Static mixing spacers for spiral wound modules

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The University of Toledo
A Thesis
entitled

Static Mixing Spacers for Spiral Wound Modules

by
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Submitted to the Graduate Faculty as partial fulfillment of
the requirements for The Master of Science Degree in Chemical Engineering

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The University of Toledo
December 2012
Membranes play a critical role in many separation processes ranging from nitrogen production to desalination. Membranes are used most commonly in the form of fine hollow fibers or sheets. The sheet form is used to produce spiral wound modules that permit the efficient contacting of process streams with the membrane in a compact form. Spiral wound modules are the dominant form used in reverse osmosis and Nanofiltration membrane processes.

Spacers are used in spiral wound modules to create feed and permeate flow channels and to enhance mass transfer rates by reducing concentration polarization. Most spacers possess a ladder or mesh structure and rely on the generation of turbulence and eddies to enhance mass transfer. The literature contains numerous experimental and theoretical studies of how pressure drop and mass transfer rates depend on the geometry of these spacers.

We present a new spacer paradigm. The spacer acts as a static mixer for planar flow channels and effect mixing without generating turbulence and eddies. Simulations of flow
and mass transfer with the new spacer were performed using the computational fluid dynamics program, FLUENT. Flow visualizations clearly show how the spacer mixes the fluid. Furthermore, spacer prototypes were constructed and evaluated for mass transfer performance and pressure drop-flow rate characteristics. Significant enhancement in mass transfer was observed by experimental measurements for fabricated static mixer spacer. Experimental results were compared for the static mixer spacer, a commercial spacer and an empty channel and results in terms of Sherwood number, Power number and friction factor. Future works are proposed to have a better comparison for experimental and simulation results.
Acknowledgements

I wish to express my sincere gratitude to my advisor Dr. Glenn Lipscomb. I would also like to thank Dr. Sasidhar Varanasi and Dr. Maria Coleman for their guidance and useful suggestions.

I would like to thank Dr. Glenn Lipscomb for giving me admission in University of Toledo. I am grateful to the United States Bureau of Reclamation and Department of Chemical and Environmental Engineering for financial support throughout the course of my study.

I would like to thank my labmates and friends, Rahul Patil and Xi Du, for their help, support and encouragement.
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Chapter 1

Overview of Membrane Filtration

1.1. Introduction

More than 1 million people have insufficient access to water in developing countries. Consequently, there is great interest in developing novel, effective methods for desalination and other drinking water production processes. Membrane separation is one of the cost effective methods for fresh water production. Removing organic and inorganic compounds and microorganisms from water to produce high quality drinking water is an important advantage of membrane processes. A good example of the effectiveness of membrane filtration is microorganism disinfection where UV irradiation and chlorine disinfection have lost effectiveness as organisms resistant to removal by these techniques have emerged; such organisms, however, can be removed using membranes.

Additionally, membrane separation often requires fewer consumables in comparison with other commercial water treatment techniques where chemicals are added for water purification. Additional advantages are lower energy requirements, ease of operation and maintenance. Membrane separation costs can be significantly lower than other commercial methods [1].

A membrane is a thin layer of material which is made from an organic or inorganic material. This layer has the ability to separate molecules or particles by
preventing transport of unwanted species across the membrane. Solute or particle rejection may be based on size exclusion or electrostatic repulsion and the separation is driven by applying a differential pressure, or other chemical potential difference, across the membrane. Membranes have found extensive application in a number of situations. For instance, reverse osmosis technique has been used in the desalination industry since 1960. Since late 1980s, nanofiltration has been used for water softening and total organic carbon removal [2].

Color removal, water disinfection, industrial effluent cleaning, pathogen and suspended solids removal in medical applications, and toxin removal from the blood are various examples of membrane filtration in different industries [3].

