3-D NUMERICAL SIMULATIONS OF CONJUGATE HEAT TRANSPORT
IN VACUUM MEMBRANE DISTILLATION SYSTEMS
WITH APPLIED MEMBRANE HEATING

by

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A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Masters of Science (Mechanical Engineering).

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ABSTRACT

Membrane distillation has gained attention recently for its capabilities to treat hyper-saline brine and its compatibility with renewable heat. But the effects of temperature and concentration polarization are major inhibitors to its permeate production and ultimately its commercial viability. To alleviate these effects, we investigate an improvement to vacuum membrane distillation (VMD) such that a thin, thermally conductive, porous metal mesh is placed beneath the membrane. This mesh is heated laterally with low-grade heat to actively heat the membrane and feed, thereby countering effects of temperature polarization. We develop a three-dimensional CFD code to simulate heat and vapor transport conjugately in the feed, membrane, and mesh for this system, which included deriving new equations governing heat and mass in the membrane and mesh. We discretize these governing equations with second-order accurate finite volume methods. These methods are verified using manufactured solutions. We then perform a comprehensive parametric study of fully developed duct flow over a heated plate. We identify the optimal combination of plate properties, duct dimensions, and operating conditions to maximize uniform heating of the duct-plate interface. With this, we identified that decreasing channel width, decreasing inlet flow rate, and increasing plate thickness provided the best results of uniform heating. We then validate our solver against experimental measurements of vapor flux, and determined the best fit for membrane vapor permeability $A_m$. For best fit $A_m$, we were able to reproduce experimental results to within 9% mean error. Following that, we performed a second comprehensive parametric study of the VMD system to investigate the effect of operating conditions, mesh properties, and system geometry on temperature polarization and vapor flux measurements. We observe that polarization effects could be reversed for systems with a high input heat, faster flow rate, slim channel width, thicker mesh, and high vacuum pressure.
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ACKNOWLEDGMENTS

Firstly, I would like to thank my advisor, Dr. Nils Tilton, for the guidance, support, and opportunity to be a part of this project. I have learned so much in the last two years that would not have been possible without your teaching, and I have grown substantially because of it. Additionally, I would like to thank my other committee members: Many thanks to Dr. Tzahi Cath, whose wisdom has been invaluable to keep the code modeling realistic scenarios of MD. And great appreciation to Dr. Jason Porter, who helped to bridge a number of conceptual gaps for the heat transport processes and offered words of encouragement.

I would also like to thank everyone in the fourth floor office. The support I got from all of you for both research aspects and becoming a better person is honestly something I won’t forget. Even if it was just a random question of the day, lamenting late work schedules, or nonstop 502 homework, being there with all of you made it truly so much more bearable. Of that group, I’d like to specifically thank the Computational Fluid Dynamics Group: Jincheng Lou, Jacob Johnston, Nick Yearout, and Zahra Khalifa. Your insight about code was invaluable. Your conversations in the office were fun. And I think you’re one of a couple who pulled me back from insanity and more than once. So I thank you for that.

I have nine best friends in this world. I cannot thank them enough for all of the support that they’ve give me and the motivation to consistently be better and better:

To the seven from Fort Collins, David Andales, Kyle Johnson, Jason Krbec, Dennis Shi, Logan Newman, Frankie Caballero and Derek Holland: You have kept me on track for an entire decade, almost even more. If it were not for you seven, I would not be finishing this thesis right now. You turned my life around back then, though some of you might not know that. I thank you guys. And I can firmly say, my family thanks you guys too. We’ll assemble sometime soon.

And to the two I met here at Mines, Jacob Wilkinson and Nick Hill: You two have seen me through some of my biggest hardships, and the two of you have been there for me all the way. And I don’t think I can ever repay you for it. Whether it was the 3 AM talks, the
Voodoo Donut runs, top 5 lists, bands upon bands, or the late night Civilization Games. I’d do it again, every time, you mad lads. Mines got so much quieter without you here.

I’d also like to thank my family. To all of you in Georgia, Texas, Virginia, New York, and Las Vegas: thank you. Your constant love and support has made this so much more bearable. Especially to my siblings, Catie and Chip. I love you guys more than I say.

And last, but furthest from least, is my mother, Doreen Dudley. She is the wind at my sails when I get deflated and the best sanity check there is. I don’t think a thousand lifetimes would give me the opportunity to love you back enough. You’re my biggest cheerleader and I wouldn’t trade that ever. I love you and thank you for everything you’ve sacrifice (mostly sanity) to help me get to this point.
To my father, Jim Dudley.
CHAPTER 1
INTRODUCTION

Membrane distillation (MD) is a membrane separations process with emerging applications to desalination and the treatment of complex wastewaters. Though there are several modes of MD, such as direct contact and air gap MD, the current study focuses on vacuum MD (VMD). With this approach, warm liquid feed solution flows over a hydrophobic microporous membrane that separates the feed from a channel filled with water vapor that is maintained at a low pressure by a vacuum pump, as illustrated in Figure 1.1. The hydrophobic membrane creates vapor-liquid interfaces on the feed surface of the membrane. The difference in partial vapor pressure between the warm feed and the vacuum channel causes volatile components (i.e. H$_2$O) to evaporate from the feed side of the membrane and travel through the vapor-filed pores, after which it is removed from the system by the vacuum pump and later condensed.

VMD has several advantages over pressure driven separation processes such as reverse osmosis. First, the transmembrane partial vapor pressure varies significantly with the feed temperature, but only weakly with the feed salinity [1–3]. This allows VMD to 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 VMD is approximately 300 g/L [4, 5]. Second, VMD systems do not require

![Figure 1.1: Illustration of 2-D plate-and-frame VMD system. The arrows marked $j_v$ and $q_e$ depict transmembrane vapor flux and heat transfer due to evaporation, respectively.](image)
high-pressure pumps, and can be built with inexpensive plastics. Third, VMD operates at feed inlet temperatures below 90 °C that are readily produced by renewable energy and low-grade industrial heat. Additionally, in comparison to other modes of membrane distillation, VMD has significantly lower conductive heat losses through the membrane due to the low thermal conductivity of the rarefied vapor in the permeate channel [6, 7].

Two major challenges to commercializing VMD, as well as all other modes of MD, are temperature polarization and concentration polarization [8, 9]. Temperature polarization is the decrease in transmembrane temperature difference due to heat loss through the membrane, as shown by the temperature profile in Figure 1.1. Concentration polarization is the accumulation of solute in the feed solution near the membrane, as shown by the solid dots in Figure 1.1. Both phenomena lower the transmembrane partial vapor pressure difference, and consequently reduce permeate production. Additionally, concentration polarization leads to mineral scaling, which is the of solutes onto the membrane surface. Scaling can block membrane pores and cause pore-wetting and even permanent membrane damage.

This current thesis investigates a modification to VMD in which a thin layer of porous, thermally conductive, metal mesh is placed beneath the membrane, as illustrated in Figure 1.2. Heat is then applied to the lateral edges of the mesh to actively heat the membrane and adjacent feed, thereby counteracting temperature polarization. This design was proposed by collaborators at UCLA and is motivated by a DOE request for novel methods of using solar thermal energy to drive desalination without passing through the intermediary step of converting solar energy into electricity, such as using solar photovoltaic panels to run a conventional reverse osmosis system. One approach of satisfying this constraint is to use solar energy to directly heat the feed before passing it to a conventional MD system. Unfortunately, with this approach, MD systems still suffers from temperature polarization. Another approach heats the membrane surface by exposing the membrane to direct sunlight [10]. That approach mitigates temperature polarization, but at the expense of spreading a membrane sheet over a large area, thereby negating a primary advantage to
considering membrane separations in the first place, which is the ability of membrane systems to tightly pack adjacent membrane sheets into small system volumes. The current approach can directly heat the membrane surface without exposing the membrane to direct sunlight, thereby mitigating temperature polarization without requiring the exposure to direct sunlight. This comes with the major challenge, however, of designing a system that somehow conducts thermal energy from the thin lateral edges of the mesh laterally into the VMD system so as to provide a uniform heating of the membrane surface.

1.1 Objectives

Thus motivated, our objective is to develop numerical methods of simulating heat transport within the proposed VMD system, and to then use those methods to perform a parametric study that explores the impacts of feed channel geometry, membrane and mesh properties, and operating conditions on heat transport and vapor production. We do not consider concentration polarization, which is left to future work. Our objective presents several major challenges. (1) The problem involves conjugate heat transport between the mesh, membrane, and feed channel. (2) Heat transport in the feed channel also requires
the solution of the 3D Navier-Stokes and continuity equations to determine the feed velocity field. (3) The question of how to best model heat and vapor transport in the membrane remains a topic of considerable discussion [11]. Common models of VMD neglect heat conduction through the membrane altogether. In our case, that assumption is not valid, and we must derive equations that account for heat transport through the mesh and membrane. This transport occurs due to a combination of advection and diffusion through both solid and vapor phases. (4) Due to the manner in which heat is supplied to the lateral edges of the mesh, the resulting heat transport problem is inherently three-dimensional, and cannot be approximated as two-dimensional.

We approach these challenges by developing our numerical code incrementally in a series of simpler problems, in which we add the relevant physics one-by-one. We begin by developing a finite volume code to simulate 3D heat transport in a feed channel for which the membrane is replaced with an impermeable heated plate. This removes the influence of transmembrane vapor flow, and allows us to use an analytical solution for laminar duct flow. This in turn allows us to focus on the issue of how to simulate conjugate heat transport between the channel and plate. We verify our code and then use it to find the optimal combination of plate properties, duct dimensions, and operating conditions to maximize uniform heating of the feed-plate interface.

Next, in collaboration with Dr. Steven DeCaluwe, we applied conservation of mass and energy principles to develop a finite-volume model of heat and vapor transport through a heated composite membrane. We incorporated the model into our code and verified it with manufactured solutions. To avoid the solution of the full Navier-Stokes and continuity equations, we propose a simplified model for the fluid flow that leverages the fact that the transmembrane velocity component is several order of magnitude smaller than the mean downstream velocity in the feed channel. We then validated our code by comparing with experimental measurements of vapor flux performed by our collaborator at UCLA. Finally, we use the code to explore how the membrane and mesh properties, duct geometry, and operating conditions impact the vapor productions and temperature polarization in the
Finally, we developed a 3D finite-volume code for simulating the Navier-Stokes and continuity equations in the feed channel. The code uses a fully explicit discretization in time and a fast Poisson solver to avoid building any of the large matrix systems that lead to memory issues with 3D codes. The drawback is that the code requires small time steps. The code is verified against manufactured solutions, but due to time constraints, the solution of the Navier-Stokes equations is not integrated in our VMD model, and that is necessarily left to future work.

