmembrane heat flux is maximized. For comparison, the dashed lines in Figure 4.5(b) show the membrane surface temperatures, $T_{m,Nu}^f = 48.06 \, ^\circ C$ and $T_{m,Nu}^d = 31.12 \, ^\circ C$, predicted by the Nusselt correlation (4.14). The solid line in Figure 4.5(c) shows the TPC evaluated using the CFD results for $T_m^f(x)$ and $T_m^d(x)$. The dashed line in Figure 4.5(c) shows $TPC_{Nu}$ evaluated using $T_{m,Nu}^f$ and $T_{m,Nu}^d$. The Nusselt correlation (4.14) underpredicts TPC by 57.6% at the inlet and overpredicts
Figure 4.6: (a) Temperature profiles in the feed channel at $x = L/4$, $x = L/2$, $x = 3L/4$ and $x = L$. (b) Self-similar temperature distributions. (c) Downstream growth of $\delta_T$.

TPC by 137.7% at the outlet.

Figure 4.6(a) shows cross-sectional temperature profiles in the feed channel at $x = L/4$ (*), $L/2$ ($\triangle$), $3L/4$ (□), $L$ (×). To focus on the thermal boundary layers near the membrane surface, we only show the profiles for $0 < y/H < 0.5$. As expected, the layer thicknesses increase in the downstream direction. The layers are also relatively thick, covering nearly 40% of the channels at $x = L$. To measure the thermal boundary layer thickness in the feed channel, we define the non-dimensional temperature $\hat{T}$ and coordinates $\hat{x}$ and $\hat{y}$ as

$$\hat{T}(x, y) = \frac{T(x, y) - T_m^f(x)}{T_{in}^f - T_m^f(x)}, \quad \hat{x} = \frac{x}{H}, \quad \hat{y} = \frac{y}{H}. \quad (4.19)$$

$\hat{T}$ is defined such that it varies from zero on the membrane surface ($\hat{y} = 0$) to unity when $T = T_{in}^f$. We then define the non-dimensional thermal boundary layer thickness $\hat{\delta}_T(\hat{x})$ as the location where

$$\hat{T}|_{\hat{y} = \hat{\delta}_T(\hat{x})} = 0.95. \quad (4.20)$$

Figure 4.6(b) shows that the four curves in Figure 4.6(a) collapse to a self-similar curve when we plot $\hat{T}$ as a function of $\eta_T = \hat{y}/\hat{\delta}_T$. Figure 4.6(c) shows that $\hat{\delta}_T$ (solid line) grows with $\hat{x}$ as $\hat{\delta}_T = 0.076\hat{x}^{0.36}$ (dashed line). The power law does not fit the CFD data for $\hat{x} < 1$
due to inlet effects. The exponent of the power law is close to 1/3, which often occurs in thermal boundary layers, as in the Leveque problem [151], as well as concentration boundary layers, as in De and Bhattacharya [148]. As discussed by Probstein [122], the 1/3 exponent arises due to a competition between downstream advection and transverse diffusion. The slight deviation of the numerical results from the predicted 1/3 exponent likely arises due to simultaneous temperature and concentration polarization, as well as variations of \( \mu \), \( \alpha \), and \( D \) with temperature and concentration. None of these phenomena are considered in the analyses of Leveque [151] and Probstein [122].

Figure 4.7 shows the downstream variation of the transmembrane vapor flux, \( v_m(x) \), normalized with \( U_{in} \). The secondary y-axis indicates the equivalent local permeate flux in L/m² h (LMH). We observe that \( v_m \) is four orders-of-magnitude smaller than \( U_{in} \), and decreases approximately 77 % from 61.7 LMH at the inlet to 13.9 LMH at the outlet. The dashed line in Figure 4.7 shows the average vapor flux \( v_{ave}^m = 4.40 \times 10^{-5}U_{in} \). Thin film models of DCMD systems often neglect the downstream variation of \( v_m \) by applying this constant value along the entire membrane surface. Meanwhile, DCMD models based on Graetz [152] and Leveque [151] boundary layer solutions neglect \( v_m \) altogether.

Figure 4.8(a) shows the steady-state concentration field. Because the mass diffusivity \( D \) is much smaller than the thermal diffusivity \( \alpha \), the concentration boundary layer is much
thinner than the thermal layer. Throughout our study, the Lewis number \( Le = \alpha/D \gg 1 \) is consistently greater than 50. Consequently, Figure 4.8(a) only shows the concentration for \( 0 < y/H < 0.1 \). The solid line in Figure 4.8(b) shows the variation of the membrane surface concentration, \( c_m(x) \). Though the permeate velocity \( v_m \) is small, \( c_m \) increases significantly from 100 g/L at the inlet to around 130 g/L at the outlet. As expected, \( c_m \) increases rapidly near the inlet, where the vapor flux is maximal. Though \( c_m \) increases dramatically, the average concentration at the outlet is only \( c_{out} = 101.2 \) g/L. The disparity between \( c_m \) and \( c_{out} \) arises because the solute only accumulates within a thin layer. In appendix 4.8.4, we show that the concentration boundary layer is self-similar and exhibits an approximate 1/3 downstream power law.

The dashed line in Figure 4.8(b) shows the uniform membrane concentration \( c_{m,sh} = 128.3 \) g/L predicted by Sherwood correlation (4.15). Though \( c_{m,sh} \) significantly overpredicts \( c_m \) in the inlet region, it predicts \( c_m \) within 2 % of the CFD result when \( x > 14H \). Unfortunately, in section 4.5.2, we find this agreement does not extend to counter-current operations. One drawback to modeling concentration polarization with Sherwood correlations is that such
correlations usually neglect the downstream variation of $c_m(x)$. They consequently may not accurately predict the regions of a membrane operating in supersaturated conditions, which is important in the treatment of hypersaline brines.

Though the Leveque and Graetz problems are often used to study both temperature and concentration polarization, they consider thermal boundary layers developing on an impermeable wall with a fixed temperature. In contrast, neither the temperature nor concentration are fixed on DCMD membrane surfaces. This partially explains why Nusselt and Sherwood number correlations fail to accurately predict local membrane conditions. De and Bhattacharya [148] extended the analysis of Leveque to include permeate flux. However, they too assumed that $c_m$ was constant.

### 4.5.2 Counter-current operation

To investigate polarization under counter-current operation, we repeat the simulation of the previous section in a counter-current mode. Figure 4.9(a) shows the resulting temperature field. The solid lines in Figure 4.9(b) show the membrane surface temperatures $T_{fm}^f$ and $T_{dm}^d$. We observe that $T_{fm}^f$ decreases monotonically from 60 to 38.65 °C in its downstream direction (rightward), while $T_{dm}^d$ increases monotonically from 20 to 43.11 °C in its downstream direction (leftward). As expected, the surface temperatures vary most rapidly at the channel inlets and outlets. The dashed lines show the uniform surface temperatures, $T_{fm,Nu}^f = 48.0$ °C and $T_{dm,Nu}^d = 31.2$ °C, predicted by the Nusselt correlation (4.14).

Figure 4.10(a) shows the transmembrane temperature difference predicted by CFD (solid line) and the Nusselt correlation (4.14) (dashed line). The secondary y-axis indicates the corresponding TPC. The correlation significantly overpredicts the temperature difference and thus TPC throughout the channel. Figure 4.10(b) shows that vapor flux $v_m(x)$ varies non-monotonically in a counter-current operation. Perhaps unexpectedly, the temperature difference is maximized at the feed outlet, while the vapor flux is maximized at the inlet. This occurs because the saturation pressure $P_{sat}$ varies non-linearly with temperature, such that $dP_{sat}/dT$ increases with temperature (see equation (4.2)). In addition, concentration
polarization decreases the water vapor pressure, with the largest impact at the feed outlet. These compounding phenomena cause $v_m(x)$ to be minimized near $x/L = 3/4$. For comparison, the dashed line in panel (b) shows the vapor flux in a co-current operation. Co-current operation produces a larger vapor flux in the upstream section (roughly $x<L/4$), while counter-current operation produces a larger flux in the remaining downstream section (roughly $x>L/4$). Overall, the counter-current operation produces a net permeate flux of 20.5 LMH, compared to 19.6 LMH for co-current operation.

Figure 4.10(c) shows the counter-current surface concentration $c_m(x)$ (solid line) increases by approximately 40%, compared to approximately 30% for co-current operation. Through-
out our study, we find that counter-current operation produces only a modest increase in permeate flux, but a significant increase in concentration polarization. Furthermore, in section 4.5.3, we show that the increased concentration polarization in counter-current operation is not simply a result of its modest increase in permeate flux. In fact, we will show that a co-current system can be operated such that it produces greater permeate flux while producing lower concentration polarization. We hypothesize that the maximum concentration is reduced in co-current systems due to the monotonic decrease in the permeate flux $v_m(x)$. 

Figure 4.10: (a) $\Delta T_m$ predicted by CFD (solid line) and the Nusselt correlation (4.14) (solid line). (b) $v_m(x)/U_{in}$ for counter-current (solid line) and co-current (dashed line) operation. (c) The solid line shows $c_m$ for counter-current operation. The dashed line shows $c_{m}^{sh} = 129.54$ g/L.
Figure 4.11: (a) Variation of average vapor flux with varying feed inlet temperature when $T^f_{in} = 20 \, ^\circ C$. (b) Variation of average vapor flux with varying distillate inlet temperature when $T^d_{in} = 90 \, ^\circ C$. The secondary y-axes in both panels indicate the water recovery.

This allows the concentration layer to diffuse away from the membrane, thereby producing a thicker layer with a smaller surface concentration $c_m(x)$ than in a counter-current operation. This interpretation is motivated by our observations of concentration polarization in long counter-current systems (see appendix 4.8.5) for which we find that concentration polarization eventually begins to decrease with downstream distance due to the decrease in local vapor flux and the resulting back-diffusion of solute into the bulk. The dashed line in Figure 4.10(c) shows that the concentration $c^{sh}_m = 129.5 \, g/L$ predicted by the Sherwood correlation (4.15) significantly overpredicts $c_m(x)$ near the inlet, and underpredicts $c_m$ at the outlet. This suggests that the correlation may fail to predict mineral scaling in counter-current DCMD systems.

Though not shown, we found that the temperature and concentration boundary layers remain self-similar for counter-current operation, and satisfy the power laws $\hat{\delta}_T = 0.075 \bar{x}^{0.35}$ and $\hat{\delta}_c = 0.025 \bar{x}^{0.32}$, respectively.

### 4.5.3 Influence of feed and distillate inlet temperatures

To investigate the effects of feed and distillate inlet temperatures, we simulated co-current and counter-current DCMD systems for the feed and distillate inlet temperatures $30 \leq T^f_{in} \leq 78$.
Figure 4.12: (a) Downstream variation of CPC when $T_{\text{in}}^f = 40$ (solid line) and 80 (dashed line) °C when $T_{\text{in}}^d = 20$ °C for co-current (crosses) and counter-current (squares) operation. (b) Variation of CPC$_{\text{max}}$ with feed inlet temperature when $T_{\text{in}}^d = 20$ °C.

90 °C and $20 \leq T_{\text{in}}^d \leq 80$ °C. All other parameters were maintained as in sections 4.5.1 and 4.5.2. Figure 4.11(a) shows the variation of the average vapor flux, $v_{\text{ave}}$, with increasing $T_{\text{in}}^f$ for $T_{\text{in}}^d$ maintained at 20 °C. Conversely, Figure 4.11(b) shows the variation of $v_{\text{ave}}$ with increasing $T_{\text{in}}^d$ for $T_{\text{in}}^f$ held at 90 °C. The secondary y-axis indicates the corresponding water recovery WR (%). In all cases, counter-current operation (solid lines) produces slightly higher water flux than co-current operation (dashed lines), and the fluxes increase with the difference between the two inlet temperatures (i.e, $\Delta T_{\text{in}} = T_{\text{in}}^f - T_{\text{in}}^d$). However, we also see that for a fixed temperature difference $\Delta T_{\text{in}}$, the flux increases with the distillate inlet temperature. For example, comparing panels (a) and (b) in Figure 4.11, we see that $\Delta T_{\text{in}} = 40$ °C produces 20 LMH when $T_{\text{in}}^d = 20$ °C and 30 LMH when $T_{\text{in}}^d = 50$ °C, an increase of 50%. This is due to the nonlinear variation of $P_{\text{sat}}$ with temperature (see Equation (4.2)).

Figure 4.12(a) shows the downstream variation of CPC when $T_{\text{in}}^f = 40$ (solid line) and 80 (dashed line) °C when $T_{\text{in}}^d = 20$ °C for co-current (crosses) and counter-current (squares) operation. As expected, CPC increases with the feed inlet temperature due to the increased vapor flux. Figure 4.12(b) shows the corresponding variation of the maximum CPC within the feed channel, CPC$_{\text{max}}$, for varying $T_{\text{in}}^f$. As expected, the maximum value, CPC$_{\text{max}}$=1.615,
occurs in the counter-current operation. We again note that while the transmembrane flux is small, the concentration polarization is significant, exceeding a 60% increase in the counter-current case. We again stress that the increased concentration polarization in the counter-current system is not simply a result of its marginally larger permeate flux. To demonstrate this fact, note from Figure 4.11(a) that a co-current system operating at the feed temperature $T_{in}^f = 90 \, ^\circ C$ produces more permeate flux than a counter-current system operating at the lower feed temperature $T_{in}^d = 80 \, ^\circ C$. We nevertheless observe from Figure 4.12(b) that the co-current system has a lower $CPC_{max}$ than the counter-current system with lower permeate flux.