![Figure 1-1: Membrane filtration spectrum based on pore size and removal capabilities](image)

[27]
Membranes are classified based on molecular weight cut-off. The molecular weight cut-off indicates the molecular weight of the smallest molecule which can pass through the membrane. As illustrated in Figure 1-1, the classifications include:

1. **Reverse osmosis**
2. **Nanofiltration**
3. **Ultrafiltration**
4. **Microfiltration**

### 1.1.1 Reverse Osmosis

Reverse osmosis (RO) is a membrane separation method in which pressure is applied to the feed solution to separate large molecules and ions from the feed solution by forcing the solvent across a membrane with an apparent pore size smaller than the rejected components but larger than the solvent. The solvent is collected on the permeate side of the membrane while the rejected components are removed from the retentate side of the membrane.

The apparent pore size of the membrane is critical to the separation. The pores should be large enough to let small solvent molecules pass while preventing the passage of larger solute molecules. In contrast, forward osmosis refers to a technique which equalizes the solute concentration on both sides of the membrane by permeation of the solvent through the membrane from the low solute concentration side to the high solute concentration side. When sufficient pressure is applied to reverse the osmotic pressure driven solvent flow, reverse osmosis occurs.

Reverse osmosis occurs by a solution-diffusion mechanism and the separation efficiency depends on the water flux, permeate solute concentration and required driving
pressure. For permeation to occur across the membrane, the applied pressure must overcome the osmotic pressure. Therefore, the reverse osmosis membrane should be strong enough to tolerate the applied pressure on the feed side. Reverse osmosis membranes are available as either hollow fiber or flat sheets.

### 1.1.2 Nanofiltration

Nanofiltration (NF) is similar to reverse osmosis. The degree of removal of monovalent species is the primary difference. Nanofiltration can remove 50% to 90% of the monovalent species depending on the membrane while the reverse osmosis membrane can remove monovalent ions at 97-99% level at 200 psi. However, bivalent and multivalent species are rejected by NF. The difference in monovalent ion rejection is due to the slightly larger apparent pore size of NF membranes which dramatically increases water permeation rates relative to RO.

### 1.1.3 Ultrafiltration

Ultrafiltration (UF) also is a pressure driven membrane separation technique. Water and low molecular weight solutes can pass through a membrane, but high molecular weight solutes and suspended solids are retained. Ultrafiltration membranes are used for separation of large molecules such as starch, protein and microorganisms such as viruses and bacteria [4]. An ultrafiltration membrane is capable of treating water turbidity at low pressures and used in water treatment to eliminate sedimentation and coagulation processes [5].
1.1.4 Microfiltration

The process of removing contaminants from a solution using a micro porous membrane is called microfiltration. Relative to RO and NF, microfiltration requires much smaller applied pressures to drive the separation [6].

1.2 Operational Modes

Membrane filtration systems can be operated in two modes:

1. Cross-flow and
2. Dead-end filtration

In cross-flow filtration, a feed stream flows parallel to the membrane surface while the permeate flows perpendicular to the feed across the membrane as illustrated in Figure 1-2. Feed components pass through the membrane as the permeate while larger components are rejected to form the retentate and flow along the membrane surface toward the retentate outlet. This tangential flow helps control the formation of a stagnant layer of rejected material (a cake layer) adjacent to the membrane surface which mitigates concentration polarization and fouling [7].

The feed flows normal to the membrane in dead-end filtration (see Figure 1-2). Rejected components buildup on the membrane surface to form a cake that increases in thickness with time. This cake increases the resistance to permeation and therefore requires increasing the feed pressure to maintain a constant permeation rate or results in a
reduction in permeate flow if the pressure is held constant. Back-flushing the membrane periodically can help remove the cake layer.

Figure 1-2: Cross-flow and dead-end filtration [28]

Two important factors which reduce membrane permeation rates and lifetime are concentration polarization and membrane fouling. Figures 1-3 and 1-4 illustrate fouling and concentration polarization [8].
Figure 1-3. Components of membrane fouling and concentration polarization in filtration [24].
1.2.1 Membrane Fouling

Membrane fouling is defined as internal or external pore blocking, gel formation, bacterial growth, feed particle adsorption and chemical interaction between membrane and solutes. Bacterial growth is of particular concern because it is difficult to remove. Membrane fouling reduces membrane lifetime, increases energy consumption, and reduces permeation rates across the membrane.