1.2 Organization

The remainder of this thesis is organized as follows. Chapter 2 presents a review of the pertinent literature. Chapter 3 presents the system geometry, governing equations, boundary conditions, and derivation of our transport models for the membrane and mesh. Chapter 4 presents our numerical methods and code verification. Chapter 5 shows our results for the parametric study of a feed channel with an impermeable heated plate, the experimental validation of our VMD model, and a brief parametric study showing the impact of feed velocity on the performance of our proposed VMD system. Chapter 6 presents our conclusions.
CHAPTER 2

BACKGROUND

Membrane distillation is a process in which a heated feed solution flows over a hydrophobic microporous membrane separating the feed from a permeate channel. Due to its hydrophobicity, the membrane creates vapor-liquid interfaces at which feed solvent evaporates and passes through the membrane as a vapor, leaving non-volatile solutes in the feed channel. The feed is heated to maintain a higher partial vapor pressure on the feed side of the membrane than the permeate side. This transmembrane vapor pressure difference drives the evaporation and vapor flow through the membrane [6].

2.1 Modes of Membrane Distillation

The four common types of MD are called: direct contact (DCMD), sweep gas (SGMD), air gap (AGMD), and vacuum MD (VMD). Each type differs in how it controls the partial vapor pressure in the permeate channel and in how it condenses the vapor, as shown in Figure 2.1. DCMD is likely the most common and simplest mode of MD to operate [6]. With this approach, cool distillate is pumped through the permeate channel so vapor condenses directly at the vapor-liquid interfaces on the permeate side of the membrane. Though simple to operate, the presence of warm and cold liquids in direct contact with the membrane surfaces cause DCMD to suffer large energy losses due to heat conduction through the membrane [5, 12].

SGMD flows an inert gas through the permeable channel to sweep the vapor out of the system, after which it is later condensed. To ensure a vapor pressure difference across the membrane, the sweep gas enters the permeate channel with a low water content and low temperature [13]. SGMD has less conductive heat losses than DCMD because the sweep gas has a smaller thermal conductivity than liquid permeate [1, 6].

With AGMD, the vapor passes through a layer of stagnant air in the permeate channel, after which the vapor condenses on a cool surface opposite the membrane, as sketched in
In each case, the feed is the aqueous solution to the left of the membrane and the distillate is the right side chamber. This is adapted from [6].

Figure 2.1(b). The air gap behaves as an insulator to reduce conductive heat losses [1, 6, 12]. Unfortunately, the layer of stagnant air adds resistance to vapor transport, such that AGMD tends to produce lower fluxes than other forms of membrane distillation [12, 14].

With VMD, vapor is drawn out of the system using a vacuum pump that maintains the permeate channel at a low partial vapor pressure. The rarefied gas in the permeate channel has a much lower thermal conductivity than the liquids or gasses present in the permeate channels of the other modes of MD. As a result, conductive heat loss is often approximated as zero for VMD [1, 7, 12]. Furthermore VMD directly controls the vapor pressure with a vacuum pump, rather than indirectly by controlling the permeate temperature. One drawback to VMD is the energy required to continuously run the vacuum pump. For our
purposes, VMD is likely the best mode of MD, because it minimizes heat losses between the heated mesh and the permeate channel. This helps ensure that most of the supplied heat conducts through the membrane and into the overlying feed.

2.2 Coupling MD to renewable energy and low-grade heat

MD has a lower energy efficiency than most other thermal and pressure-driven desalination processes [15, 16]. It nevertheless attracts considerable attention because it can treat high-concentration brines for which RO is not suitable, has a smaller physical footprint than conventional distillation processes, and operates at low feed temperatures readily produced by renewable energy or low grade heat produced by colocated industry. Studies often couple MD to such heat sources by directly heating the feed using solar [17–27], geothermal [28, 29] or industrial [30, 31] heat, before passing the feed to the MD system. With this approach, the MD system still suffer the effects of temperature polarization [25, 26]. Mericq et al. [23] and Summers and Lienhard [26] both attempt to alleviate temperature polarization by increasing the feed flow rate. Summers and Lienhard noted, however, that a low feed flow rate is often necessary for direct solar heating to maintain a high inlet feed temperature, given the small sunlight window that illuminates the feed.

Other studies mitigate temperature polarization by directly heating the membrane surface [8, 32–41]. The majority use sunlight to excite and heat photothermal layers deposited on the membrane-feed surface [8, 32–39]. Others use resistive heating in the membrane [40, 41]. Both modes have been shown to alleviate temperature polarization and increase thermal efficiency. However, most studies using photothermal membranes reported low permeate flux values [32–36, 38]. A challenge for photothermal-coupled systems is their incompatibility with densely-packed modules, such as spiral-wound modules. Light struggles to reach the membrane surface to provide heat to closed and packed systems [10].
CHAPTER 3

GEOMETRY AND GOVERNING EQUATIONS

We consider the 3-D flat-sheet VMD system illustrated in Figure 3.1(a) The feed channel has a length $L$, width $W$, and height $H$. For the scope of the current study, we neglect concentration polarization and assume pure water enters the feed channel with a temperature $T_{in}$ and an average inlet velocity $U_{ave}$. The feed channel is bounded below by a composite membrane, consisting of a hydrophobic membrane of thickness $\delta_1$ overlying a metallic mesh of thickness $\delta_2$. The composite membrane has a width $W$ and length $L$, identical to the feed channel. We place the coordinate system at the feed inlet, as shown in Figure 3.1(a), such that the feed-mesh interface is located at $y = 0$, the upper wall is located at $y = H$, and the system side-walls are located at $z = \pm W/2$. We apply a uniform heat flux $q_{in}$ to the lateral edges ($z = \pm W/2$) of the mesh.

During the development of our code, we also consider a simpler case in which the composite membrane is replaced with an impermeable metal plate of thickness $\delta_p$, as sketched in Figure 3.1(b). From a practical perspective, this allowed us to initially focus our code development on the issue of how to best couple conjugate heat transport without addressing the equally challenging questions of how to model heat and vapor transport through the composite membrane. It also allowed us to simplify the fluid flow in the channel, as discussed in section 3.4. Beyond that practical motivation, however, the simulations of the heated plate are valuable in their own right. Specifically, in Chapter 5, we perform a thorough parametric study of heat transport in the simpler geometry to gain a physical understanding of what combinations of operating conditions, channel geometry, and plate parameters produce the most uniform heating of the plate surface. Performing such a thorough study is far harder for the full problem.
3.1 Transmembrane vapor transport

We first present our model of vapor transport across the composite membrane because it helps our discussion of the governing heat transport equations and boundary conditions discussed in sections 3.2 and 3.3. We assume the vapor mass flux, $j_v$, (see Figure 3.2) is linearly proportional to the transmembrane vapor pressure difference [6, 42, 43]

$$j_v = A_m(P_{mf} - P_{vac}),$$

(3.1)

where $A_m$ is the membrane vapor permeability, $P_{mf}$ is the partial vapor pressure at the membrane-feed interface, and $P_{vac}$ is the applied vacuum pressure. Though there is some discussion in the literature as to whether $A_m$ may vary with temperature and pressure [6,
Figure 3.2: Sketch (not to scale) showcasing the mass transport through the hydrophobic membrane and mesh via an idealized pore, where \( j_v \) is defined by equation (3.1).

7], multiple studies show that approximating \( A_m \) as a constant membrane property produces good agreement with experimental flux measurements [42–44]. In the current study, we define \( A_m \) as an effective vapor permeability for the composite membrane, i.e. including the mesh. In Chapter 5, we determine \( A_m \) by fitting our numerical results to experimental measurements of vapor flux.

For MD with pure water, the feed-membrane pressure \( P_{mf} \) is often approximated as saturation pressure of water computed at the feed-membrane temperature [6, 45]. We use that approach, and approximate \( P_{mf} \) as the empirical Antoine equation for water

\[
P_{sat}(T) = \exp \left( 23.238 - \frac{3841}{T + 228.15} \right),
\]

(3.2)

where \( P_{sat} \) and \( T \) are given in units Pa and °C. Note that \( T_{mf} \), \( P_{sat} \), and \( j_v \) all vary with \( x \), \( z \), and time \( t \), as shown in Figure 3.2.

### 3.2 Governing equations in the feed channel

Heat transport in the feed channel is governed by the thermal energy equation,

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

(3.3)

where \( \mathbf{u} = [u \ v \ w] \), \( \rho \), \( c_p \), and \( k \) are the feed water velocity vector, density, specific heat capacity, and thermal conductivity, respectively. The thermophysical properties of the feed
\( (\rho, c_p, k) \) are fixed to those corresponding to the inlet temperature. Fluid flow in the feed channel is governed by the incompressible continuity equation and Navier-Stokes equations,
\[
\nabla \cdot \mathbf{u} = 0, \quad \rho \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right] = -\nabla p + \mu \nabla^2 \mathbf{u},
\]
where \( p \) and \( \mu \) are the feed channel pressure field and dynamic viscosity, respectively. We fix \( \mu \) to that of pure water at the inlet temperature. Though we present the Navier-Stokes and continuity equations here, our simulations of VMD systems all use simpler analytical models for the feed velocity. These are discussed in section 3.4. These models were used to simplify our initial code development and allow us to provide faster preliminary results to our collaborators at UCLA. We have since developed a numerical solver for the Navier-Stokes and continuity equations, but that is not included here.