Figure 4.13(a) shows the variation of GOR with varying $T_{in}^f$ when $T_{in}^d = 20 \, ^\circ C$. The monotonic increase in GOR with the feed inlet temperature arises because the transmembrane latent heat transfer rate, $Q_v$, increases more rapidly with $T_{in}^f$ than $Q_{in}$, as illustrated in Figure 4.13(b). In Figure 4.13(a), we also observe that co-current operation produces a higher GOR than counter-current.
4.5.4 Influence of feed concentration

To investigate the effects of feed concentration, we simulated co-current and counter-current operations for $0 < C_{in} < 300$ g/L in increments of 50 g/L. All other parameters were fixed as in sections 4.5.1 and 4.5.2. Figure 4.14(a) shows the variation of $v_{m}^{ave}$ with $C_{in}$. For both operations, $v_{m}^{ave}$ decreases almost linearly with increasing $C_{in}$, due to the decrease in vapor pressure on the membrane feed surface. For counter-current operation, the net transmembrane flux decreases over 50% from 24.6 LMH at $C_{in} = 0$ g/L to 12.0 LMH at $C_{in} = 300$ g/L. Figure 4.14(b) shows that the decrease in the transmembrane flux causes a decrease in concentration polarization. For counter-current operation, $CPC_{max}$ decreases from 1.42 at $C_{in} = 50$ g/L to 1.22 at $C_{in} = 300$ g/L. The latter value corresponds to 366 g/L, which exceeds the saturation value $c_{sat} = 364$ g/L, computed at the feed outlet membrane temperature $T = 41.2$ °C. Though not shown, we found that the GOR of both co-current and counter-current operations decreased around 25% with increasing feed concentration.
4.5.5 Influence of inlet velocity

To investigate the effects of inlet velocity, we simulated co-current and counter-current operations for $0.041 \leq U_{in} \leq 0.248 \text{ m/s}$, corresponding to the laminar Reynolds numbers of $175 < Re_f < 1048$ and $131 < Re_d < 783$. All other parameters are set as in section 4.5.1 and 4.5.2. Figure 4.15(a) shows the variation of $v_m^{ave}$ with $U_{in}$. For both operations, $v_m^{ave}$ increases approximately 40% with increasing $U_{in}$. However, Figure 4.15(b) shows that the single-pass water recovery ($WR$) decreases, because the inlet flow rate increases faster than $v_m^{ave}$.

The increase in permeate flux with $U_{in}$ occurs due to a decrease in temperature and concentration polarization, which occurs due to the increase in the downstream advection of heat and solutes. Figure 4.16(a) shows the TPC for $U_{in} = 0.083$, 0.165, and 0.248 m/s. At mid-length ($x = L/2$), TPC increases 29% from 0.22 for $U_{in} = 0.083$ m/s to 0.28 for $U_{in} = 0.248$ m/s. Intuitively, we would expect the increase in vapor flux to cause an increase in concentration polarization, as observed in Figure 4.11, for example. Figure 4.16(b) shows, however, that the CPC decreases marginally with increasing $U_{in}$, despite the increase in vapor flux. The decrease likely occurs due to the increased downstream advection. We
conclude that the increase in permeate flux is due primarily to the decrease in temperature polarization.

Though permeate production increases with $U_{in}$, Figure 4.17(a) demonstrates that the GOR decreases by approximately 80%. Figure 4.17(b) shows that this occurs due to an increase in $Q_{in}$, which occurs due to a decrease in heat exchanger effectiveness, $\epsilon_{H_X}$, at higher flow rates. Consequently, the GOR could likely be improved by selecting a different heat exchanger tailored to operating at higher flow rates, i.e. an exchanger with a larger
4.5.6 Influence of channel length

To investigate the effects of channel length, we simulated co-current and counter-current operations for lengths $10 \leq L \leq 40$ cm, and $T_{m}^{f} = 90$ °C. All other parameters are set as in section 4.5.1 and 4.5.2. As expected, we found that increasing the length of a co-current operation simply extends the downstream decrease in permeate flux. Figure 4.18(a) and Figure 4.18(b) show the local vapor flux, $v_{m}(x)$, and average flux, $v_{m}^{ave}$, respectively, for $L = 10$, 20, 30, and 40 cm in counter-current operation. Vapor flux decreases with

downstream area. However, this is beyond the scope of our study.
increasing $L$, because longer systems have more heat exchange between the feed and distillate channels, which results in a smaller transmembrane temperature difference at a fixed $x$ location. Though $v_{m}^{ave}$ decreases with channel length, Figure 4.18(c) shows that the net permeate production per unit width, $L \cdot v_{m}^{ave}$, increases because longer channels provide larger heat and mass exchange areas.

Figure 4.18(d) shows the variation of GOR with $L$. For short channels, most of the recycling heat comes from the feed outlet, while for long channels, most of the recycling heat comes from the distillate outlet. We find that GOR increases with increasing $L$. This shows that in a DCMD system with heat recycling, long channels are systematically more efficient than short channels.

Figure 4.19(a) and Figure 4.19(b) show the downstream variation of TPC and CPC, respectively, with $L$ for counter-current operation. We find that temperature polarization increases with channel length. We also find that though the CPC decreases at a fixed $x$ location, $CPC_{max}$ increases with channel length. Note that the corresponding downstream variations of TPC and CPC with $L$ for co-current operation are provided in appendix 4.8.5.
4.5.7 Case study

We conclude by considering a case-study in which a counter-current system is tasked with treating an inlet concentration \( C_{in} = 300 \, \text{g/L} \) subject to a constant distillate inlet temperature \( T_{in}^d = 20 \, ^\circ\text{C} \) and channel length \( L = 17.78 \, \text{cm} \). The feed inlet temperature and mean velocity are varied between \( 40 \leq T_{in}^f \leq 80 \, ^\circ\text{C} \) and \( 0.165 \leq U_{in} \leq 0.413 \, \text{m/s} \), respectively. Though we demonstrate the procedure here for a NaCl solution, it could of course be repeated using the properties of a sparingly soluble salt. Figure 4.20 shows the resulting variation of the maximum concentration \( c_{max} \), average vapor flux \( v_{ave} \), water recovery \( WR \), and GOR. To aid the visualization of the four surfaces, we have plotted the temperature and velocity axes such that \( T_{in}^f \) and \( U_{in} \) increases in the leftward direction. Figure 4.20(a) shows that \( c_{max} \) increases dramatically with \( T_{in}^f \), but decreases only slightly with \( U_{in} \). In all panels, the region above the red solid line shows combinations of \( T_{in}^f \) and \( U_{in} \) for which \( c_{max} \) exceeds the saturation concentration, measured at the outlet membrane surface.

The solid line in Figure 4.21(a) shows the maximum feed inlet temperatures \( T_{in,\text{max}}^f \) that avoid supersaturation for different \( U_{in} \). As expected from our discussion in section 4.5.5, \( T_{in,\text{max}}^f \) increases only moderately with \( U_{in} \) due to the fact that concentration polarization is not sensitive to \( U_{in} \). However, the dashed line in Figure 4.21(a) shows that the corresponding maximum average vapor flux, \( v_{ave,\text{max}} \), increases substantially with \( U_{in} \) due to the fact that temperature polarization is sensitive to \( U_{in} \). As expected, the maximum flux occurs when the inlet velocity and feed inlet temperature are both maximized. This operating condition is marked as a solid dot symbol in panels (a)-(d) of Figure 4.20.

Figure 4.21(b) shows the maximum water recovery and GOR obtained by operating the system at \( T_{in,\text{max}}^f \) for different \( U_{in} \). We see that maximizing permeate production minimizes the single pass water recovery and GOR. This is due to the decrease in the heat and mass transfer efficiency of the DCMD module and heat exchangers with increasing \( U_{in} \). Consequently, water recovery and GOR are maximized by operating the system at the maximum allowable temperature corresponding to the minimum flow rate. This condition is marked
Figure 4.20: Variation of $c_{\text{max}}$ (a), $v_{\text{ave}}$ (b), WR (c), and GOR (d) with $T_{\text{in}}^f$ and $U_{\text{in}}$ for counter-current operation. The region above the red solid line shows operating conditions for which $c_{\text{max}}$ exceeds the saturation concentration measured at the outlet membrane surface, as a solid square symbol in panels (a)-(d) of Figure 4.20.

4.6 Conclusions

Consistent with Leveque [151] and De & Bhattachrya [148], we found that the temperature and concentration layer thicknesses follow 1/3 power laws with downstream distance. Contrary to these analyses, however, we found that the temperature and concentration vary considerably along the membrane surfaces, such that common Nusselt and Sherwood relationships do not accurately predict local membrane conditions, producing errors on the order of 100%. We conclude that such correlations will fail to predict the onset of mineral scaling.
The temperature boundary layers are relatively thick, covering up to 40% of the channel width. As expected, the transmembrane temperature difference $\Delta T_m(x)$ and vapor flux $v_m(x)$ in co-current operations decrease monotonically in the downstream direction. In counter-current operations, however, $\Delta T_m(x)$ and $v_m(x)$ vary non-monotonically. Furthermore, due to the non-linear dependence of vapor pressure on temperature and concentration, the local vapor flux is not necessarily maximized at the same location where $\Delta T_m$ is maximized. Temperature polarization and permeate production are also sensitive to the inlet velocity, such that we observed 40% increases in permeate production with increasing $U_{in}$.

We found that the concentration boundary layers are relatively thin, covering around 10% of the channel width near the feed outlet. Because the concentration layers are thin, the increase in concentration within them is dramatic, even for small permeate fluxes that are four orders-of-magnitude smaller than the feed velocity. Concentration polarization increases with feed inlet temperature and is also much stronger in counter-current operations, producing CPC coefficients above 1.6. Concentration polarization reduces the water activity $a_w$ and consequently reduces permeate production. For the parameters considered, we observed 50% decreases in permeate production with increasing $C_{in}$. Though temperature polarization decreases significantly with inlet flow rate $U_{in}$, concentration polarization de-

Figure 4.21: (a) Variation of $T_{in,max}^f$ (solid line) and corresponding $v_{ave,m, max}^m$ (dashed line) with $U_{in}$. (b) Corresponding variation of $WR_{max}$ (solid line) and $GOR_{max}$ (dashed line).
creases only marginally. Consequently, though increasing $U_{in}$ increases permeate production, it only marginally decreases the risk of mineral scaling for laminar flow regimes considered in this study.

To investigate system level performance, we computed the average vapor flux ($v_{ave}^m$), single pass water recovery ($WR$), maximum concentration polarization coefficient ($CPC_{max}$), and gained output ratio (GOR) of a DCMD system with heat recovery. We report the following conclusions. (1) Increasing the operating temperature difference $\Delta T_{in} = T_{in}^f - T_{in}^d$ increases $v_{ave}^m$, $WR$, and GOR, but also increases $CPC_{max}$ and the risk of mineral scaling. (2) Increasing the feed concentration reduces $v_{ave}^m$, $WR$, and GOR, but also reduces $CPC_{max}$. (3) Increasing the flow rate $U_{in}$ increases $v_{ave}^m$, but decreases both the $WR$ and GOR. (4) Longer systems have a smaller $v_{ave}^m$, but have a greater $WR$ and GOR. (5) Overall, counter-current systems produce slightly larger water recoveries, but are at significantly greater risk of mineral scaling. Their GOR is also often nearly indistinguishable from that for co-current systems. (6) We found that permeate production was maximized by maximizing both the feed inlet temperature and flow rate. In contrast, the water recovery and GOR are maximized by maximizing the feed inlet temperature while minimizing the flow rate.

Ongoing work is now focused on extending our analysis to three-dimensional flow effects, onset of turbulent mixing, and the effects of membrane spacers.

### 4.7 Acknowledgements

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### 4.8 Appendices

The appendices present supplemental materials for this paper.
4.8.1 Thermo-physical correlations for NaCl solution or water

Dynamic viscosity $\mu(T, c)$ of NaCl solution is evaluated as,

$$A_v(T) = 4.0912 \times 10^{-21} T^4 - 9.8135 \times 10^{-19} T^3 + 8.9878 \times 10^{-17} T^2$$
$$- 3.3743 \times 10^{-15} T + 2.5617 \times 10^{-14},$$

$$B_v(T) = -1.1551 \times 10^{-18} T^4 + 3.1028 \times 10^{-16} T^3 - 3.1776 \times 10^{-14} T^2$$
$$+ 1.2275 \times 10^{-12} T + 4.7647 \times 10^{-13},$$

$$C_v(T) = 6.6306 \times 10^{-16} T^4 - 1.6487 \times 10^{-13} T^3 + 1.5945 \times 10^{-11} T^2$$
$$- 6.9728 \times 10^{-10} T + 1.0827 \times 10^{-08},$$

$$D_v(T) = -8.3450 \times 10^{-14} T^4 + 1.8820 \times 10^{-11} T^3 - 1.5232 \times 10^{-09} T^2$$
$$+ 4.1167 \times 10^{-08} T + 1.0124 \times 10^{-06},$$

$$E_v(T) = 3.3922 \times 10^{-11} T^4 - 8.6874 \times 10^{-09} T^3 + 9.0999 \times 10^{-07} T^2$$
$$- 5.1893 \times 10^{-05} T + 1.7415 \times 10^{-03},$$

$$\mu(T, c) = A_v(T) c^4 + B_v(T) c^3 + C_v(T) c^2 + D_v(T) c + E_v(T).$$

Specific heat capacity $c_p(T, c)$ of NaCl solution is evaluated as,

$$A_h(T) = 3.2167 \times 10^{-08} T^2 - 9.1455 \times 10^{-06} T + 2.4487 \times 10^{-03},$$

$$B_h(T) = 2.2508 \times 10^{-05} T^2 - 2.2851 T \times 10^{-03} - 4.6391,$$

$$C_h(T) = -6.1128 \times 10^{-04} T^2 + 0.75986 T + 4129.8,$$

$$c_p(T, c) = A_h(T) c^2 + B_h(T) c + C_h(T).$$

Latent heat of water is evaluated as,

$$\lambda(T) = -2438.18 T + 2502800.$$

Thermal conductivity of NaCl solution is evaluated as [140],

$$k(T, c) = 0.5621 + 0.001997 T - 8.6 \times 10^{-6} T^2$$
$$+ (-0.01394 + 0.000294 T - 2.3 \times 10^{-6} T^2) m$$
$$+ (0.00177 - 6.3 \times 10^{-5} T + 4.5 \times 10^{-7} T^2) m^2, m = 0.01716 c.$$
Mass diffusivity of NaCl solution is evaluated as [141],

\[
\alpha = 0.02, \\
\lambda_{Na,25} = 50.11, \lambda_{Na} = \lambda_{Na,25}(1 + \alpha(T - 25)), \\
\lambda_{Cl,25} = 76.35, \lambda_{Cl} = \lambda_{Cl,25}(1 + \alpha(T - 25)), \\
D(T) = 17.872 \times 10^{-14}(T + 273.15) \frac{\lambda_{Na}\lambda_{Cl}}{\lambda_{Na} + \lambda_{Cl}}
\]

(4.25)

4.8.2 Numerical method

We discretize Navier-Stokes, heat, and concentration equations temporally using a second-order semi-implicit method in which the diffusive terms and nonlinear terms are discretized with the Crank-Nicolson and Adams-Bashforth methods, respectively. For example, the Navier-Stokes equation is discretized as

\[
\rho \frac{u^{n+1} - u^n}{dt} + \frac{3}{2}(u^n \cdot \nabla)u^n - \frac{1}{2}(u^{n-1} \cdot \nabla)u^{n-1} = \\
- \nabla p^{n+1} + \frac{\mu_{in}}{2} \left[ \nabla^2 u^n + \nabla^2 u^{n+1} \right] + \frac{3}{2} \nabla \cdot \left[ \tilde{\mu}(\nabla u^n + (\nabla u^n)^T) \right] \\
- \frac{1}{2} \nabla \cdot \left[ \tilde{\mu}(\nabla u^{n-1} + (\nabla u^{n-1})^T) \right],
\]

(4.26)

where \(dt\) is the time step, and the superscript denotes the field at the time \(t = n \cdot dt\). To account for temporal variations in diffusive coefficients, we decompose the viscosity, thermal conductivity, and mass diffusivity into sums of the form \(\mu = \mu_{in} + \tilde{\mu}(x, y, t)\), where \(\mu_{in}\) is the constant inlet value, and \(\tilde{\mu}(x, y, t)\) denotes the variation due to temperature and concentration. As demonstrated in equation (4.26), this allows us to discretize diffusive terms semi-implicitly.