1.2.2 Concentration Polarization

During membrane filtration, rejected feed components accumulate along the retentate side of the membrane. This results in the formation of a concentration boundary layer in which the concentration of rejected components is higher than in the bulk solution. Concomitantly, the concentration of permeating components is reduced at the membrane surface which reduces the driving force for permeation and the permeation rate. Figure 1-4 illustrates the concentration polarization in the cross-flow filtration.
The degree of concentration polarization depends on the balance between convective transport of rejected components towards the membrane and diffusive transport away from the surface. The polarization layer can be reversible or irreversible. Polarization is reversible for non-aggregating rejected components such as molecular solutes but can result in the formation of a fouling gel layer for aggregating components especially in UF [9].

Membrane permeability and selectivity do not change as a result of concentration polarization. However, concentration polarization increases the osmotic pressure at the membrane surface in RO and NF which requires a higher applied pressure to generate the driving force for permeation.
1.3 Methods to Reduce Concentration Polarization and Membrane Fouling

Hydrodynamic, chemical and physical methods are the three main classes of techniques used to reduce concentration polarization and membrane fouling. Hydrodynamic methods rely on increasing the shear rate at the membrane surface to increase back transport of rejected components from the membrane surface to the bulk fluid. Chemical methods use a coagulant, such as a hydrophilic polymer, to aggregate the rejected component and hence increase effective size which reduces fouling potential [10].

Physical methods utilize an external field such as ultrasound or electric potential, to remove rejected components that accumulate along the membrane surface. All three methods are summarized in Figure 1-5 along with methods for implementing each that have been reported in the literature.

![Figure 1-5: Hydrodynamic, chemical and physical methods to reduce concentration polarization and membrane fouling [24].](image-url)
1.3.1. Spacer

Spacers are used widely in membrane filtration processes to create flow channels between two membrane sheets in spiral wound modules and promote mixing in the flow channels. Concentration polarization and membrane fouling can be minimized with spacer-induced mixing but the mixing process increases pressure drop and the energy required for flow through the channel.

The requirements for feed and permeate spacers are different. Feed and permeate spacers both create flow channels when a module is formed as shown in Figure 1-6. However, only the permeate spacer is required to keep the flow channel open in operation since the pressurized feed will push the membrane into the permeate channel. Concentration polarization and fouling typically are more significant in the feed channel so the mixing requirements for the feed spacer are greater than the permeate spacer.

![Figure1-6: Schematic of spacer for permeate and feed side.](image)
Commercial spacers commonly consist of cylindrical filaments that are either woven or overlain at different angles. The diamond and ladder configurations are shown in Figure 1-7. Mesh length, filament diameter, filament angle relative to the flow direction, and the angle between filaments are design variables [11].

![Diamond and Ladder Configurations](image)

**Figure 1-7:** Schematic of the diamond and ladder configuration mesh type spacer [13].

Woven and non-woven configurations are illustrated in Figures 1-8 and 1-9.

![Woven and Non-Woven Spacers](image)

**Figure 1-8:** Woven and non-woven spacers [12].
Figure 1-9: Woven and non-woven spacer textile [13].

Figure 1-10 illustrates a number of alternative spacer designs that have been reported in the literature. Relative to the conventional designs shown in Figure 1-10, the nonconventional alternatives include use of non-circular filaments, helical screw-like elements that possess characteristics similar to the static mixers used to mix fluids in circular pipes, wavy elements, and asymmetrical element arrangements.

Figure 1-10: Conventional and unconventional spacers [14].
1.4 Static Mixing Spacer

A theoretical and experimental study of new static mixing spacer element is reported in this thesis. The spacer mixes fluid in a rectangular flow channel without vorticity or turbulence. This mixing reduces concentration polarization and the potential for fouling. The mixing differs from that achieved with conventional static mixers for pipes in that the streamlines adjacent to the flow channel surface are moved from the surface to the middle of the flow channel.

A section of the proposed spacer design is illustrated in Figure 1-11 which also indicates how fluid flows through the element. The fluid is divided into two part flows to the top and bottom of front plate and then changes its direction by touching the static mixing spacer. Figure 1-12 illustrates how fluid is forced from the upper flow channel into the lower on the left and vice versa on the right.