At the channel side-walls \( (z = \pm W/2) \) and upper wall \( (y = H) \) we assume insulated conditions
\[
\frac{\partial T}{\partial z} \bigg|_{z=\pm W/2} = \frac{\partial T}{\partial y} \bigg|_{y=H} = 0.
\]
At the channel outlet \( (x = L) \), we apply a Neumann condition
\[
\frac{\partial T}{\partial x} \bigg|_{x=L} = 0.
\]
At the channel inlet \( (x = 0) \), we apply a uniform desired temperature \( T = T_{in} \). At the feed-membrane interface \( (y = 0) \), conservation of energy requires the sum of heat conduction and advection within the liquid feed to balance the sum of heat conduction and advection within the membrane. Following conservation of energy principles for liquid-vapor interfaces with phase change [46], this can be written as
\[
T \bigg|_{y=0^-} = T \bigg|_{y=0^+}, \quad -k_1 \frac{\partial T}{\partial y} \bigg|_{y=0^-} + k_f \frac{\partial T}{\partial y} \bigg|_{y=0^+} = j_v \lambda,
\]
where \( \lambda \) is the latent heat of vaporization of water and \( k_1 \) and \( k_f \) are the thermal conductivities of the membrane and feed water, respectively. The “+” and “-” superscripts indicate evaluation of \( T \) and \( \partial T/\partial y \) from the feed or membrane side of the interface. We
account for variations of $\lambda$ with temperature using the following relation

$$\lambda(T) = -2438T + 250300,$$

(3.8)

where $T$ has units of °C and $\lambda$ has units of kJ/kg. This empirical equation was derived using the OLI Stream Analyzer database [47]. Note that $\lambda$ also varies with $x$, $z$, and $t$.

We do not include boundary conditions for the Navier-Stokes equations here.

### 3.3 Governing equations in the membrane and mesh

To simplify the derivation of our model for heat transport through the composite membrane, suppose that we consider the case of 2D transport within the $x$-$y$ plane. Furthermore, suppose we neglect the presence of the mesh, which will be addressed later. Consistent with our use of finite-volume methods in Chapter 4, we derive our model of heat transport by first dividing the membrane into small cells, as sketched in Figure 3.3(a). We also assume the cell volumes are nevertheless much larger than the pore structures within the membrane. This allows us to interpret the flow fields within each cell as effective volume-averaged quantities.

Figure 3.3(b) shows a single cell across which mass enters or leaves the four faces. Conservation of mass requires the time rate-of-change of mass within a cell to equal the net

![Figure 3.3](image)

Figure 3.3: (a) Each finite volume is much larger than the pore-structures within. (b) Application of conservation of mass principles.
rate of mass crossing the control surface,

$$\frac{dm_{CV}}{dt} = \dot{m}_w + \dot{m}_s - \dot{m}_n - \dot{m}_e, \quad (3.9)$$

where \(m_{CV}\) is the mass in the cell, and \(\dot{m}\) represents the mass fluxes through the cell faces, as illustrated in Figure 3.3(b). We assume the membrane pores contain only water vapor, i.e. we neglect the potential presence of air. Consistent with previous literature [11], we also assume that vapor transport through the membrane occurs due to gradients in partial vapor pressure, and that the gradient across the membrane (in the \(y\)-direction) is much larger than any pressure gradients in the \(x\) or \(z\)-directions. This allows us to assume that \(\dot{m}_w = \dot{m}_e \approx 0\). If we assume that accumulation of mass within the pore is negligible, or if we limit ourselves to steady-state conditions, then \(\dot{m}_n = \dot{m}_s\), such that

$$\dot{m}_n = \dot{m}_s = j_v. \quad (3.10)$$

We conclude that at steady-state, the mass flow rates through a vertical stack of cells is constant, and equal to mass flux \(j_v\) of vapor produced at the interface between the membrane and feed flow.

Figure 3.4 shows the conservation of energy for a cell, which can be written as

$$\frac{dE_{CV}}{dt} = q_s^a - q_n^a + q_w^d - q_e^d + q_s^d - q_n^d, \quad (3.11)$$

Figure 3.4: Application of conservation of energy principles.
where \( E_{CV} \) denotes the energy in the cell, \( q^a \) denotes advective heat fluxes, \( q^d \) denotes diffusive heat fluxes, and the subscripts denote which face of the control volume, across which, the flux is evaluated. Note that heat advection only occurs in the \( y \)-direction. We approximate the advection terms as

\[
q^a_s - q^a_n = \dot{m}_s \Delta x \left. c_{p,s} T \right|_s - \dot{m}_n \Delta x \left. c_{p,n} T \right|_n = j_v \Delta x (\left. c_{p,s} T \right|_s - \left. c_{p,n} T \right|_n),
\]

where thermophysical properties are those of only the vapor.

To approximate the diffusion terms, we must consider that heat conduction occurs through both the vapor and solid. We will approximate the conductive heat transport via an effective temperature gradient between volume-averaged temperatures. We consequently approximate \( q^d \) as,

\[
q^d \approx -(1 - \Phi)k_s \nabla \langle T \rangle \bigg|_{\text{solid}} - \Phi k_v \nabla \langle T \rangle \bigg|_{\text{vapor}},
\]

where \( \Phi \) is the porosity of the membrane, and \( k_s \) and \( k_v \) are the thermal conductivities of the solid and vapor, respectively. We then reduce the thermal conductivity relation to an equivalent effective thermal conductivity, \( k_{ave} = -(1 - \Phi)k_s - \Phi k_v \), so that \( q^d = k_{ave} \nabla T \).

To approximate the time rate-of-change \( \frac{dE_{CV}}{dt} \), we first consider that thermal energy is stored in the vapor and solid of the cell. Using an average temperature \( \langle T \rangle \) and porosity \( \Phi \), we approximate \( E_{CV} \) as,

\[
E_{CV} = V_{CV} \left[ \Phi \left( \rho_{c_p} \right)_v + (1 - \Phi) \left( \rho_{c_p} \right)_s \right] \langle T \rangle,
\]

where \( V_{CV} \) is the volume of the cell. We reduce the \( \rho \) and \( c_p \) terms to an equivalent effective relationship, \( (\rho c_p)_{ave} = \Phi (\rho c_p)_v + (1 - \Phi) (\rho c_p)_s \), so that \( E_{CV} = V_{CV} (\rho c_p)_{ave} \langle T \rangle \).

Finally, we take the derivative of equation (3.14) with respect to time, such that

\[
\frac{dE_{CV}}{dt} = V_{CV} \frac{d[(\rho c_p)_{ave} \langle T \rangle]}{dt}.
\]

This accounts for all energy terms in (3.11) within the composite membrane, and we can define (3.11) using average cell temperatures. For convenience, we combine equations
(3.11) through (3.14) and express the result in integral form as,

\[
\int_V \frac{d[(\rho c_p)_{ave} T]}{dt} dV + \int_S T(c_p)(j \cdot n) dA = k_{ave} \int_S (\nabla T \cdot n) dA,
\]

where \( j \) is the mass flux vector. Following an identical procedure, we can show that heat transport through the mesh is governed by an identical equation. The only conceptual issue there, is that while the pores of the membrane are very small, the pores within the mesh are much larger, such that our assumption that the cell is much larger than the pore is not as well satisfied within the mesh.

### 3.3.1 Boundary conditions of the for the composite membrane

We apply no-flux conditions to the inlet and outlet surfaces of the composite membrane, including both the upper membrane layer and underlying mesh,

\[
\frac{\partial T}{\partial x} \bigg|_{x=0,L} = 0, \text{ for } -\delta_1 - \delta_2 \leq y \leq 0
\]  

(3.17)

On the lateral side walls \((z = \pm W/2)\), the boundary condition for the mesh and membrane layer differ. We assume the membrane layer is thermally insulated, such that

\[
\frac{\partial T}{\partial z} \bigg|_{z=\pm W/2} = 0.
\]

(3.18)

In the mesh, we apply the heat flux \( q_{in} \),

\[
-k^2 \frac{\partial T}{\partial z} \bigg|_{z=\pm W/2} = \pm q_{in}.
\]

(3.19)

We insulate the bottom of the composite mesh bottom wall \((y = -\delta_1 - \delta_2)\)

\[
\frac{\partial T}{\partial y} \bigg|_{y=-\delta_1-\delta_2} = 0.
\]

(3.20)

At the feed-membrane surface \((y = 0)\) we apply the liquid-vapor phase change boundary condition. For this, we apply equation (3.7).

At the membrane-mesh surface \((y = -\delta_1)\), conservation of energy requires the sum of heat conduction and advection between the mesh and membrane interface to balance. We
apply principles of conservation of energy for an interface with no phase change, such that,

\[ T|_{y=-\delta^1_1} = T|_{y=-\delta^1_2}, \quad k_1 \frac{\partial T}{\partial y} \bigg|_{y=-\delta^1_1} = k_2 \frac{\partial T}{\partial y} \bigg|_{y=-\delta^1_2}, \]  

(3.21)

where \( k_1 \) and \( k_2 \) are the effective thermal conductivity of the membrane and mesh, respectively.

### 3.4 Neglecting the Navier-Stokes

During the early development of our code, we replaced the Navier-Stokes equations with the analytical solution for fully developed laminar duct flow [48]. This aligned excellently with the model goals and ambitions at the time. With the inclusion of the vaporization model discussed in section 3.3, short time constraints made it impossible to implement both the Navier-Stokes solver and conjugate vapor transport simultaneously. We prioritized including vapor transport because it better aligned with the project goals at the time. Since the inclusion of vapor transport to the model, we prioritized developing the Navier-Stokes solver. We have managed to successfully numerically discretize them and verify them through manufactured exact solutions following similar methods discussed in Chapter 4. Unfortunately, the Navier-Stokes solution could not be implemented to the VMD model prior to this study, and will be left to future work.