Each time step consists of the sequential solutions of the advection-diffusion, heat, and Navier-Stokes equations. The pressure-velocity coupling is treated using the projection method of Choi and Moin [142]. All governing equations are discretized spatially using second-order finite volume methods in which diffusive terms are approximated using central differencing and advection terms are discretized using a total variation diminishing scheme.
Using the standard practice in CFD, we verify the temporal and spatial accuracies of our discretization with respect to the following artificial, but exact, analytical solution,

\[
\begin{align*}
T_e &= \cos(x) \cos(y) \cos(\omega t), \\
c_e &= \cos(x) \cos(y) \cos(\omega t), \\
u_e &= \cos(x) \sin(y) \cos(\omega t), \\
v_e &= -\sin(x) \cos(y) \cos(\omega t).
\end{align*}
\] (4.27)

Solution (4.27) satisfies the governing equations with the addition of appropriate forcing terms. The numerical solvers were tested in each channel separately, subject to general Robin boundary conditions of the form

\[
ag^{n+1} + b \nabla g^{n+1} \cdot \mathbf{s} = q
\] (4.28)

where \( g = [u, T, c] \), is the velocity, temperature, or concentration field, \( a \) and \( b \) are constant coefficients, \( \mathbf{s} \) is the normal to the boundary, and \( q \) is the appropriate boundary source terms determined from the exact solution (4.27).

To test the spatial accuracy of the method, we set \( \omega = 0 \), \( g^0 = 0 \) and integrate in time using \( N \) finite volumes in each direction (\( N^2 \) in total) until steady state, after which we evaluate the spatial error as \( E_N = ||g - g_e||_\infty \). Figure 4.22(a) demonstrates second-order
Figure 4.23: (a) The solid line shows the variation of relative error of $v$ component, $E_{Ny}$, with $Nx$ for co-current operation. (b) The solid line shows the variation of relative error of $v$ component, $E_{Nx}$, with $Ny$ for co-current operation.

spatial accuracy. To test temporal accuracy, we set $\omega=\pi$, $N=100$, and $g^0 = g^0_e$. The fields are integrated from $t=0$ to $t=1$ s for $0.02 \leq dt \leq 0.1$. Figure 4.22(b) confirms second-order temporal accuracy.

4.8.3 Grid independence study

We performed grid independence studies to determine the appropriate number of finite volumes in the $x$ and $y$ directions to ensure relative errors below 1 %. We set the system dimensions to those of our experimental system, $L = 17.78$ cm and $H = 3.175$ mm. We set the operating conditions to $T_{in}^f = 80$ °C, $T_{in}^i = 20$ °C, $C_{in} = 100$ g/L, and $U_{in} = 0.248$ m/s. We set the permeability to $B = 8.12 \times 10^{-7}$ kg/m s Pa and the effective heat transfer coefficient $k_m/\delta = 576.72$ W/m K. This represents a challenging set of operating conditions, such that we expect the results to be valid the range of parameters considered in our study. We first set the number of volumes in the $x$ direction to $N_x=64$, and varied the number of finite volumes in the $y$ direction between $32 \leq N_y \leq 512$. Taking the solution at $N_y=512$ as
the exact answer, we evaluate the relative error as

\[ E_{N_y} = \frac{||g_{N_y} - g_{512}||}{||g_{512}||}, \]  

(4.29)

where \( g_{N_y} = [u_{N_y}, T_{N_y}, c_{N_y}] \) is the solution evaluated at volume number \( N_y \), and \( g_{512} \) is the solution at \( N_y = 512 \).

Of the considered variables \( u, v, T, \) and \( c \), the largest relative error occurred in \( v \), because \( v \) is very small compared to \( u \). Figure 4.23(\( a \)) shows the variation of relative error of \( v \) component, \( E_{N_y} \), with varying grid number \( N_y \). We can see that \( E_{N_y} \) is smaller than 1% when \( N_y = 100 \). Similarly, we then fix \( N_y \) to 64, and vary \( N_x \) from 16 to 256. As observed in Figure 4.23(\( b \)), we find that \( E_{N_x} \) is less than 1% when \( N_x = 120 \).

Table 4.1: Grid number \( N_x \) and \( N_y \) that produce relative error within 1 % for co-current and counter-current operations

<table>
<thead>
<tr>
<th></th>
<th>( N_x )</th>
<th>( N_y )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co-current</td>
<td>120</td>
<td>100</td>
</tr>
<tr>
<td>Counter-current</td>
<td>160</td>
<td>120</td>
</tr>
</tbody>
</table>

We then conduct a similar analysis for counter-current operation, and the optimal grid number are found to be \( N_x = 160 \) and \( N_y = 120 \). The optimal grid sizes for both operations are organized in table (Table 4.1).

4.8.4 Self-similarity of the concentration boundary layer

Figure 4.24(\( a \)) shows concentration profiles at the downstream locations \( x = L/4 \) (\( \ast \)), \( L/2 \) (\( \triangle \)), \( 3L/4 \) (\( \square \)), \( L \) (\( \times \)). To measure the layer thickness, we define the non-dimensional concentration as

\[ \tilde{c} = \frac{c - C_{in}}{c_m(x) - C_{in}}. \]  

(4.30)

We then define the non-dimensional concentration boundary layer thickness \( \tilde{\delta}_c(x) \) as the location where

\[ \tilde{c}_{|y=\delta_c(x)} = 0.05. \]  

(4.31)
Figure 4.24: (a) Concentration profiles in feed channel at $x = L/4$, $x = L/2$, $x = 3L/4$ and $x = L$. (b) Self-similar behavior of concentration distributions (c) Variation of the concentration boundary layer thickness under logarithm coordinates.

Figure 4.25: (a) Downstream variation of $TPC$ with channel length $L = 10$ (solid), 20 (dashed), 30 (dash-dotted), and 40 (dotted) cm, co-current operation. (b) Downstream variation of $CPC$ with channel length $L = 10$ (solid), 20 (dashed), 30 (dash-dotted), and 40 (dotted) cm, co-current operation.

The four curves in Figure 4.24(a) collapse to a single curve in Figure 4.24(b) when we plot $\hat{c}$ as a function of $\eta_c = \hat{y}/\hat{\delta}_c$. Figure 4.24(c) shows that the downstream growth of $\hat{\delta}_c$ fits the power law relationship $\hat{\delta}_c = 0.024\hat{x}^{0.34}$. 

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4.8.5 Downstream variation of $TPC$ and $CPC$ with channel length for counter-current operation

Figure 4.25 shows the downstream variation of $TPC$ (panel $(a)$) and $CPC$ (panel $(b)$) with channel length for co-current operation. Note that the curves overlap and are indistinguishable. As expected, the $TPC$ decreases monotonically in the downstream direction, indicating increased temperature polarization. However, the $CPC$ is maximized near $x/H = 20$, after which the $CPC$ decreases with $x$ due to decreasing $v_m$. 
CHAPTER 5
COMPUTATIONAL FLUID DYNAMICS SIMULATIONS OF UNSTEADY MIXING IN SPACER-FILLED DIRECT CONTACT MEMBRANE DISTILLATION CHANNELS

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5.1 Abstract

Direct Contact Membrane Distillation (DCMD) has emerged as a promising means of concentrating brines to their saturation limit. During that process, membrane spacers play a key role in temperature polarization, concentration polarization, and mineral scaling. These interactions are not well understood, because they are difficult to study experimentally and numerically, and the flow regimes are not fully charted. We consequently develop a tailored in-house CFD code that simulates unsteady two-dimensional heat and mass transport in plate-and-frame DCMD systems with cylindrical spacers. The code uses an efficient combination of finite-volume methods in space, projection methods in time, and recent advances in immersed boundary methods for the spacer surfaces. Using the code, we explore how the transition from steady flow to unsteady laminar vortex shedding affects temperature polarization, concentration polarization, and thermal efficiency of DCMD systems. We show that the impact of spacers on polarization and system performance can be explained by examining the various steady and unsteady vortical flow structures generated in the bulk and near

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5.1 Sketch (not to scale) that demonstrates concentration and temperature polarization in a co-current DCMD system. Concentration polarization is shown by the solid dots.

the bounding plates and membranes. Overall, we show that though unsteady vortex structures tend to mix temperature polarization layers with the bulk, they are not similarly able to mix the thin concentration layers. Rather, vortical structures tend to create regions of preferential salt accumulation. In the vortex shedding regime, the net result is that spacers often increase vapor production at the expense of increasing the risk of mineral scaling.

keyword: Membrane Distillation, temperature polarization, concentration polarization, immersed boundary method, vortex shedding

5.2 Introduction

Membrane distillation has emerged as a promising means of concentrating waste brines to their saturation limit, after which they can be discharged to crystallizers or small evaporation ponds [8–19]. Though there are several modes of membrane distillation, such as vacuum and air gap membrane distillation, the current study focuses on direct contact membrane distillation (DCMD). With this approach, warm feed and cool distillate water flow on opposite sides of a hydrophobic microporous membrane in a co-current or counter-current manner, as sketched in Figure 5.1. The hydrophobic membrane creates vapor-liquid interfaces on the feed and distillate sides of the membrane. The temperature difference across the membrane causes volatile components (i.e. H$_2$O) to evaporate from the feed side of the membrane, travel through the vapor-filled pores, and condense on the distillate side of the membrane.
Non-volatile solutes remain in the feed. DCMD can treat hypersaline brines because it is insensitive to osmotic pressure and rejects 99-100% of salts. While reverse osmosis (RO) can treat NaCl solutions up to approximately 70 g/L, the limit for DCMD is approximately 300 g/L [21]. Furthermore, DCMD operates at feed temperatures below 90 °C that are readily produced by renewable energy.

Temperature and concentration polarization are two crucial factors that affect DCMD treatment of hypersaline brines [9, 69]. Temperature polarization is the reduction in the transmembrane temperature difference due to heat transfer through the membrane, as illustrated in Figure 5.1. Concentration polarization is the accumulation of solutes adjacent to the feed side of the membrane, a phenomena occurring in nearly all membrane processes. Both polarization phenomena reduce the transmembrane vapor flux by reducing the transmembrane partial vapor pressure difference. Concentration polarization is also responsible for mineral scaling, which occurs when the concentration at the membrane surface exceeds the saturation limit of a solute. This blocks the membrane and can lead to pore wetting and permanent membrane damage.

Temperature and concentration polarization are further complicated by spacers, a mesh-like material that separates and supports tightly packed membrane sheets, as illustrated in Figure 5.2(a). Thinner spacers increase the membrane surface area that can be packed in a system volume, but at the expense of increasing the channel pressure drop (and pumping costs) required to drive the feed and distillate flows. Spacers also generate three-dimensional
flow structures that influence polarization and create regions of preferential solute accumulation and precipitation. Though this influence is documented for RO [51–57], there is less work on scaling in DCMD systems. Literature suggests that solute accumulation tends to occur near what are referred to as “stagnant” or “dead” zones [58–62]. The same is also said of biofouling. The definitions of “stagnant” or “dead” are not always precise, but they tend to refer to locations on the membrane surface where the flow velocity is low or mixing is weak [59, 60, 62–64]. These zones often form near spacers, particularly the contact points where spacers meet the membrane surface [59, 60, 63]. This is demonstrated in Figure 5.2(b), which shows a membrane that experienced scaling in a high-recovery RO system operated by Desalitech. An autopsy indeed suggested that the scaling occurred near contact points (personal communication).

There is potential to increase the water recovery, energy efficiency, and membrane life of DCMD systems by designing spacers that strike a balance between maximizing membrane packing while minimizing the downstream pressure drop, polarization, and scaling. Designing such spacers is complicated by the coupled heat and mass transport in the feed, membrane, and distillate. These coupled processes are not fully understood, particularly when interactions between polarization and spacers are important. Because these interactions are difficult to observe experimentally [61, 153, 154], computational fluid dynamics (CFD) offers a valuable complement because it predicts the full temperature, concentration, and velocity fields [23–50].