Figure 1-11: Three dimensional sketch of static mixing spacer.
The movement of fluid illustrated in Figure 1-12 requires the upward flowing stream to pass around the downward flow stream. How this is accomplished is illustrated in Figure 1-13. Fluid in the upper portion of the channel is forced laterally into openings that allow it to move into the lower portion of the flow channel while fluid in the lower portion is forced to the center of the channel where it may move up through a third opening.
This design moves streamlines adjacent to the membrane, in which the concentration of rejected species is higher, to the middle of the flow channel and replaces them with fluid from the center of the flow channel. This mixing occurs at both the upper and lower membrane surfaces. Thus, the static mixing spacer mixes the flow to reduce concentration polarization and increase mass transfer.

In the following chapters, spacer design variables are identified. Fluid flow and mass transfer is simulated with spacers that possess a wide range of design dimensions to identify the most promising designs. Two of the most promising designs were fabricated using stereolithography. The performance of these designs was evaluated experimentally.
Chapter 2

Numerical Analysis

2.1 Introduction

The governing equations of conservation should be solved for concentration and velocity fields for a channel with and without a spacer to study the effect of the spacer on mass and momentum transfer. The finite volume method is applied to convert the governing differential equations to a set of non-linear algebraic equations. These equations provide point values for the velocity, pressure, and concentration at specific points in the flow domain. These points correspond to the nodes of a grid or mesh used to divide the flow domain into a set of small volume elements; the nodes lie at the center of each volume element.

In the finite volume method, the governing partial differential equations are transformed into algebraic equations by integrating the equations over the flow domain and applying the divergence theorem. The divergence theorem states that the volume integral of the divergence of a vector quantity is equal to the integral of the normal outward component of the vector quantity along the surface of the volume.

The computational fluid dynamics (CFD) program FLUENT is used primarily to solve the conservation of momentum, heat, and mass equations. Some results also are
reported using COMSOL Multiphysics which utilizes the finite element method to transform the partial differential conservation equations to algebraic equations.

### 2.2 Geometry Building and Mesh Construction

To perform a simulation, the boundary of the solution domain first must be defined. This can be done using tools provided with FLUENT or a supported third party computer aided design (CAD) program. SOLIDWORKS was used to create the solution domain for the work reported here. The SOLIDWORKS is a parasolid based CAD program. SOLIDWORKS uses parametric features of surfaces to create complex geometries and models. Parameters are subdivided into two main groups:

a. **Geometric parameters:** horizontal, vertical, parallel, concentric, tangent etc.

b. **2-numeric parameters:** line length, circle diameter, thickness etc.

To draw the spacer, a 2-D projection of the 3-D object is created. Dimensions are added to define the location of geometry and size of the model. Dimensions of the 2D sketch are controlled by entering specific values or defining relationships between dimensions in the drawing. The 2D sketch is extruded to create the desired 3D geometry; multiple objects may be combined or assembled by addition or subtraction to create complex features that cannot be extruded. SOLIDWORKS has an ability to save files in the Microsoft structured storage file format. The Parasolid (*.x_t, *.x_b) format is used to save drawings for import into FLUENT. All dimensions were specified in units of millimeters.
Figure 2-1: 2D sketch of the Static Mixing Spacer.

Figure 2-2: 3D sketch of the Static Mixing Spacer.
The 2-D sketch in Figure 2-1 was used to create the 3-D domain shown in Figure 2-2. The 2-D sketch was divided into multiple elements that when extruded and combined by addition yielded the desired 3-D object.

To define the flow domain in which the conservation equations will be solved, the spacer element is subtracted from a solid rectangular slab with a length equal to the desired flow domain length and thickness equal to the flow channel height. The width of the slab is selected such that the boundaries correspond to planes of symmetry as discussed later.

![3D sketch of flow](image)

**Figure 2-3: 3D sketch of the fluid domain.**

This process led to the creation of the flow domain illustrated in Figure 2-3.