#### 3.4.1 Approximate fluid flow models

Our simulations of heat transport in a duct with a heated impermeable plate replace the full Navier-Stokes and continuity equations with an analytical solution for fully developed laminar duct flow [48]

\[ u(y, z) = \sum_{n=1,3,...}^{\infty} -\frac{U_{ave}a_n}{d} \left[ 1 - \frac{\cosh\left(\frac{n\pi y}{W}\right)}{\cosh\left(\frac{n\pi H}{2W}\right)} \right] \cos\left(\frac{n\pi z}{W}\right), \quad v = w = 0, \]  

(3.22)

\[ a_n = \frac{48(-1)^{n+1}}{\pi^3 n^3}, \quad d = 1 - \frac{192W}{\pi^5 H} \sum_{m=1,3,...}^{\infty} \frac{\tanh\left(\frac{m\pi H}{2W}\right)}{m^5}, \]  

(3.23)

where \( U_{ave} \) is the mean inlet velocity. For our simulations of heat transport in the VMD system with a heated composite membrane, at a minimum we must include the effects of
heat transport in the feed due to advection in the membrane-normal $y$-direction. We consequently continue to model the downstream flow component $u$ as a fully developed duct flow, and we continue to neglect any spanwise flow in the $z$-direction, $w = 0$. However, we add a membrane normal velocity component equal to
\[ v(x, z) = \frac{j_v}{\rho}. \] (3.24)

This minimum model is no longer an exact solution of the Navier-Stokes equation. It is motivated by the fact that the transmembrane flow is typically three to four orders-of-magnitude smaller than the inlet feed velocity. Consequently, the profile for $u$ differs very little from that of fully developed duct flow. Unfortunately, the membrane-normal velocity field $v(x, z)$ does not vary in the $y$-direction, and consequently does not satisfy the no-slip conditions on the channel side walls at $z = \pm W/2$ or the no-penetration condition at the upper wall $y = H$. Our philosophy is that the error introduced is likely small, due to the fact that $v$ is so small. In any case, this simplification will be removed once we incorporate our full Navier-Stokes solver.
CHAPTER 4
NUMERICAL METHODS

We develop our numerical code by considering a series of simpler problems to which we add the relevant physics incrementally over time. First, we develop a finite-volume code to simulate 3-D heat transport in a channel. Next, we develop a finite volume code to simulate heat transport in a feed channel overlaying an impermeable plate that is heated laterally. That code is then further generalized to consider a composite plate composed of two layers of impermeable material with different thermophysical properties. Finally, we incorporate heat and vapor transport through a heated composite membrane. For each step of the code development above, we verify the codes by comparing against manufactured analytical solutions. We validate the final code by comparing with experimental measurements of vapor flux performed by our collaborator at UCLA.

4.1 Numerical discretization of the feed channel

We spatially discretize the thermal energy equation (3.3) in the feed channel (shown in Figure 4.1) using second order finite-volume methods on a uniform staggered grid. To simplify the presentation of the method, we consider a simpler 2-D slice of the finite-volume grid in the longitudinal $x$-$y$ plane. We store the temperature field $T$ at cell centroids, while $u$ and $v$ are stored at the center of the cell face, as illustrated in Figure

Figure 4.1: Illustration (not to scale) of 3-D laminar channel domain of the VMD system. The domain is length $L$, width $W$, and height $H$. 
4.2. We then write the energy equation in control volume form as

\[ \rho c_p \int_V \frac{\partial T}{\partial t} dV + \rho c_p \int_S T(\mathbf{u} \cdot \mathbf{n})dA = k \int_S (\nabla T \cdot \mathbf{n})dA + \int_V f dV, \tag{4.1} \]

where \( V \) and \( S \) are the volume and surface of a finite-volume cell, and the forcing term \( f \) is introduced for benchmarking purposes, as explained later.

We approximate the volume integrals in equation (4.1) as

\[ \int_V \frac{\partial T}{\partial t} dV \approx \frac{\partial T_p}{\partial t} \Delta x \Delta y, \quad \int_V f dV \approx f \Delta x \Delta y, \tag{4.2} \]

where \( \Delta x \) and \( \Delta y \) are the cell dimensions, and \( T_p \) is the temperature at the cell center, as indicated in Figure 4.2.

We approximate the surface integral representing advection as

\[ \int_S T^n(\mathbf{u} \cdot \mathbf{n})dA \approx T_e u_e \Delta y - T_w u_w \Delta y + T_n v_n \Delta x - T_s v_s \Delta x, \tag{4.3} \]

where the subscripts denote evaluation at the points labeled in Figure 4.2. The face temperatures are approximated using the trapezoidal rule, for example,

\[ T_e \approx \frac{T_E + T_P}{2}. \tag{4.4} \]

Figure 4.2: 2-D interior cell \( x-y \) staggered grid. \( T, u, \) and \( v \) are stored at the locations indicated by the circles, squares, and triangles, respectively.
We approximate the surface integral representing diffusion as
\[
\int_S (\nabla T^n \cdot \mathbf{n}) \, dA \approx \left\{ \frac{\partial T}{\partial x} \bigg|_e - \frac{\partial T}{\partial x} \bigg|_w \right\} \Delta y + \left\{ \frac{\partial T}{\partial y} \bigg|_n - \frac{\partial T}{\partial y} \bigg|_s \right\} \Delta x,
\]
(4.5)
where subscripts denote evaluation at the four face centers labeled in Figure 4.2. We approximate derivatives using second-order centered differences. For example,
\[
\frac{\partial T}{\partial x} \bigg|_e \approx \frac{T_E - T_P}{x_E - x_P}.
\]
(4.6)

We discretize the thermal energy equation in time using a first order forward Euler method
\[
\frac{\partial T}{\partial t} \approx \frac{T^{n+1} - T^n}{\Delta t},
\]
(4.7)
where \(\Delta t\) is the time step, and the superscript \(n\) denotes a field evaluated at time \(t = n \Delta t\). With this, we solve for temperature \(T^{n+1}_P\) explicitly
\[
T^{n+1}_P = T^n_P + \frac{\Delta t}{\Delta V} \left[ \int_S -T^n (\mathbf{u} \cdot \mathbf{n}) \, dA + \alpha \int_S (\nabla T^n \cdot \mathbf{n}) \, dA \right],
\]
(4.8)
where \(\Delta V = \Delta x \Delta y\) and \(\alpha = \frac{k}{\rho c_p}\) is the thermal diffusivity of the feed corresponding to the inlet temperature.

At the external surfaces of the numerical domain, we apply boundary conditions by introducing grid points on the boundary faces, such as the point labeled B in Figure 4.3.

![Figure 4.3: 2-D boundary cell. Additional temperature nodes are added to the wall, as shown by B.](image-url)
We then generalize the boundary conditions as Robin conditions of the form

\[ aT^{n+1} + b(n \cdot \nabla T^{n+1}) = g, \tag{4.9} \]

where \(a\) and \(b\) are coefficients, \(n\) is the unit normal to the boundary, and \(g\) is the boundary source term. We discretize condition (4.9) using finite difference methods. Using the boundary point B in Figure 4.3 as an example,

\[ aT_B + b \left[ \frac{T_P - T_B}{x_P - x_B} \right] = g. \tag{4.10} \]

Given an initial temperature field \(T^n\), our fully explicit discretization allows us to solve for \(T^{n+1}\) using only information from the previous time step, i.e. without the need to solve a large matrix problem. Using the standard practice in CFD, we verify the spatial accuracy of our discretization with respect to a manufactured analytical solution,

\[ T_e = \sin(x) \sin \left( \frac{\pi y}{H} \right) \cos(z), \quad u_e = \sin(z) \cos(y), \tag{4.11} \]

\[ v_e = \cos(z) \sin(x), \quad w_e = \sin(y) \sin(x). \tag{4.12} \]

These fields satisfy the thermal energy equation (3.3) with the inclusion of an appropriate forcing term \(f\). To test the spatial accuracy, we initialize \(T^0 = 0\) and integrate in time using \(N^3\) total finite volumes (\(N\) in each direction) until we reach a steady-state. We then evaluate the spatial relative error using an infinity norm,

\[ E_N = \frac{||T - T_e||_\infty}{||T_e||_\infty}. \tag{4.13} \]

This current study is only interested in steady-state results. Therefore, evaluating the temporal accuracy is not necessary, but will be considered in the future. Figure 4.4 shows a log-log plot of \(E_N\) vs \(N\) when we set \(L = W = 1\) and \(H = 4\). Dirichlet conditions (a=1, b=0) were applied on all boundaries. We see that the error decreases as \(E_N \sim N^{-2}\), i.e. with second-order spatial accuracy. We repeated the analysis for several combinations of Neumann and Dirichlet conditions, and consistently observed second order accuracy.
Figure 4.4: Error results for temperature $T$, showing $E_N$ vs. $N$. The dashed line shows $1/N^2$.

4.2 Fully-developed duct flow over a heated plate

We next consider conjugate heat transport between a duct flow and an underlying impermeable plate heated laterally, as illustrated as in Figure 4.5. Heat transport in the plate is governed by the heat equation without advection

$$\rho_p (c_p)_p \int_V \frac{\partial T}{\partial t} dV = k_p \int_S (\nabla T \cdot \mathbf{n}) dA + \int_V f_p dV, \quad (4.14)$$

where $\rho_p(c_p)_p$, and $k_p$ are the density, specific heat, and thermal conductivity of the plate, respectively.

This equation is discretized spatially and temporally exactly as in the duct,

$$T_{p}^{n+1} = T_{p}^{n} + \frac{k_p \Delta t}{\Delta \rho_p (c_p)_p V} \int_S (\nabla T^n \cdot \mathbf{n}) dA + \frac{\Delta t}{\rho_p(c_p)_p} f, \quad (4.15)$$

where the diffusive term is discretized using centered differences.

Conservation of energy at the duct-plate interface requires

$$k_p \frac{\partial T}{\partial y} \bigg|_{y=0^-} = k_f \frac{\partial T}{\partial y} \bigg|_{y=0^+}, \quad (4.16)$$

where $k_f$ is the thermal conductivity in the fluid. To apply the interface conditions between the plate and duct, we introduce temperature nodes on the feed-plate interface,
Figure 4.5: Illustration (not to scale) of a feed channel domain overlying an impermeable plate. The domain is length $L$, width $W$, and height $H$ while the plate has a thickness $\delta_1$.

such as those labeled I in Figure 4.6. This shared node enforces continuity of temperature, and allows us to discretize equation (4.16) as

$$-k_p \frac{T_I - T_S}{y_I - y_S} = -k_f \frac{T_N - T_I}{y_N - y_I},$$

(4.17)

where the temperature subscripts correspond to Figure 4.6. Note that discretization (4.17) uses one-sided approximations that account for the fact that $\partial T/\partial y$ is discontinuous at the

Figure 4.6: 2-D Illustration (not to scale) of the cells adjacent to the interface between the plate (shaded grey) and duct flow (unshaded). Note that additional temperature nodes (labeled I) are introduced at the interface.
interface. The code is developed to apply general Robin boundary conditions on all other external boundaries of the plate and duct.