CFD studies have made important contributions to understanding the effects of spacers on heat and mass transport in membrane processes. Reviews can be found in references [22, 65–67]. Our review finds three persistent challenges. The first is the simulation of near-membrane transport, which is difficult even in the absence of spacers. For pressure-driven processes such as RO, the dependence of the transmembrane flow on the pressure field causes traditional CFD methods to lose accuracy [68]. For DCMD, the accurate prediction of polarization requires the simultaneous simulation of the coupled feed channel, membrane,
and distillate channel flows [69]. Due in part to these complications, studies of spacers sometimes neglect the membrane altogether [70–84]. Such studies focus on the effects of spacers on the downstream pressure drop and near-membrane shear stress, for which the small transmembrane flow likely has a minimal role. Nevertheless, one could argue that this assumption needs validation, because spacers generate hydrodynamic instabilities, and instabilities can be surprisingly sensitive to small velocity components [85].

A second challenge arises because the flow regime in spacer-filled channels is not fully understood. Though spacers are often called “turbulence promoters,” it is not clear whether membrane systems actually operate in turbulent regimes. RO and DCMD systems typically operate with cross-flow Reynolds numbers in the range of $Re \leq 1000$, where $Re = \frac{U_{in}H}{\nu}$ is defined using the mean feed inlet velocity $U_{in}$ and feed channel height $H$ (see Figure 5.3). In this range, experiments [34, 67, 84, 86, 87] and simulations [34, 35, 67, 79–84, 86–94] suggest that the flow is steady at low Reynolds numbers, and transitions to unsteady laminar vortex shedding at higher Reynolds number. These studies show that the critical Reynolds number $Re_c$ for transition to vortex shedding varies between roughly $70 \leq Re_c \leq 500$, depending on the spacer geometry [34, 67, 79, 81, 82, 84, 86, 91–93]. Studies suggest that vortex shedding reduces polarization and scaling by increasing shear stress near the membrane and directing bulk fluid towards the membrane surface [34, 88–92]. Comparatively little work exists on the transition to turbulence [35, 77, 78, 84], and studies sometimes assume turbulent flow by incorporating Reynolds-averaged models [35, 77, 78].

A third challenge arises because CFD studies typically rely on software that simulate spacers using body-fitted grids. Such grids are time-consuming to generate and limit the number of simulations that can be reasonably performed. A similar situation is faced in the CFD community simulating porous media [95, 96]. In that case, the state-of-the-art has turned to Immersed Boundary Methods (IBM) [97] that use a simple Cartesian grid, with grid points located in both the fluid and solid regions. Solid surfaces are then modeled by introducing a body force in the governing equations to force the fluid velocity to zero in
the solid. Depending on the implementation, this achieves the same order-of-accuracy as body-fitted grids.

In the current study, we investigate how transition from steady flow to unsteady laminar vortex shedding affects polarization in DCMD systems. For that purpose, we develop a 2-D CFD code that solves the Navier-Stokes, continuity, advection-diffusion, and heat equations using a finite-volume method in space and an efficient projection method in time. To investigate the influence of vortex shedding, we consider idealized 2-D spacer filaments, as illustrated in Figure 5.3. The spacers are simulated using recent advances in IBM. Though spacers are inherently 3-D, we focus on idealized 2-D spacers because their hydrodynamic stability is much better understood in the fluid mechanics literature [98], and their simplicity allows us to perform a comprehensive parametric study and identify fundamental transport phenomena. It is our philosophy that elucidating such phenomena is prerequisite to intelligently designing 3-D spacers. Finally, though beyond the scope of the current study, 2-D spacers are more amenable to quantitative experimental study, which is the topic of ongoing work in our group. Considering the various spacer geometries encountered in industry and literature [61], our geometry is closest to ladder-type spacers with filaments perpendicular to the downstream flow direction [61, 99, 100].

The remainder of this study is organized as follows. Section 5.3 presents the system geometry, governing equations, and boundary conditions. Section 5.4 summarizes the numerical methods and code validation. Section 5.5 discusses the impact of the Reynolds number, spacer diameter, and spacer vertical location on polarization and system performance. Section 5.6 presents our conclusions.

5.3 Geometry and governing equations

We consider a plate-and-frame DCMD system with feed and distillate channels of length $L$ and height $H$, as illustrated in Figure 5.3. Both channels have an idealized cylindrical spacer of diameter $D_{sp}$, centered at $x = L/2$ and a distance $y_c$ from the membrane. NaCl solution enters the feed channel with temperature $T_{in}^f$, concentration $C_{in}$, and mean velocity
Figure 5.3: Sketch (not to scale) of the 2-D DCMD flow channels considered in this study. Each channel has a length $L$ and height $H$. The membrane is shaded gray. Both channels have a cylindrical spacer filament centered at $x = L/2$ and $y = \pm y_c$. NaCl solution enters the feed channel with temperature $T_{in}^f$, concentration $C_{in}$, and mean velocity $U_{in}$. Pure water enters the distillate channel with temperature $T_{in}^d$ and mean velocity $U_{in}$.

We focus on counter-current operation because it is preferred in the literature. Though Figure 5.3 shows the membrane as a shaded region about $y = 0$, we model transmembrane heat and mass transport using effective interface conditions that couple the feed ($0 \leq y \leq H$) and distillate ($-H \leq y \leq 0$) channels. We set $H = 2$ mm, which is typical of DCMD systems. We set $L = 2$ cm, which was found to sufficiently minimize the impact of outlet conditions on upstream flow.

5.3.1 Transmembrane heat and mass transport

We model heat and mass transport through the membrane as previously described in Lou et al. [69]. We only highlight the key features here. As in most previous literature, we assume that the transmembrane mass flux, $j_v$, is linearly proportional to the transmembrane vapor pressure difference [20],

$$j_v = -B(p_{m}^f - p_{m}^d), \quad (5.1)$$

where $B$ is the vapor permeability and $p_{m}^f$ and $p_{m}^d$ are the local partial vapor pressures on the feed and distillate membrane surfaces, respectively. These pressures are functions of the
local temperature and concentration at the membrane surface [101], and are evaluated as the product of the saturation pressure $P^{\text{sat}}$ and water activity $a_w$,

$$ p_m = a_w P^{\text{sat}}, \quad P^{\text{sat}} = \exp \left( 23.238 - \frac{3841}{T_m + 228.15} \right), \quad (5.2) $$

where $P^{\text{sat}}$ is determined using the Antoine equation [102], and $T_m$ is the local temperature on the membrane surface. The activity is determined from the expression $a_w = 1 - 0.03112b - 0.001482b^2$ [22], where $b$ is the NaCl molality (mol/kg). This expression is valid from zero salinity to saturation [22]. We assume complete salt rejection, such that $a_w = 1$ in the distillate.

As in most previous literature, we model transmembrane heat conduction as

$$ q_c = -\frac{k_m}{\delta} (T^f_m - T^d_m), \quad (5.3) $$

where $\delta$ and $k_m$ are the membrane thickness and thermal conductivity, respectively, and $T^f_m$ and $T^d_m$ are the temperatures on the feed and distillate membrane surfaces, respectively. Conservation of energy for liquid-vapor interfaces with phase change (see Leal [104]) requires that on the membrane feed surface, conductive heat transport within the liquid phase must equal

$$ -k \frac{\partial T^f_m}{\partial y} \bigg|_{y=0^+} = j_v \lambda - \frac{k_m}{\delta} (T^f_m - T^d_m) \quad (5.4) $$

where $\lambda$ is the latent heat per unit mass, and the “$+$” superscript signifies that the derivative is evaluated from the feed side of the membrane. We set $\lambda$ to

$$ \lambda = (\lambda^f_m + \lambda^d_m)/2, \quad (5.5) $$

where $\lambda^f_m$ and $\lambda^d_m$ are evaluated using the feed and distillate conditions, respectively. Similar conditions are applied on the distillate surface. Finally, total salt rejection requires the summation of advective and conductive salt flux on the feed side of the membrane to be zero,

$$ \frac{j_v c_m}{\rho} - D \frac{\partial c}{\partial y} \bigg|_{y=0^+} = 0, \quad (5.6) $$
where $c_m$ is the salt concentration on the feed side of the membrane, and $D$ is the effective mass diffusivity.

Consistent with much MD literature, we approximate the vapor permeability $B$ as a constant membrane property, and the ratio $k_m/\delta$ as an effective heat transfer coefficient. Hereinafter, we set these to $B = 1.87 \times 10^{-6}$ kg/m$^2$ s Pa and $k_m/\delta = 576.72$ W/m$^2$ K. These were determined experimentally in Lou et al. [69] for a 0.2 m pore size polypropylene 3M membrane.

5.3.2 Transport in the feed and distillate channels

The channel flows are governed by the incompressible continuity and Navier-Stokes equations for Newtonian fluids,

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \mu \nabla^2 \mathbf{u},$$

where $\mathbf{u} = [u \ v]$, $p$, $\rho$ and $\mu$ are the fluid velocity vector, pressure, density, and dynamic viscosity, respectively. Within each channel, we neglect variations in density with temperature and concentration, because the maximum variation of density is typically within 3%. In each channel, we set the density to the inlet value. Heat and solute transport in the flow channels are governed by the thermal energy and advection-diffusion equation,

$$\rho c_p \left[ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right] = k \nabla^2 T,$$

$$\frac{\partial c}{\partial t} + (\mathbf{u} \cdot \nabla)c = D \nabla^2 c,$$

where $c_p$ is the fluid heat capacity [105]. As shown in appendix 5.8.1, the variation of thermo-physical properties with temperature and concentration has only a small impact on the numerical results (approximately 4% or less) for the system lengths considered in the current study. We consequently neglect these variations, because including them substantially increases the computational time. In each channel, we set the thermo-physical properties to
those evaluated at the inlet conditions.

At the plates \((y = \pm H)\) and spacer surfaces, we apply the no-slip, no-penetration, and no-flux conditions, \(u = v = \nabla c \cdot n = \nabla T \cdot n = 0\), where \(n\) is the normal vector. On the membrane surfaces, we apply the no-slip condition, \(u = 0\), and the following conditions determined from the models discussed in section 5.3.1. The feed side conditions are,

\[
v = \frac{j_v}{\rho f}, \quad -k \frac{\partial T}{\partial y} \bigg|_{y=0^+} + \frac{k_m}{\delta} T_{m}^f = j_v \lambda + \frac{k_m}{\delta} T_{m}, \quad vc_m - D \frac{\partial c}{\partial y} \bigg|_{y=0^+} = 0, \quad (5.11)
\]

and the distillate side conditions are,

\[
v = \frac{j_v}{\rho f}, \quad -k \frac{\partial T}{\partial y} \bigg|_{y=0^-} - \frac{k_m}{\delta} T_{m}^d = j_v \lambda - \frac{k_m}{\delta} T_{m}^d. \quad (5.12)
\]

At the channel inlets, we apply uniform temperature and concentration, and fully developed laminar velocity profiles with desired mean velocity \(U_{in}\),

\[
u = 6U_{in} \left[ \frac{y}{H} - \frac{y^2}{H^2} \right], \quad v = 0, \quad T = T_{in}, \quad c = C_{in}. \quad (5.13)
\]

For all cases, the feed and distillate channels have identical mean inlet velocities, \(U_{in}\). At the channel outlets, we apply convective conditions \([107, 108]\),

\[
\frac{\partial g}{\partial t} + U_{in} \frac{\partial g}{\partial x} = 0,
\]

where \(g = [u, T, c]\), is the velocity, temperature and concentration field.

### 5.4 Methodology

We solve Eqns. (5.7)–(5.10) using the numerical methods previously described and validated in Lou et al. [69]. The simulation of the spacer surfaces uses an immersed boundary method similar to that of Fadlun et al. [123]. Details and benchmarking are provided in appendix 5.8.1.

We set the initial flow fields to the inlet conditions, and integrate in time until the fields reach a steady-state or transition to vortex shedding. In the latter case, the simulation is run sufficiently long to minimize transient effects from the initial start-up. For the Reynolds
numbers considered, we found that all simulations produce laminar flows.

5.4.1 Measure of critical Reynolds number and Strouhal number

Transition to vortex shedding depends on the size and location of the spacer filaments. For that purpose, we define the blockage ratio \( \beta = D_{sp}/H \) and non-dimensional offset \( \hat{y}_c = y_c/H \). We define the Reynolds number \( Re = U_{in}H/\nu \), where \( \nu \) is the kinematic viscosity. The feed and distillate channels have different Reynolds numbers, because \( \nu \) in each channel is evaluated using the channel’s inlet temperature and concentration. To compute the critical Reynolds numbers \( Re_c \) for transition to vortex shedding, we perform simulations to determine a pair of Reynolds numbers \( Re_1 \) and \( Re_2 \), for which \( Re_2 - Re_1 \leq 2 \), and for which the flow is steady at \( Re_1 \) and unsteady at \( Re_2 \). We then set \( Re_c = (Re_1 + Re_2)/2 \). For cases with vortex shedding, we compute the shedding frequency by measuring the velocity \( u \) in time at \( x = 3L/5 \) and \( y = H/2 \) (downstream of the feed spacer). We then perform a Fourier transform to extract the dominant frequency \( f \), and define the Strouhal number \( St = f_0H/U_{in} \).

Table 5.1: For the blockage ratios shown in column 1, columns 2 and 3 show our computed critical Reynolds numbers \( Re_c \) and Strouhal numbers \( St_c \) for the feed channel of a DCMD system with \( \hat{y}_c = 0.5 \), \( T_{in}^f = 80 \, ^{\circ}C \), \( T_{in}^d = 20 \, ^{\circ}C \) and \( C_{in} = 100 \, g/L \). Columns 4 and 5 show the corresponding predictions of Sahin and Owens [111] for a cylinder in a channel with two impermeable walls.