The solution domain is meshed to discretize it into a set of small volume elements within which point values of velocity, pressure, and concentration are determined. Each volume element is referred to as a cell or element and the collection of elements as the mesh or grid. The solution accuracy is affected by the quality of mesh.
A fluid domain can be meshed manually or auto-meshed. The hexahedron (HEX) elements or brick elements are used when a user meshes the geometry manually while the tetrahedron (TET) elements are used for automatically generated meshes. The tetra/auto mesh approach often is preferred because it is fast and easy to use for simple geometries. However, manual meshing is preferred for complex geometries.

Hex element types typically are more accurate due to the degree of interpolation they possess as well element shape (aspect ratio, distortion) but the creation of structured hex meshes is time consuming. Thus, the user must balance the time required for meshing against the accuracy of the mesh elements (lower accuracy will require finer meshes and longer solution times to achieve the same solution accuracy) when generating a mesh. Additionally, the user may consider increasing mesh refinement in regions where large gradients are expected to improve solution accuracy.

In this work the solution domain is subdivided to allow manual meshing when creating the mesh structure. The number of nodes in each edge is controlled to increase refinement and solution accuracy in regions where large gradients are expected including adjacent to the membrane surface and near the surface of the spacer.
Figure 2-4: Subdivided fluid domain.

Figure 2-5: Subdivided fluid domain in detail.
Figures 2-4 and 2-5 show how the fluid domain is subdivided into small regions and how these regions are meshed. The number and location of nodes in common edges of the subdivided regions must be compatible for assembly of the entire mesh from the meshes for each sub-region.

Figure 2-6: Subdivided cubes are meshed.

Figure 2-6 indicated the procedure to mesh small cubes in order to have structured mesh for all domains. So the number of nodes was selected for first couple of edges and for the following cubes we used the number of node in each direction to mesh all subdivided sections.
Figure 2-7 indicated the complete fluid domain had structured mesh following the procedure which explained for Figure 2-6.

Increasing the number of nodes on an edge is the most common way of refining the mesh. The flow behavior adjacent to a membrane and spacer surfaces are important issues in our model. Therefore, the boundary adaption option was used to create additional nodes between first the five nodes near membrane and spacer surfaces.

A rigorous estimate of the error associated with discretization of the solution domain and the algorithm used to convert the governing partial differential equations to algebraic equations with CFD cannot be provided. However, an error estimate can be obtained by increasing the number of nodes until the changes in the solution are sufficiently small.
2.3 Boundary Condition

The boundary conditions used to solve the conservation equations are described here. The top and bottom surfaces of fluid are named top and bottom membrane, respectively. The fluid surface adjacent to the spacer wall is referred to as spacer.

Boundary conditions for solution of the conservation of momentum and continuity equation are:

1. membrane and spacer boundaries: no-slip, zero velocity boundary condition
2. inlet boundary: specified inlet velocity
3. outlet boundary: pressure outlet with zero gauge pressure at one node on boundary
4. left and right side boundaries: symmetry

Boundary conditions for solution of the species conservation of mass equation are:

1. membrane boundaries: constant concentration
2. spacer boundaries: zero normal mass flux
3. inlet boundary: constant concentration
4. outlet boundary: convective flow (negligible concentration gradients along flow direction)
5. left and right side boundaries: symmetry

Liquid water was used as the fluid with specific properties tabulated in Table 2-1
Table 2.1: Properties of fluid used in the simulation

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid (water)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg/m$^3$]</td>
<td>1014.65</td>
</tr>
<tr>
<td>Viscosity [kg/m·s]</td>
<td>0.00215</td>
</tr>
<tr>
<td>Thermal Conductivity [W/m·K]</td>
<td>0.6</td>
</tr>
</tbody>
</table>

2.4 Solution of Conservation Equation

The boundary conditions and mesh described previously were used to solve the governing conservation equations. The finite volume method was used for converting the governing differential equations to non-linear algebraic equations and the 3D double precision solver was used to solve these equations. Double precision refers to the number of bytes used to represent a real number in the calculation.