We verify the spatial accuracy of our discretization with respect to the following manufactured solution,

$$\begin{align*}
T_e &= \begin{cases}
\sin(x) \sin \left( \frac{\pi y}{H} \right) \cos(z) & 0 \leq y \leq H \\
\frac{k_f H}{k_p \delta_p} \sin(x) \sin \left( \frac{\pi y}{\delta_1} \right) \cos(z) & -\delta_1 \leq y \leq 0
\end{cases} \\
\left(4.18\right)
\end{align*}$$

$$\begin{align*}
u_e &= \begin{cases}
\sin(z) \cos(y) & 0 \leq y \leq H \\
0 & -\delta_1 \leq y \leq 0
\end{cases} \\
\left(4.19\right)
\end{align*}$$

$$\begin{align*}
v_e &= \begin{cases}
\cos(z) \sin(x) & 0 \leq y \leq H \\
0 & -\delta_1 \leq y \leq 0
\end{cases} \\
\left(4.20\right)
\end{align*}$$

$$\begin{align*}
w_e &= \begin{cases}
\sin(y) \sin(x) & 0 \leq y \leq H \\
0 & -\delta_1 \leq y \leq 0
\end{cases} .
\left(4.21\right)
\end{align*}$$

Figure 4.7: Error results for temperature $T$, showing $E_N$ vs. $N$. $T_D$ (circles) shows the error in all Dirichlet conditions, where $T_N$ (triangles) shows the error in all Neumann except for the inlet. The dashed line shows $1/N^2$. 

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These fields satisfy the thermal energy equation in the feed channel and plate with the inclusion of appropriate forcing terms. They also satisfy the interface conditions between the feed and mesh. To test the spatial accuracy of our discretization method, we initialize $T^0 = 0$ in both the plate and duct. We set $L = 4$, $W = 4$, $H = 4$, $\delta_p = 2$, $k_f = 1$, and $k_p = 2$. We separately test for the case of Dirichlet conditions on all boundaries. We then test Neumann conditions ($a=0$, $b=1$) to all but the inlet, at which we apply a Dirichlet condition. We then integrate in time using $N^3$ total finite volumes, such that both the duct and plate were discretized into $N_x = N_z = N$ and $N_y = N/2$, until we reach a steady-state, then we evaluate the spatial error using equation (4.13). Figure 4.7 depicts second-order spatial accuracy for both $T_D$ and $T_N$.

4.3 VMD system with transmembrane heat and vapor model

Finally, we consider the heated VMD system of a feed channel above a composite membrane, as illustrated in Figure 4.8. We write the energy equation for the mesh and membrane in control volume form as

$$\int_V \frac{d[(\rho c_p)_{ave}T]}{dt} dV + \int_S (c_p)vT(j \cdot n)dA = k_{ave}\int_S (\nabla T \cdot n)dA + \int_V f_{ave}dV,$$

where the effective thermophysical properties vary depending on whether equation (4.22) is solved in the membrane or mesh. The spatial terms of equation (4.22) are discretized using an identical procedure to those in the channel. However, the temporal discretization is slightly different with the inclusion of $(\rho c_p)_{ave}$ within the time derivative

$$\frac{d[(\rho c_p)_{ave}T]}{dt} = \frac{[(\rho c_p)_{ave}T]^{n+1} - [(\rho c_p)_{ave}T]^n}{\Delta t},$$

where $[(\rho c_p)_{ave}T]^n = (\rho c_p)_{ave}^n T^n$. We extrapolate from the previous time step ($n - 1$), so that

$$(\rho c_p)_{ave}^{n+1} \approx 2(\rho c_p)_{ave}^n - (\rho c_p)_{ave}^{n-1},$$

where $(\rho c_p)_{ave}^n = (\rho c_p)_{ave}^{n-1}$ at the first time step.
We discretize the interface condition (4.25) at the interface as

\[-k_1 \frac{T_I - T_S}{y_I - y_S} + k_f \frac{T_N - T_I}{y_N - y_I} = j_v \lambda,\]

(4.25)

where the subscripts I, S, and N refer to points labeled in Figure 4.6. We also discretize equation (4.25) in time as

\[-k_1 \frac{T_{I}^{n+1} - T_{S}^{n}}{y_I - y_S} + k_f \frac{T_{N}^{n} - T_{I}^{n+1}}{y_N - y_I} = j_v^{n} \lambda^{n},\]

(4.26)

where \(j_v^{n}\) and \(\lambda^{n}\) are both evaluated using the temperature field at the previous time step. Generalized robin boundary conditions are applied to the external surface of the domain.

We verify the spatial accuracy of our discretization with respect to the following manufactured solution

\[T_e = \begin{cases} 
\sin(x) \sin\left(\frac{\pi y}{H}\right) \cos(z) & 0 \leq y \leq H \\
\frac{k_f H}{k_1 \delta_1} \sin(x) \sin\left(\frac{\pi y}{\delta_1}\right) \cos(z) & -\delta_1 \leq y \leq 0 \\
\frac{k_f \delta_2}{k_2 H} \sin(x) \sin\left(\frac{\pi (y+\delta_1)}{\delta_2} - \pi\right) \cos(z) & -\delta_2 - \delta_1 \leq y \leq -\delta_1
\end{cases},\]

(4.27)

\[u_e = \sin(z) \cos(y), \quad v_e = \cos(z) \sin(x), \quad w_e = \sin(y) \sin(x).\]

(4.28)

These fields satisfy the thermal energy equations in the feed channel (4.1), membrane, and mesh (4.22) with the inclusion of appropriate forcing terms. Unlike the system shown in
Figure 4.9: Error results for temperature $T$, showing $E_N$ vs. $N$. $T_D$ (circles) shows the error for the Dirichlet conditions and $T_N$ (triangles) shows the error for all Neumann except for the inlet. The dashed line shows $1/N^2$.

Figure 4.8, we apply mass flux in all directions within the membrane and mesh via $u_e$, $v_e$, and $w_e$ in equation (4.28). Additionally, these fields do not satisfy the phase-change boundary at $y = 0$ (4.25), and instead they solve a simpler thermally conductive interface condition

$$k_1 \frac{\partial T}{\partial y} \bigg|_{y=0^-} = k_f \frac{\partial T}{\partial y} \bigg|_{y=0^+},$$

which we spatially discretize the same as the duct-plate interface condition (4.17). For the membrane-mesh $y = -\delta_1$, these fields satisfy that interface condition. We test the numerical solver for cases with Dirichlet boundary conditions ($a=1,b=0$) applied to each wall of the domain.

To test the spatial accuracy of our discretization method, we set $L = 2\pi$, $W = 2\pi$, $H = 2\pi$, $\delta_1 = 2\pi$, $\delta_2 = 2\pi$, $k_f = 2$ $k_1 = 2$, and $k_2 = 2$. We then initialize $T^0 = 0$ and integrate in time using $N^3$ total finite volumes, such that each of the duct, membrane, and mesh discretized to $N_x = N_z = N$ and $N_y = N/3$ until we reach a steady-state. Figure 4.9 shows second-order spatial accuracy for both $T_D$ and $T_N$. 
CHAPTER 5

RESULTS

We then consider the system configurations for duct flow over a heated plate and VMD with an actively heated composite membrane, for which we showed governing equations in Chapter 3. Using the numerically discretized equations from Chapter 4, we investigate the effects of system geometry, operating conditions, and the properties of the heated material on heat and mass transport in the system. First, we perform a series of parametric studies on the plate system configuration to characterize temperature polarization and temperature uniformity across the channel. Then, we validate our numerical solver with measurements of vapor flux performed by UCLA experiments. Finally, we perform a second parametric study for the VMD system configuration exploring temperature polarization, temperature uniformity spanning the channel, and vapor production.

5.1 Fully-developed duct flow over a heated plate

To investigate the impact of module geometry, operating conditions, and plate properties on heat transfer in the plate and duct flow configuration (Figure 5.1), we performed a parametric study in which we fixed the feed duct length and height, $L = 1 \text{ m}$. 

![Figure 5.1: Sketch (not to scale) of 3-D laminar heated duct flow.](image-url)
and $H = 2$ mm, and the inlet feed temperature $T_{in} = 30$ °C. We chose $L$ and $H$ to emulate those of an industrial membrane [49]. The thermophysical properties of the plate were set to those of copper. We then systematically varied the feed flow rate $U_{ave}$, system width $W$, and plate thickness $\delta_p$. For each combination of conditions, we ran a series of simulations to find the required input heat $q_{in} = q_{100}$ to attain a maximum temperature of 100 °C on the interface between the plate and feed channel. In all cases, the maximum temperature occurred at the system outlet. For $q_{in} = q_{100}$, we also compute the average plate temperature defined as

$$T_{ave} = \frac{1}{LW} \int \int_{A_p} T_p dA,$$

(5.1)

where $A_p$ and $T_p$ are the plate surface area and surface temperature, respectively.

Figure 5.2(a) shows results for the case $W = 8$ cm, $U_{ave} = 10$ cm/s, and $\delta = 0.2$ mm. The four curves show cross section temperature profiles along the plate surface, as sketched in panel (c). We see that lateral heating tends to preferentially heat the fluid near the side

![Figure 5.2](image-url)

Figure 5.2: Downstream temperature profiles on the plate surface at $x = L/4$, $x = L/2$, $x = 3L/4$, and $x = L$ for $W = 8$ cm, $U_{ave} = 10$ cm/s, and $q_{in} = q_{100}$ when (a) $\delta_p = 0.2$ mm and (b) $\delta_p = 1$ mm. (c) Shows downstream location of each temperature profile.
walls, leaving the temperature in the center of the plate relatively cool. This is because the plate behaves as a heat fin. Energy enters laterally to the plate. As it conducts toward the plate center \((z\text{-direction})\), it also conducts toward the duct-plate interface \((y\text{-direction})\). Because \(W \gg \delta_p\) for this system \((W/\delta_p \sim 10^2)\), the heat transfer resistance to the duct-plate interface will be lower than that to the plate center. This causes the large increase in temperature near the lateral edges of the system. The maximum temperature \(T = 100 \, ^\circ\text{C}\) occurs at the side walls at the outlet. Figure 5.2(b) shows equivalent results when we increase the membrane thickness to 1 mm. The thicker plate transports heat much further into the channel, raising the temperature of the plate center to roughly 65 \(^\circ\text{C}\) at the outlet, compared to only 36 \(^\circ\text{C}\) for \(\delta_p = 0.2 \, \text{mm}\). We repeated the simulations demonstrated in Figure 5.2 for the thickness \(\delta_p = 0.2, 0.4, 0.6, 0.8, 1.0 \, \text{mm}\), keeping \(W = 8 \, \text{cm}\), and \(U_{\text{ave}} = 10 \, \text{cm/s}\). The blue circle symbols in Figure 5.3 show our results for \(q_{100}\) (a) and \(T_{\text{ave}}\) (b). We see that increasing the plate thickness increases the amount of heat, \(q_{100}\), that can be supplied to the system and the resulting average plate temperature. For a thicker plate, the heat transport resistance to the duct-plate interface increases, which means the resistance to the plate center is relatively smaller for thinner plates. The system will reach the maximum temperature \(T = 100 \, ^\circ\text{C}\) at the lateral walls, and therefore this