<table>
<thead>
<tr>
<th>( \beta )</th>
<th>DCMD system</th>
<th>Sahin and Owens</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( Re_c )</td>
<td>( St_c )</td>
</tr>
<tr>
<td>0.3</td>
<td>213.0±1.0</td>
<td>1.0429±0.01</td>
</tr>
<tr>
<td>0.5</td>
<td>166.0±1.0</td>
<td>1.0193±0.01</td>
</tr>
<tr>
<td>0.7</td>
<td>106.0±1.0</td>
<td>1.0076±0.01</td>
</tr>
</tbody>
</table>

Our code was previously validated without spacers in reference [69]. We validate our simulation of spacers by comparing with a theoretical analysis performed by Sahin and Owens [111] of vortex shedding over a cylinder placed on the centerline of a channel with two impermeable walls. Table Table 5.1 summarizes our computed \( Re_c \) and \( St_c \) for the feed channel of a DCMD system with blockage ratios \( \beta = 0.3, 0.5, \) and \( 0.7 \). The spacers are
placed in the middle of the channels \((\hat{y}_c = 0.5)\). Columns 2 and 3 present the results for the DCMD system when we set the operating temperatures and concentration to \(T_{in}^f = 80 ^\circ C\), \(T_{in}^d = 20 ^\circ C\), and \(C_{in} = 100 \text{ g/L}\), respectively. Columns 4 and 5 show there is excellent agreement (within 1 \% relative difference) with the corresponding theoretical predictions of Sahin and Owens [111]. We conclude that the membrane-normal velocity component has a negligible effect on transition to vortex shedding for the cases in Table Table 5.1.

5.4.2 System performance criteria

We investigate the system-level performance of DCMD systems by computing the transmembrane thermal efficiency [114],

\[
\eta = \frac{q_v^{net}}{q_v^{net} + q_c^{net}} = \frac{\int_0^L j_v \lambda dx}{\int_0^L j_v \lambda dx + \int_0^L \frac{k_m}{\delta} (T_{in}^f - T_{in}^d) dx},
\]

where \(q_v^{net}\) is the net latent heat flux, and \(q_c^{net}\) is the net conductive heat flux. The definition of \(\eta\) quantifies the fraction of total heat transport across the membrane that contributes to water evaporation. It does not account for the fact that some of the energy spent heating the feed exits the system at the feed outlet. Though we explored the computation of a gained output ratio, we found that for our small system lengths, the physical relevance of the results were unclear. They are consequently not reported.

We compute the pressure drop in the feed channel as,

\[
\Delta P/L = \frac{P_{in} - P_{out}}{L},
\]

where \(P_{in}\) and \(P_{out}\) are the area-averaged feed pressures at the channel inlet and outlet. In the vortex shedding regime, we average \(\Delta P/L\) in time. We characterize concentration polarization using a concentration polarization coefficient,

\[
\text{CPC}(x) = \frac{c_m(x)}{C_{in}},
\]

where CPC = 1 denotes no concentration polarization, and CPC \(\gg 1\) indicates strong polarization. We denote the maximum CPC as CPC\(_{max}\).
5.5 Results

We investigate the effects of spacers on flow regime and polarization by performing a parametric study in which we fix the operating temperatures $T_{f}^{i} = 80 \degree C$, $T_{d}^{i} = 20 \degree C$, and feed concentration $C_{in} = 100 \text{g/L}$, which are realistic conditions for DCMD. In the following sections, we systematically vary $U_{in}$, $D_{sp}$, and $y_{c}$ to investigate the effects of the Reynolds number and spacer geometry.

5.5.1 Influence of Reynolds number

We investigate the effects of the Reynolds number by considering spacers positioned on the channel centerline ($\hat{y}_{c} = 0.5$), blocking 50% of the channel ($\beta = 0.5$). We then vary the inlet velocity between $1.06 \times 10^{-2} < U_{in} < 6.34 \times 10^{-2} \text{ m/s}$. This varies the feed and distillate Reynolds numbers between $50 < Re_{f} < 300$ and $42 < Re_{d} < 126$. To demonstrate the impact on the flow regime, the left column of Figure 5.4 shows instantaneous streamlines downstream of the feed spacer for $Re_{f} = 50$ (a and b), 150 (c and d), 200 (e and f), and 300 (g and h), when $\beta = 0.5$ and $\hat{y}_{c} = 0.5$.

![Figure 5.4: Streamlines (left column) and vorticity field (right column) downstream of the feed spacer for $Re_{f} = 50$ (a and b), 150 (c and d), 200 (e and f), and 300 (g and h), when $\beta = 0.5$ and $\hat{y}_{c} = 0.5$.](image_url)

We investigate the effects of the Reynolds number by considering spacers positioned on the channel centerline ($\hat{y}_{c} = 0.5$), blocking 50% of the channel ($\beta = 0.5$). We then vary the inlet velocity between $1.06 \times 10^{-2} < U_{in} < 6.34 \times 10^{-2} \text{ m/s}$. This varies the feed and distillate Reynolds numbers between $50 < Re_{f} < 300$ and $42 < Re_{d} < 126$. To demonstrate the impact on the flow regime, the left column of Figure 5.4 shows instantaneous streamlines downstream of the feed spacer for $Re_{f} = 50$ (a), 150 (c), 200 (e), and 300 (g), respectively. The axes are
non-dimensionalized as $x/H$ and $y/H$. The right column shows the corresponding vorticity fields $\Omega = \partial v/\partial x - \partial u/\partial y$. Note that vorticity is a measure of fluid rotation generated by viscous effects. Consistent with $Re_c = 166$ reported in Table 5.1, panels (a) and (c) show steady regimes with counter-rotating vortices in the cylinder wakes. We observe that the downstream length of the wakes grows with Reynolds number. Panels (e) and (g) show that for supercritical Reynolds numbers ($Re > Re_c$), the flows are strongly unsteady, and exhibit two types of vortical flow structures. First, the vortices in the wake are periodically shed from the cylinder and advected downstream in the bulk. This generates a procession of staggered vortex structures, akin to the von Kármán vortex street. These structures are more clearly observable in the vorticity fields than the streamlines. Second, we observe that vortical structures with closed streamlines periodically form and travel downstream along both the outer plate and membrane surface. These structures are more clearly observable in the streamlines. The strength and number of these vortices increase with Reynolds number. We refer to the vortices on the outer plates as “plate-vortices,” and those on the membrane as “membrane-vortices”.

Figure 5.5 shows our results for a full DCMD system operated at $U_{in} = 2.11 \times 10^{-2}$ m/s, for which $Re_f = 100$ and $Re_d = 42$. The streamlines in panel (a) show that both the feed and distillate channels are steady. The wake is larger in the feed channel, because the feed Reynolds number is larger than in the distillate. Panel (b) shows a color plot of the temperature field. We use different color scales for the distillate and feed channels to highlight cooling of the feed and heating of the distillate. Focusing on the feed channel, we observe that the fluid temperature remains constant, except in a thermal boundary layer adjacent to the membrane surface. The thermal boundary layer thickness grows with downstream distance from the inlet, until it approaches the leading edge of the spacer. From the streamlines in panel (a), it is evident that the upstream cylinder surface acts as a converging nozzle, i.e. it decreases the cross-sectional flow area, accelerates the feed, and redirects warm fluid from the channel center toward the membrane surface. This decreases the boundary layer
thickness as feed flows around the cylinder, after which the boundary layer relaxes and continues to grow in the remaining downstream feed channel. Similar behavior is observed in the distillate channel, with the downstream distance pointing in the negative $x$-direction.

Overall, the thermal layers are relatively thick, covering nearly 50% of the channel widths at the outlets. Panel (c) shows the concentration field near the membrane, $0 < y/H < 0.2$. The concentration of the feed channel is constant, except in a thin concentration boundary layer at the membrane surface. This layer is much thinner than the thermal layer because the Lewis number in the feed channel is $Le = \alpha/D = 42$. As observed for the thermal layer, the concentration layer grows with downstream distance, except in a region near the upstream half of the cylinder, where the cylinder redirects lower-concentration feed flow towards the membrane surface. For comparison, appendix 5.8.3 shows corresponding results from a simulation without spacers.
Figure 5.6: The solid lines show the downstream variation of (a) the thermal boundary layer thickness $\hat{\delta}_T$, (b) the concentration boundary layer thickness $\hat{\delta}_c$, and (c) the feed membrane surface shear stress $\tau_m = \mu \partial u / \partial y$. The dashed lines show the corresponding results without spacers.

Figure 5.6 shows the downstream variation of the thermal boundary layer thickness $\hat{\delta}_T$ (panel (a)) and the concentration boundary thickness $\hat{\delta}_c$ (panel (b)) measured in the feed channel. The definitions of the boundary layer thicknesses follow that of Lou et al. [69], as detailed in appendix 5.8.4. The hat symbol denotes that $\hat{\delta}_T$ and $\hat{\delta}_c$ are non-dimensionalized with respect to $H$. The solid line in panel (c) shows the downstream variation of the shear stress on the feed side of the membrane $\tau_m = \mu \partial u / \partial y$. In all panels of Figure 5.6, the dashed lines show the corresponding results when the simulation is run without spacers. Consistent with our discussion of Figure 5.5, the boundary layer thicknesses decrease from those observed without spacers. We also see a sharp increase in the membrane shear stress. However, the influence of the spacer is limited to a region extending roughly two cylinder diameters up and downstream from the cylinder center.
Figure 5.7: Solid lines show (a) the transmembrane temperature difference $\Delta T_m$, (b) the membrane surface concentration $c_m$, and (c) the transmembrane vapor flux $v_m$ for the simulation with spacers. Dashed lines show corresponding results for simulation without spacers. The transmembrane vapor flux in panel (c) is shown in units of both LMH (Lm$^{-2}$/hr$^{-1}$) and m/s.

The solid lines in Fig. 5.7 show the transmembrane temperature difference $\Delta T_m$ (a), transmembrane vapor flux $v_m$ (b), and membrane surface concentration $c_m$ (c) for the simulation with spacers. Note that we define $v_m = |j_v|/\rho_f$, i.e. the local transmembrane vapor flux is defined using the feed density, and is a positive quantity. The dashed lines show corresponding results without spacers. In a region roughly two diameters up and downstream from the cylinder center, redirection of the bulk flows towards the membrane surfaces increases $\Delta T_m$. Panel (b) shows that this increases the local transmembrane vapor flux. Counterintuitively, however, panel (c) shows that the increase in $v_m$ does not produce an increase in $c_m$. Rather, we see a decrease in $c_m$. This is because the reduced boundary layer thickness $\delta_c$ creates a steeper concentration gradient $\partial c/\partial y$ that increases back diffusion of solutes away from the membrane surface. Outside the near-cylinder region, the cylinder has
Figure 5.8: Results when $Re_f = 300$. (a) Streamlines. (b) Vorticity field. (c) Temperature field, using different color scales in the distillate and feed channels. (d) Concentration field for $0 < y/H < 0.2$.

Minimal impact. Overall, the spacers decrease temperature and concentration polarization, and produce an average transmembrane vapor flux of 43.9 LMH ($1.22 \times 10^{-5} \text{ m/s}$), compared to 39.6 LMH ($1.10 \times 10^{-5} \text{ m/s}$) without spacers, an increase of 11.3%. Note that the short length ($L = 2 \text{ cm}$) of the simulated system produces higher average vapor flux values than typically observed in larger bench or pilot-scale systems.

Figure 5.8 shows snapshots of the instantaneous streamlines (a), vorticity field (b), temperature field (c), and concentration field (d) when we increase the inlet velocity to $U_{in}$.
Figure 5.9: Instantaneous streamlines superimposed on the temperature (panel a) and concentration (panel b) fields in the vicinity of the leading membrane-vortex nearest the cylinder. Panel (c) is a sketch demonstrating how converging streamlines at the leading edge of the membrane-vortex tend to eject cool fluid into the bulk.

\[ \dot{m} = 6.34 \times 10^{-2} \, \text{m/s}, \text{ producing } Re_f = 300 \text{ and } Re_d = 126. \] The feed flow is now strongly supercritical, while the distillate flow remains steady. The streamlines show the presence of at least 3 membrane-vortices near \( x/H = 6.5, 8, \) and 9. Panel (b) shows that in addition to the vorticity generated on the cylinder surface, considerable vorticity is generated on the plate and membrane around \( x/H = 5 \), where the cross-sectional flow area is minimized due to the spacer. Downstream from the cylinder, this vorticity separates from the plate and membrane, and interacts with the vortical structures in the bulk. In panel (c), we find that unsteady flow in the feed channel strongly mixes the thermal boundary layer with the bulk flow. However, panel (d) shows that the concentration layer is not similarly mixed, likely because it is much thinner than the thermal layer.

Closer inspection suggests that the membrane-vortices play an important role in temperature and concentration polarization. This is demonstrated in Figure 5.9, which shows instantaneous streamlines superimposed on the temperature (panel a) and concentration (panel b and c) fields in the vicinity of the membrane-vortex nearest the cylinder. Panel (a)
suggestions that the leading edge of the vortex ejects cool fluid from near the membrane into the bulk flow. The concentration plots in panels (b) and (c) suggests that the vortex does not similarly eject high concentration fluid into the bulk flow. Panel (c) shows that the reverse flow beneath the vortex advects salt upstream, accumulating salt near the leading edge of the vortex. Indeed, throughout this study, our simulations consistently show that solutes tend to accumulate near the leading edge of membrane-vortices, whether these vortices are steady or traveling along the membrane.

Figure 5.10 shows sequential snapshots of the streamlines in the downstream feed channel. Membrane-vortices periodically form at multiple downstream locations, initially growing as they travel downstream, before dissipating. The first vortex forms near $x/H = 6.1$, and dissipates near $x/H = 6.7$. Though not shown, for brevity, our inspection of the pressure field suggests that the leading membrane-vortex forms due to an adverse pressure gradient,
Figure 5.11: The solid lines in (a), (b), and (c) show the $\Delta T_m$, the $c_m$, and the $v_m$ for simulation with spacers operated when $Re_f = 300$, respectively. The dashed lines show the results for the simulation without spacers.

$\partial p/\partial x > 0$, in the downstream region of the feed spacer. This adverse gradient occurs due to the rapid expansion of cross-sectional flow area over the rear surface of the spacer. Additional adverse gradients occur along the downstream membrane surface, due likely to interactions between the membrane and overlying vortical structures in the bulk flow.