Figure 5.3: Variation of (a) \(T_{\text{ave}}\) and (b) \(q_{100}\) versus plate thickness \(\delta_p\) when \(W = 8 \, \text{cm}\). For each case, results for \(U_{\text{ave}} = 10 \, \text{cm/s}\) (blue circles) and \(U_{\text{ave}} = 1 \, \text{cm/s}\) (red stars) are shown.
Figure 5.4: Temperature profiles on the plate surface at the outlet when $W = 8$ cm for (a) $\delta_p = 0.2$ mm and (b) $\delta_p = 1$ mm. Results for $U_{ave} = 1$ cm/s (dashed line) and $U_{ave} = 10$ cm/s (solid line) are shown with corresponding values of $q_{in} = q_{100}$ listed above each profile.

acts as a bottleneck for the total applied heating. Thicker plates have better pathways for lateral conductive heat transport and conduct a larger relative percent of the $q_{in}$ to the channel center, thus requiring higher values of $q_{in}$ before the system sidewall reaches $T = 100$ °C. Additionally, better heat distribution to the plate center results in better temperature uniformity across the channel, thus contributing to the higher average plate temperature.

We then investigate the impact of duct velocity ($U_{ave}$) on the system. We repeat simulations for $U_{ave} = 1$ cm/s and 10 cm/s, keeping the channel width fixed $W = 8$ cm for two plate thicknesses, $\delta_p = 0.2$ mm and 1 mm. Figure 5.4(a) shows temperature profiles along the plate surface at the outlet for the feed velocities $U_{ave} = 1$ cm/s (dashed line) and $U_{ave} = 10$ cm/s (solid line) for a plate thickness $\delta_p = 0.2$ mm, and channel width $W = 8$ cm. The corresponding $q_{100}$ for the two cases are marked in the Figure. We see that decreasing the feed velocity produces more uniform heating for a much lower $q_{100}$. This occurs because decreasing $U_{ave}$ decreases downstream heat advection from the plate surface, allowing heat in the plate to conduct further toward the channel center. Panel (b) shows results when the plate thickness is then increased to 1 mm. We see that the combination of a thicker plate and slower feed velocity provides a nearly uniform
Figure 5.5: (a) Downstream temperature profiles along the plate surface for $q_{in} = 109$ W, $U_{ave} = 1$ cm/s, $\delta_p = 1$ mm, and $W = 4$ cm. (b) Temperature profiles on the plate surface at the outlet for $U_{ave} = 1$ cm/s and $\delta_p = 1$ mm. Note that both temperature and $z$-position are presented as normalized values $T/T_{max}$ and $z/W$, respectively. Results for $W = 4$ cm (dashed line) and $W = 8$ cm (solid line) are shown with corresponding values for $q_{in} = q_{100}$ listed over each profile.

This excellent temperature uniformity is attributable to the relationship of heat...
transport resistances once again. With a large $\delta_p = 1$ mm, the conductive heat transport resistance to the duct-plate interface increases significantly in comparison to a thinner plate. The slow velocity $U_{ave}$ diminishes the convection coefficient at the duct-plate interface, which increases the convective heat transport resistance to the bulk duct flow. Additionally, a lower duct flow velocity reduces the rate at which energy in the duct flow is advected out of the system. Thus, the average temperature of the bulk fluid in the duct increases and the thermal gradient between the plate and bulk flow decreases. Finally, for low width channels, we expect the conductive heat transfer resistance between the lateral plate wall and the plate center to decrease. A heat fin is prone to convective heat transport throughout the entire fin length, i.e. the plate is prone to convective transport along the entire $z$-direction. By decreasing $W$, heat more easily conducts from the lateral plate wall ($z = \pm W/2$) to the plate center ($z = 0$) because the conductive pathway is simply exposed to less convective heat losses in the bulk flow. All of these physical effects combine to create the uniform temperature profiles present in Figure 5.5.

We can conclude from our parametric study that thicker plates, slower feed velocities, and smaller channel widths all compound to produce more uniform temperature distributions. These three design factors can also be varied to compensate for constraints. For example, though thicker plates improve heat transport to the channel center, we see that if we limit the thickness to the smallest considered $\delta_p = 0.2$ mm, we can compensate by decreasing $U_{ave}$ and $W$, as shown in Figure 5.5.

5.2 Actively heated composite membrane VMD

5.2.1 Comparison to experiments

To validate our numerical model of heat and mass transport in VMD systems with active mesh heating, we compare our numerical results to experiments performed at UCLA. The experimental system used is sketched in Figure 5.6. The channel dimensions are $L = 10$ cm, $W = 4$ cm, and $H = 4$ mm. The experiments used a composite membrane composed of a $0.2 \mu$m 3M polypropylene membrane overlying an aluminum mesh. The
The porosity and thickness of the 3M membrane are $\Phi_1 = 0.85$ and $\delta_1 = 100\,\mu$m, respectively.

The porosity and thickness of the mesh are $\Phi_2 = 0.27$ and $\delta_2 = 203.2\,\mu$m, respectively. The mesh is heated from only one side wall ($z = W/2$). For all experiments, the pressure in the vacuum chamber was held at $P_{\text{vac}} = 0.01$ bar. Experiments were performed for a range of heat inputs $q_{in}$, inlet temperature $T_{in}$, and inlet flow rates $U_{ave}$.

Figure 5.7: (a) Experimental and simulated data of permeate flux versus active heat input when $U_{ave} = 4.06$ cm/s. The red stars represent UCLA flux measurements. The blue circles and black triangles represent simulated flux values from our initial and best fit $A_m$, which has units of kg m$^{-2}$ s$^{-1}$ Pa$^{-1}$. (b) Comparison of mean error for each $A_m$ when $U_{ave} = 4.06$ cm/s. Our initial $A_m$ from Vanneste et al. [50] is shown via the red line.
The red symbols in Figure 5.7(a) show experimental results performed for a constant inlet velocity $U_{\text{ave}} = 4.06 \text{ cm/s}$ and three different values of input heat $q_{\text{in}}$. Note that error bars are only present for $q_{\text{in}} = 3.73 \text{ W}$ and 7.26 W. The blue circles show corresponding results from three simulations. All thermophysical properties and operating conditions are set to those of the experiments except for the membrane vapor permeability $A_m$. To determine $A_m$, we first use the value $A_m = 1 \times 10^{-6} \text{ kg m}^{-2} \text{s}^{-1} \text{ Pa}^{-1}$, reported in an experimental study by Vanneste et al. [50]. This produced the blue circles shown in Figure 5.7(a). Because the value reported by Vanneste et al. is an estimate, we repeat simulations for a range of vapor permeabilities and measure the mean percentage error

$$Err = \frac{100}{m} \sum_{i=1}^{m} \frac{|j_n - j_e|}{j_e},$$

(5.2)

where $m$ is the number of data points, $j_n$ is the vapor flux predicted by the simulations, and $j_e$ is experimentally measured vapor flux. Figure 5.7(b) shows the variation of $Err$ for a range of $A_m$ about our initial guess. We see that the value of $A_m = 7.4 \times 10^{-7} \text{ kg m}^{-2} \text{s}^{-1} \text{ Pa}^{-1}$ provides the best fit, shown by the black triangles in Figure 5.7(a), producing an error below 6%.

Figure 5.8 shows results from two additional series of experiments. Panel (a) shows

![Figure 5.8: Experimental and simulated data of permeate flux versus active heat input when (a) $U_{\text{ave}} = 9.97 \text{ cm/s}$ and (b) $U_{\text{ave}} = 16.29 \text{ cm/s}$. The red stars represent UCLA flux measurements. The blue circles represent simulated flux values from our best fit $A_m$, as identified in Table 5.1.](image)
Table 5.1: Summary of $A_m$ and mean percentage error for varying inlet feed velocities $U_{ave}$

<table>
<thead>
<tr>
<th>$U_{ave}$ (cm/s)</th>
<th>$A_m$ (kg m$^{-2}$s$^{-1}$Pa$^{-1}$)</th>
<th>Err (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.06</td>
<td>7.4E-7</td>
<td>5.9</td>
</tr>
<tr>
<td>9.97</td>
<td>6.6E-7</td>
<td>5.5</td>
</tr>
<tr>
<td>16.29</td>
<td>7.6E-7</td>
<td>8.6</td>
</tr>
</tbody>
</table>

results for $U_{ave} = 9.97$ cm/s, while panel (b) shows results for $U_{ave} = 16.29$ cm/s.

Unfortunately, only two data points are available in panel (a) and only three data points are available in panel (b). For each series of experiments we repeated the best fit procedure described above. The blue circle symbols in panel (a) were produced using the best fit $A_m = 6.6 \times 10^{-7}$ kg m$^{-2}$ s$^{-1}$ Pa$^{-1}$, while those in panel (b) were produced using $A_m = 7.6 \times 10^{-7}$ kg m$^{-2}$ s$^{-1}$ Pa$^{-1}$. We repeated the fitting procedure to confirm agreement with the data in panels (a) and (b). Using $A_m = 7.4 \times 10^{-7}$ kg m$^{-2}$ s$^{-1}$ Pa$^{-1}$, agreement was found for the data in panel (a) to just over 6% and for the data in panel (b) to just over 9%. This indicates that $A_m = 7.4 \times 10^{-7}$ kg m$^{-2}$ s$^{-1}$ Pa$^{-1}$ is also a suitable fit for all three data sets. All three of the data points in panel (b) have error bars because they were performed in either triplicate or duplicate. Table 5.1 summarizes the optimal vapor permeabilities and associated mean percentage error for the three sets of experiments. We see that the simulations reproduce the experiments to within 8.6%.

5.2.2 Parametric study of the actively heated VMD system

Now we perform a parametric study showing how the operating conditions, system geometry, and plate properties influence heat transport and vapor production in our VMD system with a composite heated membrane. We apply heat to both lateral sides of the composite membrane via the mesh, as sketched in Figure 5.9. We fix the channel length $L = 1$ m and height $H = 2$ mm. We also fix the inlet feed temperature $T_{in} = 30^\circ$C. The thermophysical properties of the membrane are set to those of the 0.2µm 3M polypropylene membrane used in the experiments at UCLA. The mesh porosity $\Phi = 0.27$ and the thermophysical properties of the mesh are set to those of the mesh used at UCLA.
Figure 5.9: Sketch of 3-D composite membrane case, with active heating on both laminar walls \((z = \pm W/2)\) only into the mesh, which is beneath the membrane.

We then systematically vary the inlet feed velocity \(U_{\text{ave}}\), vacuum pressure \(P_{\text{vac}}\), channel width \(W\), and plate thickness \(\delta_2\) for a series of simulations that vary the mesh heat input \(q_{in}\) between 1 to 400 W.

To investigate the impact of mesh heating \((q_{in})\), we consider a system with an inlet feed velocity \(U_{\text{ave}} = 10\) cm/s, vacuum pressure \(P_{\text{vac}} = 0.01\) bar, mesh thickness \(\delta_2 = 200\) µm, and channel width \(W = 8\) cm. Figure 5.10(a) shows cross-sectional temperature profiles along the membrane surface at downstream locations \(x = L/4, L/2, 3L/4,\) and \(L\) (the outlet) when \(q_{in} = 20\) W. The highest temperatures occur near the lateral walls, where the

![Figure 5.10(a)](image)

Figure 5.10: Downstream temperature profiles on the membrane surface at \(x = L/4, x = L/2, x = 3L/4,\) and \(x = L\) for \(U_{\text{ave}} = 10\) cm/s, \(P_{\text{vac}} = 0.01\) bar, \(W = 8\) cm, and \(\delta_2 = 200\) µm, when (a) \(q_{in} = 20\) W and (b) \(q_{in} = 400\) W.
heating is applied. The maximum temperature is always below the inlet value $T_{in} = 30^\circ C$, and also decreases with downstream distance. This occurs because the low heat input does not match that lost to evaporation. Figure 5.10(b) shows the corresponding results when the heating is increased to $q_{in} = 400$ W. The maximum temperature is now always above the inlet value, reaching $T = 55^\circ C$ at the outlet. The maximum temperature also increases with downstream distance. Meanwhile, the lowest membrane temperatures occur in the middle of the membrane, and remain near the inlet value $T_{in} = 30^\circ C$. We conclude that for this high heating value, $q_{in}$ exceeds the heat lost to evaporation, such that the temperature polarization is not only removed, but actually reversed. We also observe the profile near the lateral walls suddenly flattens on the nodes at each wall. This is an artifact of the discretization method of the insulated boundary condition at the lateral walls of the membrane and channel domains ($H \geq y \geq -\delta_1$, $z = \pm W/2$), as shown in equation (3.5). We discretize these boundary condition with a first order finite difference approximation, as shown in equation (4.10). Therefore, to satisfy the insulated boundary, the temperature gradient at the wall must equal zero so that,

$$T_B = T_P,$$  \hspace{1cm} (5.3)

where subscripts $B$ and $P$ are defined by Figure 4.3 on page 21. We could implement a higher ordered accuracy discretization on the boundary in future iterations to alleviate this flattening effect, but it will not be done here. The impacts of heating on vapor production are demonstrated in Figure 5.11, which shows the downstream variation of local vapor flux averaged over the channel width, $j_w(x)$. We see that for $q_{in} = 20$ W, the vapor flux decreases with downstream distance due to temperature polarization. In contrast, when $q_{in} = 400$ W we see $j_w(x)$ increase with downstream distance.

To explore the effects of inlet flow rate, we repeated the simulations shown in Figure 5.10 for the inlet flow rates $U_{ave} = 1$ and 10 cm/s, and for a mesh thickness $\delta_2 = 200 \mu m$, vacuum pressure $P_{vac} = 0.01$ bar, and channel width $W = 8$ cm. Figure 5.11 shows that for
low heat input, faster velocities result in a higher \( j_w(x) \). Alternatively, slow velocities result in higher \( j_w(x) \) when the system is subjected to high heat input. Figure 5.11 also indicates that a slow inlet flow rate and high heat will cause \( j_w(x) \) to approach a constant value at downstream locations. Figure 5.12(a) shows the effect of flow rate on the outlet membrane temperature profiles. We see that for high heat input \( q_{in} = 400 \text{ W} \), the faster feed velocity has a more uniform temperature profiles than the slower velocity. Panel (b) shows the inlet velocity effects on net vapor transport. For low input heat, faster inlet

Figure 5.12: Impact of inlet velocity \( U_{ave} \) on the (a) outlet temperature profiles when \( q_{in} = 400 \text{ W} \) and (b) net flux. We set \( P_{vac} = 0.01 \text{ bar} \), \( \delta_2 = 200 \text{ \mu m} \), and \( W = 8 \text{ cm} \).
velocity will produce higher vapor flux while the slower velocity produces higher fluxes at high input heat. We conclude that feed velocity may be leveraged to optimize vapor flux as a result of design constraints and available heat use within a VMD system.

We then investigate the impact of channel width. We repeated the simulations for channel widths \( W = 4 \) cm and 8 cm, and for a mesh thickness \( \delta_2 = 200 \mu m \), inlet flow rate \( U_{ave} = 10 \text{ cm/s} \), and vacuum pressure \( P_{vac} = 0.01 \text{ bar} \). Figure 5.13(a) shows the downstream temperature profiles on the membrane surface over a normalized channel width \((z/W)\) for an input heat \( q_{in} = 400 \text{ W} \) and channel width \( W = 4 \) cm. We observe an increasing temperature with downstream distance spanning the width of the channel. This is indicative that temperature polarization is reversed over the entire channel width. Figure 5.13(b) shows the outlet temperature profiles on the membrane surface for \( W = 4 \) cm (dashed) and \( W = 8 \) cm (solid), where \( q_{in} = 400 \text{ W} \). We see that the slimmer channel widths have a more relative uniform temperature profile than wider channels. When \( W = 4 \) cm the outlet temperature profile is higher than the inlet temperature \( T_{in} = 30 \degree C \), while the \( W = 8 \) cm case is lower than \( T_{in} \) at the center channel. Figure 5.14(a) shows the effect of channel width on the width-average vapor flux \( j_w(x) \) when \( q_{in} = 400 \text{ W} \). We see for \( W = 4 \) cm that \( j_w(x) \) increases to nearly twofold higher values than for \( W = 8 \) cm at...
Figure 5.14: (a) Downstream variation of the width-average vapor flux $j_w(x)$ when $W = 4$ cm (dashed) and $W = 8$ cm (solid) and $q_{in} = 400$ W. (b) Impact of channel width $W$ on net vapor production in $L/hr$. We set $P_{vac} = 0.01$ bar and $\delta_2 = 200 \mu$m.

downstream locations. Panel (b) shows the vapor volumetric flow rate in L/hr at each $q_{in}$, where the red dots show $W = 4$ cm and the blue circle symbols show $W = 8$ cm. We notice that the volumetric vapor flow rate for wider channels is larger than for slimmer channels. The membrane area of a slimmer channel is smaller, so while vapor flux may increase for smaller channel widths, the net vapor volumetric flow rate will decrease. We can compensate for this by using multiple small channel systems to increase the membrane area.

To explore the impact of mesh thickness, we repeated the simulations for mesh thickness $\delta_2 = 200 \mu$m, $400 \mu$m, $600 \mu$m, and $800 \mu$m, and for a channel width $W = 8$ cm, inlet flow rate $U_{ave} = 10$ cm/s, and vacuum pressure $P_{vac} = 0.01$ bar. Figure 5.15 shows temperature profiles on the membrane surface. Panel (a) shows profiles at downstream locations for $\delta_2 = 800 \mu$m and $q_{in} = 400$ W. We observe increasing temperature with downstream distance spanning the channel width, which shows the reversal of temperature polarization effects. Additionally, we see all profiles are higher than the inlet temperature at $T_{in} = 30^\circ$C spanning the entire channel. Panel (b) shows the profile at the outlet for $q_{in} = 400$ W. We see that thicker meshes provide better temperature uniformity spanning the channel when compared to a thinner mesh. Figure 5.16(a) shows the mesh thickness.
effects on width-averaged vapor flux $j_w(x)$ when $q_{in} = 400$ W. We observe slightly raised vapor flux values at all downstream locations for $\delta_2 = 200\, \mu m$ over $W = 800\, \mu m$. Panel (b) shows the variation in net vapor flux $j_v$ with respect to input heat $q_{in}$ for $\delta_2 = 200\, \mu m$ and $\delta_2 = 800\, \mu m$, which are shown by the red star symbols and blue circle symbols, respectively. At increasing heat input, we see that a thinner mesh will produce a slightly raised vapor flux over a thicker mesh. As the mesh thickness increases, more energy is

Figure 5.16: (a) Downstream variation of the width-average vapor flux $j_w(x)$ when $\delta_2 = 200\, \mu m$ (dashed) and $\delta_2 = 800\, \mu m$ (solid) and $q_{in} = 400$ W. (b) Impact of mesh thickness $\delta_2$ on net vapor flux. We set $P_{vac} = 0.01$ bar and $W = 8$ cm.
stored in the larger mesh when it is heated and the resistance to center-channel heat transport decreases. A thinner mesh stores less heat in the mesh, so that more heat conductively transfers to the evaporative interface and raises the vapor flux. At low heat inputs, we see very little change in vapor flux values relative to mesh thickness.