The solid lines in Figure 5.11 show $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) for the simulation with spacers when $Re_f = 300$. The dashed lines show corresponding results without spacers. We begin by stressing that though the bulk flow is strongly unsteady, the results for $\Delta T_m$, $c_m$, and $v_m$ in Figure 5.11 are all essentially steady, showing negligible variations in time. We offer a physical explanation for this behavior in appendix 5.8.5. Specifically, we perform an order-of-magnitude analysis that suggests the dominant mechanisms for heat and salt transport near the membrane surface have much longer characteristic time-scales compared to the period of vortex shedding.
Figure 5.11(a) shows that the cylinder increases $\Delta T_m$, not only near the cylinder, but also in the far downstream region. Figure 5.11(b) shows that though $c_m$ is reduced near the cylinder, it increases in the downstream region $x/H > 6$. The increase in $c_m$ in the far-downstream region is likely due to the increased transmembrane flow $v_m$ in that region. We also observe a localized region of salt accumulation near $x/H = 6.2$, where $c_m$ reaches a local maximum of 153 g/L. This is consistent with our observation in Figure 5.9 (b). Though literature often attributes mineral scaling to “stagnant” or “dead” zones associated with contact points between the spacer and membrane, our results show that spacers can create regions of salt accumulation without actually contacting the membrane. Moreover, the fluid structures causing salt accumulation are the same structures that effectively mix the temperature field. Overall, the simulation at $Re_f = 300$ produces an average transmembrane vapor flux of 63.0 LMH ($1.75 \times 10^{-5}$ m/s) with spacers, compared to 54.0 LMH ($1.50 \times 10^{-5}$ m/s) without, an increase of 16.5 %.

The squares ($\Box$) in Figure 5.12 show the variation of the average vapor flux $\dot{m}_{ave}$ (a), thermal efficiency $\eta$ (b), feed pressure drop $\Delta P/L$ (c), and maximum concentration polarization coefficient $CPC_{max}$ (d) with $Re_f$. The triangles ($\triangle$) show the corresponding results without spacers. The dashed lines show the relative change (secondary y-axis) between cases with and without spacers. The supercritical regime ($Re_f > Re_c$) is shaded gray. Panel (a) shows that simulations with spacers produce more vapor flux than those without, particularly at supercritical Reynolds numbers. In panel (b), the cases with spacers produce only slightly higher $\eta$ than those without. This is because although spacers increase the permeate production and transmembrane latent heat transfer, the decrease in temperature polarization also increases the transmembrane conductive heat transfer. Panel (c) shows that though spacers increase vapor production and thermal efficiency, this comes at the expense of much larger pressure drops, and consequently pumping costs. At $Re_f = 300$, the system with a spacer requires 4 times the pressure drop in a system without. In panel (d), we find that transition to vortex shedding causes a sudden increase in $CPC_{max}$. In the steady regime,
Figure 5.12: Impact of the Reynolds number on system-level performance when $\beta = 0.5$ and $\hat{y}_c = 0.5$. The squares (□) show the variation of the average vapor flux $v_{\text{ave}}$ (a), thermal efficiency $\eta$ (b), feed pressure drop $\Delta P/L$ (c), and maximum concentration polarization coefficient $\text{CPC}_{\text{max}}$ (d) with $Re_f$. The triangles (△) show corresponding results without spacers. The dashed lines shows the relative change (right axis) between cases with and without spacers. The supercritical regime ($Re_f > Re_c$) is shaded gray in the plots.

$\text{CPC}_{\text{max}}$ of the cases with spacers decreases with increasing $Re_f$, and is less than that observed in systems without spacers. This is explained by our results in Figure 5.7(b), where we observed that the acceleration of the flow around spacers tends to decrease $\text{CPC}_{\text{max}}$ in the steady regime. However, in the unsteady regime, $\text{CPC}_{\text{max}}$ of the cases with spacers increases rapidly and shows higher values than cases without spacers. This is explained by our discussion of Figure 5.11(b).
Overall, the results in Figure 5.12 suggest that vortex shedding impacts system performance by increasing permeate production at the expense of increased concentration polarization. This trend persists throughout our parametric study in subsequent section. This suggests that when treating low-concentration feed solutions, one can increase the feed flow rate to operate in a vortex shedding regime that increases vapor production. However, when treating high-concentration feeds, one may prefer to operate at lower feed flow rates that produce steady flow regimes for which the risk of precipitation is reduced. Naturally, these results are subject to our consideration of idealized 2D spacers. The key conclusion is that the same fluid structure responsible for decreasing temperature polarization can simultaneously increase concentration polarization and mineral scaling.

5.5.2 Influence of blockage ratio $\beta$

To investigate the effects of the blockage ratio, we repeated the analysis demonstrated in the previous section, but we set $\beta = 0.3$ and 0.7. The spacers remain on the channel centerlines ($\hat{y}_c = 0.5$). Overall, we found that the small blockage ratio ($\beta = 0.3$) produced qualitatively similar results to those observed for $\beta = 0.5$, though the impact of small spacers on polarization and vapor production is less than for $\beta = 0.5$. For brevity, these results are not presented.

In contrast to our results for $\beta = 0.3$, we found that large blockage ratio produce markedly different results. Figure 5.13(a) shows the feed and distillate channel streamlines at $Re_f = 100$ when $\beta = 0.7$. In this case, the flow in both channels is steady. Panel (b) shows that when $Re_f$ is increased to 200, the feed flow transitions to vortex shedding, generating large vortices on the plate and membrane due to the sudden expansion downstream of the cylinder. Panel (c) shows that when $Re_f$ is further increased to 240, the feed flow transitions back to a steady regime characterized by a large plate-vortex and a small membrane-vortex. Panel (d) shows that when $Re_f$ is further increased to 300, the asymmetry in the feed channel reverses, such that the membrane vortex is much larger than that on the outer plate. Meanwhile, the distillate channel finally transitions to vortex shedding.
The steady asymmetric feed flows observed in Figs. Figure 5.13(c) and Figure 5.13(d) are examples of what are called “bi-stable states” in the fluid mechanics community. To our knowledge, they have never previously been observed in membrane filtration systems. A theoretical analysis by Sahin and Owens [111] has shown that they can occur when a cylindrical obstacle is placed in a channel flow with two impermeable plates. In that case,
either state is chosen randomly. To explore the selection of these bi-stable states in a DCMD system, we repeated the simulations demonstrated in panels (c) and (d) with the addition of random noise in the initial conditions. We indeed found that either state can be randomly selected, such that the larger vortex can appear on either the membrane or plate. This again suggests that the small transmembrane velocity does not impact the flow regime from what is observed in channels with two impermeable plates. Consequently, studies can explore the effects of spacers on flow regimes by neglecting the membranes. However, neglecting the membranes will not allow the accurate simulation of polarization.

Figure 5.14 shows the temperature field when $\beta = 0.7$, $\gamma_c = 0.5$, and $Re_f = 200$ (a), 240 (b), and 300 (c), respectively. The most striking results occur in panels (b) and (c). In panel
Figure 5.15: Concentration field when $\beta = 0.7$, $\hat{y}_c = 0.5$, and $Re_f = 200$ (a), 240 (b), and 300 (c), respectively. The concentration field is shown for $0 < y/H < 0.5$, and the aspect ratio causes the circular cylinders to appear ovoid. Panel (d) shows the corresponding downstream variation of $c_m$ when $Re_f = 200$ (solid), 240 (dashed), and 300 (dash-dotted).

(b), the presence of the small membrane-vortex causes the formation of a small region of cool fluid near the membrane at $x/H = 7$. In panel (c), the large membrane-vortex causes the formation of a large region of cool fluid along much of the downstream membrane surface. These cool regions form because the closed streamlines within the membrane-vortices only allow heat to be exchanged with the outside bulk flow through diffusion normal to the streamlines. This diffusion is a slow process compared to heat advection within the vortices.

Figs. Figure 5.15(a)-(c) shows the concentration field when $\beta = 0.7$, $\hat{y}_c = 0.5$, and $Re_f = 200$, 240, and 300, respectively. In all cases, we observe regions of salt accumulation associated with the leading edges of the membrane-vortices, no matter whether these vortices are unsteady (as in panel a) or steady (as in panels b and c). This again demonstrates the key role that membrane vortices play in concentration polarization. Panel (d) shows the
Figure 5.16: The solid lines show the variations of (a) $v_{\text{ave}}^m$, (b) $\eta$, (c) $\Delta P/L$, and (d) $\text{CPC}_{\text{max}}$ with $Re_f$ when $\hat{y}_c = 0.5$, and $\beta = 0.3$ (□), 0.5 (△), and 0.7 (⋆). The dashed lines show the results for simulations without spacers.

The solid lines in Figure 5.16 shows the variations of $v_{\text{ave}}^m$ (a), $\eta$ (b), $\Delta P/L$ (c), and $\text{CPC}_{\text{max}}$ (d) with $Re_f$ when $\hat{y}_c = 0.5$, and $\beta = 0.3$ (□), 0.5 (△), 0.7 (⋆). The dashed lines show the corresponding results without spacers. Panels (a) and (b) show that vapor production and thermal efficiency both improve with increasing blockage ratio when the feed Reynolds number is below $Re_f \leq 240$. However, for $Re_f \geq 250$, the performance of
spacers with blockage ratio $\beta = 0.7$ suddenly drops due to the appearance of the steady bi-stable states with large membrane-vortices. Panels (c) and (d) show that the increase in vapor production and efficiency with increasing blockage is countered by an increase in the required pressure gradient $\Delta P/L$ and maximum concentration polarization coefficient, $\text{CPC}_{\text{max}}$. At $Re_f = 300$, the pressure gradient for $\beta = 0.7$ is nearly 550% of that for $\beta = 0.3$. Note that $\text{CPC}_{\text{max}}$ shows significant variations with $Re_f$ due to the early transition to vortex shedding followed by the subsequent transition to the bi-stable states.

Overall, the results in Figure 5.16 suggest that when treating low-concentration feeds for which mineral scaling is not a risk, one can increase vapor production and thermal efficiency by increasing the blockage ratio. However, at high blockage ratios, one must avoid the bi-stable steady states. When treating feeds for which mineral scaling is a risk, small blockage ratios may be preferred, because they delay transition to vortex shedding such that there is a greater operating region with steady flow and decreased concentration polarization. No matter the feed condition or flow regime, increasing the blockage ratio always increases the downstream pressure drop and pumping costs.

5.5.3 Influence of spacer offset $\hat{y}_c$

To investigate the effects of the spacer offset, we consider $\hat{y}_c = 0.3$ and 0.7, while maintaining the blockage ratio $\beta = 0.5$. Figure 5.17(a) shows streamlines for $\hat{y}_c = 0.3$ when $Re_f = 800$. Placing the spacers near the membrane surface substantially delays transition to vortex shedding, such that both channel flows are steady, despite the large Reynolds numbers. Both channels have large membrane-vortices that cover the full membrane surfaces downstream from the spacers. In the feed channel, there is an additional vortex pair between the cylinder and the downstream membrane vortex. Note that there is a small gap between the cylinders and the membrane surfaces. Flow through this gap likely plays a role in the formation of the vortex pair in the feed channel, and may explain why the membrane-vortex in the distillate channel is displaced downstream from the cylinder surface. The zoom-in view upstream of the feed cylinder (indicated in the red box) shows that a small vortical structure with re-
Figure 5.17: Streamlines for $\hat{y}_c = 0.3$ when $Re_f = 800 (a)$ and $900 (b)$, respectively.

Reverse flow forms on the membrane near $x/H = 4.5$. The structure appears because there is a region of diverging streamlines upstream of the cylinder, between the membrane surface and the streamline that terminates at the stagnation point on the upstream edge of the cylinder. Figure 5.17(b) shows streamlines when the feed Reynolds number is increased to $Re_f = 900$. Additional simulations estimate the critical Reynolds number $Re_c = 895$. We observe that the feed flow is unsteady, with large vortical structures traveling along the membrane and outer plate. The membrane-vortices are generated immediately behind the cylinder, while the plate-vortices appear further downstream, near $x/H = 7$.

Figure 5.18 shows the corresponding temperature and concentration fields when $Re_f = 800 (a$ and $b)$, and $900 (c$ and $d)$. Panel (a) shows that the steady membrane-vortices significantly exacerbate temperature polarization, forming a large region of recirculating cool fluid in the downstream feed channel, and a similar region of recirculating warm fluid.
Figure 5.18: Temperature and concentration fields for $\hat{y}_c = 0.3$ when $Re_f = 800$ (a and b), and 900 (c and d), respectively. Note that the concentration field is shown for $0 < y/H < 0.6$.

in the distillate channel. Panel (b) shows that regions of salt accumulation form not only downstream of the cylinder, but also at the upstream location $x/H = 4.5$. This additional region of accumulation is due to the vortical structure near $x/H = 4.5$, shown in the zoom-in view in (a). Figure 5.18(c) shows that the appearance of large energetic membrane-vortices strongly mix the thermal boundary layer with the bulk. However, panel (d) shows that these membrane-vortices also generate several downstream regions of preferential salt accumulation on the membrane. Overall, the results in Figure 5.18, as well as those earlier in Figure 5.14, show that when membrane-vortices are fixed on the membrane surface, they exacerbate both temperature and concentration polarization. Only translating membrane-
vortices reduce temperature polarization, albeit at the expense of concentration polarization.

Figure 5.19 shows the downstream variation of $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) for $\hat{y}_c = 0.3$ when $Re_f = 800$ (solid), 900 (dashed). Panel (a) shows that when $Re_f = 900$, membrane-vortices dramatically increase $\Delta T_m$ for $x/H > 6$. Panel (b) shows that membrane-vortices also produce multiple downstream regions of salt accumulation, consistent with our observation in Figure 5.18(d). Panel (c) shows that at $Re_f = 900$, $v_m$ significantly increases for $x/H > 6$ due to increased $\Delta T_m$.

Figure 5.20 shows the streamlines (a), temperature field (b), and concentration field (c) when the cylinders are near the outer plates ($\hat{y}_c = 0.7$) and $Re_f = 800$. Panel (a) shows that the streamlines are essentially the mirror image of those for $y_c = 0.3$ in Figure 5.17(a). The flow is steady, with large plate-vortices behind the spacers. The feed and distillate flows accelerate between the spacers and the membrane, thereby decreasing both temperature and concentration polarization on the membrane, such that the spacers have a net beneficial
effect. Figure 5.21 shows the corresponding results when the Reynolds number is increased to $Re_f = 900$. The acceleration of the feed and distillate flows between the spacers and the membrane once again reduces polarization phenomena in a region downstream of the cylinders. However, the appearance of membrane-vortices further downstream, near $x/H = 7$, mixes the temperature layer and causes salt accumulation near $x/H = 9$. Results for $y_c = 0.7$ are further illustrated in Figure 5.22, showing the downstream variation of $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) for $y_c = 0.7$ when $Re_f = 800$ (solid) and 900 (dashed). We find that spacers placed near the outer plates decrease both temperature and concentration polarization in the steady regime. With the transition to vortex shedding, vapor production is further increased, but at the expense of increasing concentration polarization.

The solid lines in Figure 5.23 shows the variations of (a) $\eta^\text{ave}$, (b) $\eta$, (c) $\Delta P/L$, and (d) CPC$_{max}$ with $Re_f$ for $y_c = 0.3$ (□) and 0.7 (△). The dashed lines show the corresponding
results without spacers. Panel (a) shows that spacers placed near the outer plates ($\hat{y}_c = 0.7$) always produce more $v_{ave}^m$ than systems without spacers. In contrast, spacers near the membrane ($\hat{y}_c = 0.3$) always produce less, particularly in the steady regime, for which $v_{ave}^m$ is nearly constant. Panel (b) shows that $\eta$ increases substantially for $\hat{y}_c = 0.3$ and 0.7 after transition to vortex shedding ($Re_f \leq 900$) due to sudden increase in $v_{ave}^m$. Panel (c) shows that $\hat{y}_c = 0.3$ and 0.7 essentially produce same pressure drop at different $Re_f$ due to their symmetry along the channel centerlines. Panel (d) shows that $\hat{y}_c = 0.7$ decreases $CPC_{max}$ in the steady regime. However, transition to vortex shedding causes a sudden increase in $CPC_{max}$, exceeding that observed without spacers. Finally, we observe that $\hat{y}_c = 0.3$ always increases $CPC_{max}$ in comparison to that without spacers.

When interpreting the results of spacers placed near an outer feed plate, it is worth noting that though bench-scale membrane systems are often plate-and-frame, industrial membrane
separation systems usually replace the feed plate with a second membrane, as in spiral-wound systems. In that case, a spacer filament placed near one of the membrane surfaces will increase concentration polarization on that membrane, while decreasing concentration polarization on the opposite membrane. Furthermore, for the diamond spacers commonly used in industry, the displacement $\hat{y}_c$ of a filament varies along the membrane surface. The blockage ratio of the filaments also varies substantially, and reaches 100 % blockage at nodes where perpendicular filaments are welded [61].

### 5.5.4 Influence of multiple spacers

A detailed parametric study of multiple cylinders in the feed and distillate channels is beyond our scope. We nevertheless consider two select cases to determine whether our observations for single spacer filaments are likely to extend to systems with multiple filaments. For that purpose, we place three equispaced cylinders in both channels at $x/H = 2.5, 5,$ and

Figure 5.22: Downstream variation of $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) for $\hat{y}_c = 0.7$ when $Re_f = 800$ (solid) and 900 (dashed).
Figure 5.23: The solid lines show the variations of (a) $v_{m}^{ave}$, (b) $\eta$, (c) $\Delta P/L$, and (d) $C_{P_{\max}}$ with $Re_f$ for $\hat{y}_c = 0.3$ (□) and 0.7 (△). The dashed lines show the corresponding results without spacers.

7.5, thereby maintaining a distance of 2.5 diameters between each cylinder. All spacers have a blockage ratio of $\beta = 0.5$, and we fix the flow rates such that $Re_f = 300$.

Figure 5.24(a) shows streamlines when all spacers are placed on the channel centerlines ($\hat{y}_c=0.5$). In the distillate channel, the flow is steady and the cylinders are sufficiently far apart that the downstream wakes have a negligible impact on the downstream cylinder. However, in the feed channel, the downstream propagation of shedding vortices is interrupted by the appearance of downstream cylinders. Panel (b) shows that in the feed channel, the cool
fluid ejected by membrane-vortices further couples with the downstream spacers, producing stronger mixing with the bulk. Panel (c) shows three major regions of salt accumulation near \( x/H = 4, 6, \) and 8.5 due to the leading membrane-vortex behind each spacer. Figure 5.25 shows the corresponding downstream variation of \( \Delta T_m \) (a), \( c_m \) (b), and \( v_m \) (c). As predicted by our analysis of single spacer filaments, \( \Delta T_m \) and \( v_m \) increase near the cylinders, but at the expense of salt accumulation near \( x/H = 3.8, 6, \) and 7.8.

To investigate the case of staggered cylinders, we first consider Figure 5.26(a) showing streamlines in a system with a single cylinder placed in each channel at \( L/H = 5 \) and \( \hat{y}_c = 0.3 \). We then consider Figure 5.26(b) showing streamlines when additional cylinders are placed near the outer plates \( (\hat{y}_c = 0.7) \) at \( L/H = 2.5 \) and 7.5. The additional spacers redirect the flow such that the central spacers have a much larger upstream membrane-vortex and much smaller downstream-vortex. Figure 5.26(c) and Figure 5.26(d) consequently show...
Figure 5.25: Downstream variation of $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) when all spacers are placed on the centerline.

strong temperature and concentration polarization both upstream and downstream of the central spacer. Figure 5.27 shows the downstream variation of $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) for the cases in Figs. Figure 5.26(a) and (b). Panels (a) and (c) show that due to the smaller downstream membrane-vortices, the staggered arrangement shows increased $\Delta T_m$ and $v_m$ compared to the single spacer case. Panel (b) shows that the upstream local salt accumulation for the staggered case occur at $x/H = 4$ due to a larger upstream membrane-vortex.

Overall, our brief consideration of multiple spacers suggests that the fundamental mechanisms we observed for single filaments help explain what occurs in systems with multiple spacers. We do not perform a more detailed parametric study of multiple spacer arrangements, because it is our philosophy that 3D effects are also required for such analysis. Ongoing work in group is consequently focused on expanding our methods to 3D, including the parallelization of our codes for computer clusters.
5.6 Conclusions

We show that the impact of 2D spacers on temperature and concentration polarization can be physically explained by examining the rich variety of vortical structures generated in both steady and unsteady flow regimes. The impact of these structures on polarization depends on whether the structures occur in the bulk, on the membrane surface, or on the outer plate, and whether they are steady (as in subcritical regimes, $Re < Re_c$) or translate downstream (as in supercritical regimes, $Re > Re_c$). In steady regimes, vortical structures decrease both temperature and concentration polarization when the structures occur in the
Figure 5.27: Downstream variation of $\Delta T_m$ (a), $c_m$ (b), and $v_m$ (c) for the cases in Figs. Figure 5.26(a) and (b).

bulk or on the outer plates. In those cases, the structures accelerate and redirect bulk fluid towards the membrane surface. Steady vortical structures can be generated in the bulk by placing filaments on the channel centerline ($\hat{y}_c = 0.5$). In that case, the reduction of temperature and concentration polarization increases with the blockage ratio $\beta$, but at the expense of increasing pumping costs. Increasing the blockage ratio also decreases the critical Reynolds number $Re_c$. This limits the range of flow rates for which one can decrease both temperature and concentration polarization. Vortical structures can be generated on the outer plate by placing the spacer filament near the plate. In that case, the vortical structures grow with Reynolds number, and the critical Reynolds number is $Re_c \sim 900$, providing a wider range of flow rates for which one can leverage the decrease in polarization.

In contrast to steady vortical structures in the bulk or on the outer plate, steady vortical structures on the membrane surface increase both temperature and concentration polariza-
tion. This occurs when spacer filaments are placed near the membrane surface. Temperature polarization increases because the closed streamlines of the structures inhibit heat transfer with the bulk. Concentration polarization increases because the structures advect solutes upstream, where they accumulate at the leading edge of the vortex.

In cases of unsteady vortex shedding, we found that membrane-vortices play a central, but counter-intuitive, role in temperature and concentration polarization. Membrane-vortices periodically form on the membrane, and translate downstream. The translating vortices mix the thermal boundary layers and decrease temperature polarization. Unfortunately, the vortices do not similarly mix the thin concentration layers. Rather, they form regions of salt accumulation at the vortex leading edge. We consequently find that transition to vortex shedding tends to decrease temperature polarization at the expense of increasing concentration polarization. However, we found that an interesting situation occurs for spacers with large blockage ratios. In that case, we observed that with increasing Reynolds number, transition to vortex shedding is superseded by a bi-stable steady state with large steady membrane-vortices. These bi-stable states should be avoided because they increase both temperature and concentration polarization.

Overall, our results show that optimal operating conditions and spacer designs depend on the feed conditions. When treating low-concentration feeds without risk of mineral scaling, vortex shedding is preferable because it increases vapor production. In that case one should design spacers to minimize the critical Reynolds number $Re_c$. Conversely, when treating high-concentration feeds with risk of mineral scaling, it may be safer to operate in a steady regime without membrane-vortices. One may even suggest that the safest spacer is perhaps no spacer at all, so as to avoid vortex shedding altogether. In that case, however, the membrane still requires structural support, such as filaments oriented parallel to the downstream flow. Such filaments likely generate low-velocity regions at their contact lines, and could generate vortical structures of their own, such as those known to occur in duct flows [155]. Ongoing work in our group now focuses on extending our codes to 3D, so that we can ex-
plore flow regimes and polarization in exactly such cases, and extend our analysis to more realistic spacer geometries. The results of our current study are also the topic of an ongoing experimental study.

5.7 Acknowledgements

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5.8 Appendices

The appendices present supplemental materials for this paper.

5.8.1 Code benchmarking

In all the simulations, the cells in the $y$-direction are concentrated near the membrane and outer plate using Gauss-Lobatto points in both channels,

\[ y_i = -(H/2) \cos(\pi i/N_y), \quad i = 0, 1, ..., N_y, \]  

(5.18)

where $N_y$ is the number of cells in the $y$-direction. For the simulations with multiple spacers in section 5.5.4, the cells are equispaced cells in the $x$-direction. For all other simulations, we refine the grid near the cylinder by decomposing the $x$-direction into three sections, as demonstrated in Figure 5.28. A core section of length $L_1 = H$ is centered about the cylinder, and has $N_1$ equispaced cells. The inlet section has a length $L_2$ and $N_2$ equispaced cells. The outlet section has a length $L_3$ and $N_3$ equispaced cells.

The governing equations are discretized using the procedure described in our previous work [69]. Spacers are implemented using an immersed boundary method similar to that
Figure 5.28: Sketch that demonstrates mesh grids for simulated DCMD system for $N_x = 120$, $N_y = 40$. We typically concentrate grid points near the membrane, outer plate, and spacers to capture the rapid variations in boundary layers.

of Fadlun et. al [123], with modifications for the application of Neumann conditions to the temperature and concentration fields. Using the standard practice in CFD, we verify the temporal and spatial accuracies of our discretization with respect to the following artificial, but exact, analytical solution,

$$
c_e = \sin(x)y^2 \cos(\omega t), \quad p_e^f = p_e^d = \sin(x)\sin(y)\cos(\omega t)
$$
$$
T_e^f = 3/\pi \cos(x)y^2 \cos(\omega t), \quad T_e^d = 1/\pi \cos(x)y^2 \cos(\omega t),
$$
$$
u_e^f = -\sin(x)\cos(\pi y/2) \cos(\omega t), \quad u_e^d = \sin(x)\cos(\pi y/2) \cos(\omega t)
$$
$$
v_e^f = 2/\pi \cos(x)\sin(\pi y/2) \cos(\omega t), \quad v_e^d = -2/\pi \cos(x)\sin(\pi y/2) \cos(\omega t).
$$

Solution (5.19) satisfies the governing equations with the addition of appropriate forcing terms. The numerical solvers were tested with the feed and distillate channels coupled, subject to general Robin boundary conditions of the form

$$
ag^{n+1} + b \nabla g^{n+1} \cdot s = q,
$$

where $g = [u, T, c]$, is the velocity, temperature, or concentration field, $a$ and $b$ are constant coefficients, $s$ is the normal to the boundary, and $q$ is the appropriate boundary source terms determined from the exact solution (5.19).

To test the spatial accuracy of the method, we set $L = 4$, $H = 2$, $D_sp = 1$, $y_c = 2$, $N_x = N_y = N$, $\omega=0$, $g^0 = 0$ and integrate in time using $N$ finite volumes in each direction ($N^2$ in total) until steady state, after which we evaluate the spatial error as $E_N = ||g - g_e||_\infty$. 

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Figure 5.29: (a) Variation of spatial error $E_N$ for temperature ($T$), $u$ component ($u$) and pressure ($p$) as function of grid number $N$. (b) Variation of temporal error $E_t$ for temperature ($T$), $u$ component ($u$) and pressure ($p$) as function of time size $dt$.

Figure 5.30: Transmembrane temperature difference $\Delta T_m$, membrane concentration $c_m$, and transmembrane vapor flux $v_m$ for the cases of $N_x=160$ and $N_y=80$ at $Re_f=600$.

Figure 5.29(a) demonstrates second-order spatial accuracy. To test temporal accuracy, we set $L = 3$, $H = 2$, $N_x = 120$, $N_y = 80$, $\omega=\pi$, and $g^0=g^0_\omega$. The fields are integrated from $t=0$ to $t = 1$ s for $0.01 \leq dt \leq 0.1$. Figure 5.29(b) confirms second-order temporal accuracy.
Figure 5.31: (a) The solid line shows the variation of relative error of \( v \) component \( E_{N_x} \) with \( N_x \) at \( Re_f = 100 \) and \( Re_d = 42 \). (b) The solid line shows the variation of relative error of \( v \) component on the membrane \( Eb_{N_x} \) with \( N_x \) at \( Re_f = 300 \) and \( Re_d = 126 \).