To investigate the effects of the vacuum pressure, we repeated the simulations for vacuum pressure $P_{\text{vac}} = 0.01 \text{ bar}$, $0.04 \text{ bar}$, and $0.07 \text{ bar}$, and for a channel width $W = 8 \text{ cm}$, inlet flow rate $U_{\text{ave}} = 10 \text{ cm/s}$, and mesh thickness $\delta_2 = 200 \mu\text{m}$. Figure 5.17 shows temperature profiles on the membrane surface when $q_{\text{in}} = 20 \text{ W}$. Panel (a) shows downstream profiles when $P_{\text{vac}} = 0.04 \text{ bar}$. We observe reversed temperature polarization effects near the lateral walls, even at low heat input $q_{\text{in}} = 20 \text{ W}$. Also the center-channel temperature is slightly under the inlet temperature $T_{\text{in}} = 30^\circ \text{C}$ and the temperature uniformity changes little with increasing downstream distance. Panel (b) shows outlet profiles when $P_{\text{vac}} = 0.01 \text{ bar}$ (dashed) and $0.04 \text{ bar}$ (solid). We observe both profiles are similarly uniform, but $P_{\text{vac}} = 0.04 \text{ bar}$ has a higher average temperature spanning the channel width. Figure 5.18 shows similar temperature profiles to Figure 5.17, but for $q_{\text{in}} = 400 \text{ W}$ instead. Panel (a) shows downstream temperature profiles on the membrane surface when $P_{\text{vac}} = 0.04 \text{ bar}$. We observe the increasing temperature with increasing

![Figure 5.17](image.png)

Figure 5.17: (a) Downstream temperature profiles on the membrane surface when $P_{\text{vac}} = 0.04 \text{ bar}$. (b) Comparison of outlet temperature profiles on the membrane surface for $P_{\text{vac}} = 0.01 \text{ bar}$ (dashed) and $P_{\text{vac}} = 0.04 \text{ bar}$ (solid). We set $\delta_2 = 200 \mu\text{m}$, $W = 8 \text{ cm}$, and $q_{\text{in}} = 20 \text{ W}$. 

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downstream position, indicating reversed temperature polarization effects spanning the channel width. Panel (b) shows outlet profiles for \( P_{\text{vac}} = 0.01 \text{ bar} \) (dashed) and 0.04 bar (solid). Like the case for \( q_{\text{in}} = 20 \text{ W} \), we observe similar effects of temperature uniformity between the both cases of vacuum pressure. However, \( P_{\text{vac}} = 0.04 \text{ bar} \) does have a slight improvement in temperature uniformity and higher average temperature in comparison to \( P_{\text{vac}} = 0.01 \text{ bar} \).

Figure 5.19 shows effects of vacuum pressure on width-averaged vapor flux \( j_w(x) \) when \( q_{\text{in}} = 400 \text{ W} \). We note the difference in \( j_w(x) \) at the inlet between these two cases is approximately 6 LMH as compared to 3 LMH at the outlet. This indicates that the width-averaged vapor flux of a weaker vacuum pressure (like \( P_{\text{vac}} = 0.04 \text{ bar} \)) is more sensitive to input heat \( q_{\text{in}} \) at downstream locations. We also note a lower vapor flux for \( P_{\text{vac}} = 0.04 \text{ bar} \) than \( P_{\text{vac}} = 0.01 \text{ bar} \) over the entire channel length. Panel (b) shows variations of vapor flux \( j_v \) with respect to input heat \( q_{\text{in}} \) for \( P_{\text{vac}} = 0.01 \text{ bar}, 0.04 \text{ bar}, \) and 0.07 bar, which are represented by the red star, blue circle, and black triangle symbols, respectively. We initially observe that the simulations for \( P_{\text{vac}} = 0.07 \text{ bar} \) resulted in negative values of flux at low heat inputs. This indicates that for high vacuum pressures,
the transmembrane vapor pressure difference in equation (3.1) is negative. This occurs if the saturation pressure \((P_{sat})\) is lower than the vacuum pressure \((P_{vac})\). This phenomenon causes vapor to flow back into the feed channel and condense at the liquid-vapor interface instead. For this reason, we neglect showing other temperature profiles and flux results for \(P_{vap} = 0.07\) bar. In panel \((b)\), we also observe an approximately flat flux difference between \(P_{vac} = 0.01\) bar and \(0.04\) bar, where the difference is \(\sim 5\) LMH for low heat input and reduces to \(\sim 4\) LMH for high heat input. This indicates vacuum pressure has a small sensitivity to input heat, in that increasing \(q_{in}\) for a higher vacuum pressure will increase vapor flux more than for a lower vacuum pressure. We conclude that vacuum pressure may be varied for an desired vapor flux and uniform temperature profile as a result of design constraints and useable heat within VMD systems.
CHAPTER 6
SUMMARY AND CONCLUSIONS

This study details the development of 3-D numerical methods to simulate heat and vapor transport in a VMD system with a composite heated membrane. This includes the derivation and discretization of the governing equations for conjugate heat and vapor transport in the membrane and mesh. Using these methods, we performed a parametric study for which we explored the effects of feed channel geometry, membrane and mesh properties, and operating conditions on heat transport and vapor production.

For standard VMD systems, one major advantage over other modes of MD is the lack of conductive heat loss through the membrane. As a result, numerous VMD models choose not to include the membrane in their domain of interest and instead only apply the evaporative boundary condition between the feed and membrane. Unfortunately this assumption is not valid for our system. This necessitated the development of the energy transport equations that govern the composite membrane for our VMD system. We derived these expressions by dividing our membrane domain into discrete cell volumes and applying conservation of mass and energy, so as to represent transport as fluxes at the cell faces. This membrane model, along with the channel heat equations, were discretized and verified for second order spatial accuracy against manufactured solutions.

We completed a parametric study of fully developed duct flow over a heated plate. In this, we varied the inlet flow rate, thickness of the plate, and channel width over a large range of input heats. We observed that slow flow rates, thicker plates, and smaller width channels provide results with the most uniform temperature profiles on the membrane surface. We also observe that decreases in channel width ($W = 8$ to $W = 4$) could result in twofold required input heat reductions, i.e. half the necessary heat for the same or more uniform temperature profile.

Following that, we fully implemented the model for heat and vapor transport in the composite membrane and performed a validation study against experimental flux results.
provided by UCLA. We compared to fluxes for flow rates of $U_{ave} = 4.06, 9.97, \text{ and } 16.29$ cm/s and fit the membrane vapor permeability $A_m$ in these studies to provide the best replication of simulation flux results. For each flow rate, we observed differences in mean error for their corresponding best fit ranging from 5% to 9%. For the early stage of project we are at, these values are an excellent agreement. Additionally, we see that a value of $A_m = 7.4 \times 10^{-7} \text{kg m}^{-2} \text{s}^{-1} \text{Pa}^{-1}$ provided mean error percentages ranging from slightly over 6% to slightly over 9%, which is still in good agreement.

Finally, we used the full solver to explore the impact of operating conditions, system geometry, and mesh properties for the system. We specifically looked at variations in input heat ($q_{in} = 1$ to 400 W), inlet flow rate ($U_{ave} = 10$ cm/s and 1 cm/s), mesh thickness ($\delta_2 = 200, 400, 600, \text{ and } 800 \mu m$), channel width ($W = 4$ cm and 8 cm), and vacuum pressure ($P_{vac} = 0.01$ bar, 0.04 bar, and 0.07 bar). For these studies, we applied the experimentally determined vapor permeability from our comparisons with UCLA. We noted that for low input heats when $U_{ave} = 10$ cm/s, $\delta_2 = 200 \mu m$, $W = 8$ cm, and $P_{vac} = 0.01$ bar, the highest downstream temperature is always below the inlet temperature, as the input heat cannot match heat losses to evaporation. As heat increased, we observed temperature profiles eliminating or even reversing effects of temperature polarization. We also observed the width-averaged vapor flux $j_w(x)$ increased downstream with increasing heat flux, and the opposite for low heat flux due to temperature polarization. For inlet flow rate, we observed that variations only slightly impacted the outlet temperature profiles at high heat input. However, when comparing $j_w(x)$ we noted that $U_{ave} = 1 \text{cm/s}$ had lower fluxes than $U_{ave} = 10 \text{ cm/s}$ at low heat inputs ($q_{in} < 200 \text{ W}$), but transitioned to higher fluxes or high heat inputs. This shows the importance of inlet flow rate effect on vapor flux.

For variations of the channel width, we observed downstream temperature profiles over a normalized channel width ($z/W$). We see slimmer channels potentially reverse temperature polarization over the entire channel, produce more uniform temperature profiles, and produce a higher vapor flux than wider channels. However, wider channels
produce a higher total vapor volumetric flowrate than slim channels. For slim-channel VMD systems to produce comparable volumetric flowrates to wide-channel systems, multiple slim-channel systems must be used with a total equivalent membrane area to the wide-channel system. For variations of mesh thickness, we see thicker meshes reverse temperature polarization over the entire channel width and have more uniform temperature profiles than thinner meshes. Additionally we note that mesh thickness does not impact vapor flux at low heat input. At equivalent high heat input, a thinner mesh produces a higher vapor flux than a thicker mesh. Therefore, we see mesh thickness can be optimized for better temperature uniformity or more vapor flux depending on desired characteristics of the system. For variations of vacuum pressure, we observe for low heat input that temperature uniformity does not change, but the channel-averaged temperature increases with increasing vacuum pressure. When operated with a high input heat, high vacuum pressure systems raise the channel-averaged temperature and slightly improve temperature uniformity when compared to low vacuum pressure systems. However, for systems with a higher vacuum pressure we see a dramatic decrease in vapor flux. When vacuum pressure is higher than the saturation pressure, we see the direction of vapor flux reverse and condense back into the feed solution at low heat input. Vacuum pressure may be optimized for a desired vapor flux and uniform temperature profile, subject to design constraints and available heat within VMD systems.

Ultimately, we show promising results for a conjugately heated model of VMD, which, to our knowledge, has never been done before. We were able to reproduce experimentally determined flux measurements with excellent agreement, and we have been able to characterize the operating conditions, system geometry, and mesh properties of the current VMD system. We have even shown means of reversing temperature polarization in our results.

In the future, the plans for the collaboration project with UCLA are to transition to an interest in concentration polarization effects of this system. This will shift the focus to implementations of the continuity, Navier-Stokes, solute advection-diffusion, and
electrodynamic equations. However, the implementation of heat transport was the first step to this multi-mode physical solver, as understanding temperature field contributions is the most important contributor to improving VMD system performance [8, 9]. This initial solver should ultimately serve as a foundation for the next physical layers of to be added, starting with the Navier-Stokes and continuity equations. These are already completed, but had yet to be implemented at the time of this study. Future work may also include improving the performance metrics of the solver and move towards parallelization. Originally, this solver was explicitly discretized to be very conducive to parallelization in the future, as these kinds of numerical methods partition into parallel tasks extremely well. Regardless, the development of these kinds of multi-physical models will be critical to understanding the limitations of temperature and concentration polarization fully. This is a step toward making solar heated VMD, or MD in general, a commercially viable process at a larger, industrial scale.
REFERENCES