In our previous work [69], we include the variations of all thermo-physical properties, except density, with temperature and salt concentration, \( \mu(T,c) \), \( c_p(T,c) \), \( \lambda(T) \), \( k(T,c) \) and \( D(T) \). For the short systems included in the current study, we found these variations had only a small quantitative effect, on the order of 1 %. This is demonstrated in Figure 5.30, comparing typical results for transmembrane temperature difference \( \Delta T_m \), membrane concentration \( c_m \), and transmembrane vapor flux \( v_m \) at \( Re_f = 600 \) when thermophysical variations are included (solid line) and neglected (dashed line). We consequently neglect variations of thermophysical effects because this allows us to use much larger time steps, and reduces the computational time of our parametric study.

5.8.2 Grid independence study

We performed numerous grid independence studies to ensure the spatial accuracy of our reported results. For demonstration, Figure 5.31(a) shows the results of one such study, performed for \( U_{in} = 0.021 \) m/s, \( \beta = 0.5 \), \( \dot{y}_c = 0.5 \). This produces a steady case characterized by \( Re_f = 100 \) and \( Re_d = 42 \). To explore the effects of grid resolution, we first fix the ratio of grid resolution in the \( x \) and \( y \) directions as \( N_x/N_y = 3:1 \). We then vary \( N_x \) and \( N_y \) between \( 90 \leq N_x \leq 750 \) and \( 30 \leq N_y \leq 250 \), respectively. Taking the solution at \( N_x = 750 \)
as the exact answer, we evaluate the relative error as

\[ E_{N_x} = \frac{||g_{N_x} - g_{750}||}{||g_{750}||}, \tag{5.21} \]

where \( g_{N_x} = [u_{N_x}, T_{N_x}, c_{N_x}] \) is the solution evaluated at grid number \( N_x \), and \( g_{750} \) is the solution at \( N_x = 750 \). Figure 5.31(a) shows the resulting variation of the error in the plate-normal velocity field \( v \). Of the variables \( u, v, T, \) and \( c \), the largest error typically occurred in \( v \), because it is very small compared to \( u \). Figure 5.31(a) shows the error is below 1% when \( N_x = 600 \). Figure 5.31(b) shows the corresponding results for a case where \( Re_f = 300 \) and \( Re_d = 126 \). In this case, the feed flow is strongly unsteady. We consequently measure error using flow fields on the membrane surface, where \( v, T, \) and \( c \) are all quasi-steady. Fig 34(b) shows the error is around 2% when \( N_x = 600 \). Following additional mesh-independence studies, we found that \( N_x = 600 \) and \( N_y = 200 \) consistently produced spatial errors on the order of 1% or less. These values were used for all single spacer results. For unsteady cases, we ensured temporal accuracy by ensuring the time step was at least one hundred times smaller than the period of vortex shedding.

### 5.8.3 DCMD without spacers when \( Re_f = 100 \)

Figure 5.32 shows our results without spacers when \( Re_f = 100 \) and \( Re_d = 42 \). The streamlines in panel (a) are straight because there is no obstacles in the channels. Panels (b) and (c) show the temperature and concentration field, respectively. The concentration boundary layer is much thinner than the thermal layer due to a small Lewis number in the feed channel.

### 5.8.4 Definition of thermal and concentration boundary layer

To measure the thermal boundary layer thickness in the feed channel, we define the non-dimensional temperature \( \hat{T} \) and coordinates \( \hat{x} \) and \( \hat{y} \) as

\[ \hat{T}(x, y) = \frac{T(x, y) - T_m^f(x)}{T_m^f(x) - T_m^i}, \quad \hat{x} = \frac{x}{\bar{H}}, \quad \hat{y} = \frac{y}{\bar{H}}. \tag{5.22} \]
Figure 5.32: Results without spacers when $Re_f = 100$. (a) Streamlines. (b) Temperature field. Different color scales are used in the distillate and feed channels. (c) Feed concentration field for $0 < y/H < 0.2$.

$T^*$ is defined such that it varies from zero on the membrane surface ($\hat{y} = 0$) to unity when $T = T_f$. We then define the non-dimensional thermal boundary layer thickness $\hat{\delta}_T(\hat{x})$ as the location where

$$\hat{T}|_{\hat{y} = \hat{\delta}_T(\hat{x})} = 0.95.$$  \hfill (5.23)

Similarly, to measure the layer thickness, we define the non-dimensional concentration as

$$\hat{c} = \frac{c - C_{in}}{c_m(x) - C_{in}}.$$  \hfill (5.24)

We then define the non-dimensional concentration boundary layer thickness $\hat{\delta}_c(\hat{x})$ as the location where

$$\hat{c}|_{\hat{y} = \hat{\delta}_c(\hat{x})} = 0.05.$$  \hfill (5.25)
5.8.5 Order-of-magnitude analysis for near-membrane solute advection

As mentioned in section 5.5.1, we observed that the concentration on the membrane surface remains essentially steady for cases of vortex shedding where the bulk flow is strongly unsteady. To investigate this result physically, we consider the advection-diffusion equation (5.10) at the feed surface of the membrane

\[
\frac{\partial c_m}{\partial t} + u_m \frac{\partial c_m}{\partial x} + v_m \frac{\partial c_m}{\partial y} = D \frac{\partial^2 c_m}{\partial x^2} + D \frac{\partial^2 c_m}{\partial y^2},
\]

(5.26)

where the subscript \( m \) stresses that we are considering the equation on the membrane surface. This equation can be simplified by setting \( u_m = 0 \) and neglecting \( \frac{\partial^2 c_m}{\partial x^2} \), which our simulations showed to be two orders-of-magnitude smaller than \( \frac{\partial^2 c_m}{\partial y^2} \). This produces,

\[
\frac{\partial c_m}{\partial t} + v_m \frac{\partial c_m}{\partial y} = D \frac{\partial^2 c_m}{\partial y^2}.
\]

(5.27)

To estimate the order-of-magnitudes of the three terms in Eqn. 5.27, we scale derivatives of \( c \) with \( y \) as

\[
\frac{\partial c_m}{\partial y} \sim \frac{\Delta C}{\delta_c}, \quad \frac{\partial^2 c_m}{\partial y^2} \sim \frac{\Delta C}{\delta_c^2},
\]

(5.28)

where \( \Delta C = \overline{C}_m - C_{in} \), \( \overline{C}_m \) is the average concentration on the membrane surface, and \( \delta_c \) is the average thickness of the concentration boundary layer. We scale the derivative \( \partial c_m / \partial t \) as

\[
\frac{\partial c_m}{\partial t} \sim \frac{\Delta C}{\tau_m},
\]

(5.29)

where \( \tau_m \) is some characteristic time scale (to be determined) of temporal variation of \( c \) at the membrane surface. Finally, we scale \( v_m \) as \( v_m \sim V_m \), where \( V_m \) is the average velocity \( v \) at the membrane feed surface.

With these dimensional scales, we scale Eqn. 5.27 as,

\[
\frac{\Delta C}{\tau_m} \sim \frac{V_m \Delta C}{\delta_c} + \frac{D \Delta C}{\delta_c^2}.
\]

(5.30)
By multiplying Eqn. 5.30 with $H/(U_{in}\Delta C)$, we obtain the Strouhal number $St_m$ for $c_m$ as,

$$St_m = \frac{H}{U_{in}\tau_m} \sim \frac{V_m H}{U_{in}\delta_c} + \frac{1}{Pe} \left( \frac{H}{\delta_c} \right)^2, \quad Pe = \frac{U_{in}H}{D}, \tag{5.31}$$

where $Pe$ is the Peclet number. The typical Peclet number in our simulations is $Pe \approx 30000$. We estimate $V_m/U_{in} \approx 5 \times 10^{-4}$ and $H/\delta_c \approx 10$ from Figure 5.7(c) and Figure 5.6(b), respectively. Consequently, we estimate $St_m \sim 1 \times 10^{-2}$. From table Table 5.1, we see that the Strouhal number for vortex shedding, $St$, is typically on the order of 1. From the definition of Strouhal number, the characteristic time scale $\tau_m$ is estimated as,

$$\tau_m = \frac{St}{St_m} \tau_b \sim 100\tau_b, \tag{5.32}$$

where $\tau_b$ is the period for vortex shedding in the bulk flow. Finally, we conclude that because the bulk flow characteristic time length $\tau_b$ is much smaller than the membrane characteristic time length $\tau_m$, $c_m$ is not able to reflect the strong unsteadiness of the bulk flow, showing negligible variation in time. Similar analysis can be done for the membrane surface temperature.
In chapter 3, we develop a numerical approach to simulate DCMD systems using finite volume methods with immersed boundaries and projection methods. This approach achieves global second-order spatial and temporal accuracy. Our approach includes a projection method that staggers the coupled channel flows and applies Robin boundary conditions to facilitate mass conservation at the outlets. We also develop an immersed boundary method that applies Neumann boundary conditions to second-order spatial accuracy. The methods are verified and validated against manufactured solutions and theoretical predictions of vortex shedding. They are then applied to the simulation of steady and unsteady transport phenomena in membrane distillation. The methods have important applications to the broad field of chemical engineering and deal with long-standing issues in both theoretical and computational fluid dynamics.

In chapter 4, we investigate polarization and system performance of 2D DCMD systems without spacers. We perform a comprehensive parametric study of polarization phenomena for a wide range of feed and distillate operating conditions, system length, and co-current versus counter-current operation. We also investigate the system-level performance by measuring the average permeate flux, single-pass water recovery, maximum concentration polarization coefficient, and gained output ratio of DCMD systems with heat recovery. Though the transmembrane vapor flux is small, we observe dramatic increases in solute concentration at the membrane surface, exceeding 1.6 times the feed value. The temperatures, concentration, and vapor flux vary considerably in the downstream direction, and are poorly approximated by common Nusselt and Sherwood correlations.

In chapter 5, we explore how transition from laminar flow to unsteady laminar vortex shedding affects polarization and system performance in DCMD systems with spacers. We
show that the impact of spacers on polarization and system performance can be explained by examining the various steady and unsteady vortical flow structures generated in the bulk and near the bounding plates and membranes. Overall, we show that though unsteady vortex structures tend to mix temperature polarization layers with the bulk, they are not similarly able to mix the thin concentration layers. Rather, vortical structures tend to create regions of preferential salt accumulation. In the vortex shedding regime, the net result is that spacers often increase vapor production at the expense of increasing the risk of mineral scaling.

Detailed conclusions of these chapters can be found in sections 4.6, 3.7, and 5.6.

6.1 Impact and future work

This work makes fundamental contributions to the field of computational fluid dynamic, and opens many avenues for future work. For example, our numerical methods can now be expanded to three dimensions to simulate real-world spacer geometries. That expansion requires parallelization of our methods on a computer cluster, which is the topic of ongoing work in our group. The outlet conditions and immersed boundary conditions have broad applications to separation processes, such as reverse osmosis, and even more general heat and mass transport phenomena in the presence of complicated surfaces. Though beyond the current scope, the methods shown in this thesis have been successfully expanded to simulating reverse osmosis systems. An article focused on that work, lead by collaborator Jacob Johnston, is now in preparation. Additional work in our group is expanding our codes to the case of vacuum membrane distillation with a new generation of heated membranes.

Expanding our current 2D code to 3D is not trivial. The current 2D code is a serial code that uses a direct linear solver called MUMPS [156, 157]. The CPU time for a typical case to run on an Intel Skylake6154 core is around 2 days. For an unoptimized code, this was sufficient for our purposes. However, Expanding to 3D will produce much larger matrices for which direct solvers, such as MUMPS, are no longer appropriate both from a memory and CPU time perspective. To manage memory and CPU time, the 3D code will necessarily use iterative solvers with preconditioners. Some preliminary investigation has been done using
an iterative solver package called PETSc [158]. In addition, The 3D code will also need to be parallelized using techniques such as MPI. This will require a major reconstruction of the code. Lastly, we might also want to explore a fully explicit temporal discretization (such as Runge-Kutta method) for the future 3D code. This will reduce the number of matrices that need to be solved per time step from 11 to 2 (two pressure Poisson equations need to be solved implicitly) at the expense of increased time step.

Our work also makes fundamental theoretical contributions to the field of membrane separations, and particularly to our understanding of temperature and concentration polarization. We show, for example, that classic Nusselt and Sherwood relationships do not capture polarization accurately. This opens the door to developing new back-of-the-envelope relationships that can be used to estimate polarization phenomena quickly in the field. Perhaps most importantly, we show that membrane spacers can have counter-intuitive impacts on concentration polarization. This goes against the prevailing belief in the membrane separations community that vortical structures always diminish concentration polarization. We expect many of the observations of concentration polarization observed in this study to extend to reverse osmosis systems, and preliminary simulations indeed show this to likely be true.

Finally, we note that this study is part of a larger experimental-numerical study dedicated to developing and manufacturing a new generation of smart spacers that are optimized to minimize temperature and concentration polarization in DCMD systems. We propose an iterative design process in which: (1) initial spacer designs are motivated by our 2D and 3D numerical simulations; (2) prototype designs are 3D printed; (3) the printed spacers are tested in MD and RO systems at the Mines Advanced Water Technology Center (AQWATEC) and compared with conventional spacers; (4) results from both manufacturing and testing motivate improved designs, and the process continues.
REFERENCES CITED


APPENDIX A
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Jincheng Lou, Johan Vanneste, Steven C. Decaluwe, Tzahi Y. Cath, and Nils Tilton, “Computational fluid dynamics simulations of polarization phenomena in direct contact membrane distillation” is a paper published on the *Journal of Membrane Science*. No copyright permission is required from the publisher to include it in a thesis.
Computational fluid dynamics simulations of polarization phenomena in direct contact membrane distillation

Author: Jincheng Lou, Johan Vanneste, Steven C. DeCaluwe, Tzahi Y. Cath, Nils Tilton

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Cc: Johan Vanneste <vanneste@mines.edu>, Nils Tilton <ntilton@mines.edu>, Jincheng Lou <jilou@mymail.mines.edu>, Jacob Johnston <jrjohnston@mymail.mines.edu>, Tzahi Cath <tcath@mines.edu>

Dear Jincheng,

You have my permission, as well.

Congrats on a successful defense!

Best,
Steven

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All good.

Good luck!

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