2.4.1 Momentum Equation

The conservation of momentum equation is given by Equation (1):

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{\tau} + \rho \mathbf{g} + \mathbf{F}$$  \hspace{1cm} (1)

Where:

$\rho \mathbf{g}$ : Gravitational body force

$\mathbf{\tau}$ : The stress tensor
\( \mathbf{F} \): External body forces

\( p \): The static pressure

For a Newtonian fluid, the stress tensor is given by:

\[
\bar{\sigma} = \mu \left[ (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) - \frac{2}{3} \nabla \cdot \mathbf{v} \mathbf{I} \right]
\]  

(2)

\( \mu \): Molecular viscosity

\( \mathbf{I} \): Unit tensor

The second term on the right hand side of Equation (2) is the effect of volume dilation [15] which generally is negligible for liquids.

### 2.4.2 Energy Equation

Instead of solving the species conservation of mass equation, the conservation of energy is solved. The analogy between heat and mass transfer which is the basis for this is described in the next section. Solving the energy equation is significantly simpler as it does not require the coding of user defined functions.

The conservation of energy equation solved by FLUENT is given by [16]:

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\bar{\mathbf{v}} (\rho E + p)) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_i h_i \bar{J}_i + (\bar{\tau}_{\text{eff}} \cdot \bar{\mathbf{v}}) \right) + S_h
\]

(3)

Where:

\( \bar{J}_i \): The diffusion flux of species \( i \)

\( k_{\text{eff}} = \) Effective conductivity \( ((k + k_t), \text{ where } k_t \text{ is the turbulent thermal conductivity, defined according to the turbulence model}) \)
The first three terms on the right hand side of Equation (3) represent the effects of heat conduction, species diffusion and viscous dissipation, respectively. The heat of chemical reaction and other volumetric heat sources are defined in \( S_h \) term.

The energy \( E \) is the sum of three contributions:

\[
E = h - \frac{p}{\rho} + \frac{v^2}{2}
\]

(4)

For incompressible flow the sensible enthalpy \( h \) is given by:

\[
h = \sum_i Y_i h_i + \frac{p}{\rho}
\]

(5)

Where:

\( Y_i \): The mass fraction of species \( i \)

And

\[
h_i = \int_{T_{ref}}^{T} c_p \, dT
\]

(6)

where:

\( T_{ref} = 298.15 \text{K} \)

### 2.5 Heat and Mass Transfer Analogy

Even though FLUENT solves the species conservation of mass equation, it does not have the potential to calculate the mass transfer flux through surfaces. A user defined function must be created to calculate the mass transfer flux. However, one can avoid this additional work by using the analogy between mass and heat transfer and using the solution to the conservation of energy instead.
Neglecting $S_h$ and $\bar{J}_i$ since a chemical reaction does not occur and the transport of individual species is not considered, Equation (3) reduces to the following at steady-state:

$$\rho C_p \nabla \cdot (\bar{v}T) = \nabla \cdot \left( k_{\text{eff}} \nabla T + (\bar{r}_{\text{eff}} \bar{v}) \right)$$  \hspace{1cm} (7)

If viscous heating (the second term on the right) is negligible, this equation is identical to that for transport of a dilute species if concentration is replaced by temperature and the mass diffusivity by the thermal diffusivity $k_{\text{eff}}(\rho C_p)$, as discussed later. To demonstrate that viscous heating is negligible, the simulation can be run with increasing viscosities and the results compared. Figure 2-8 illustrates the effect of increasing viscosity by an order of magnitude for a test problem. The calculated heat transfer rate changes by less than 2% which is within the accuracy of the numerical approximation. Therefore, viscous heating may be neglected in Equation (7) as required for the analogy between heat and mass transfer to be valid.

Assuming $k_{\text{eff}}$ is constant and neglecting the viscous heating term, Equation (7) simplifies to:

$$\rho C_p \nabla \cdot (\bar{v}T) = k \nabla \cdot (\nabla T)$$  \hspace{1cm} (8)

The species conservation of mass equation without reaction in steady state condition is defined as

$$\rho \nabla \cdot (\bar{v} C_A) = D \nabla \cdot (\nabla C_A)$$  \hspace{1cm} (9)

$D$: Diffusion coefficient

$C_A$: is the concentration of species A

Substitute $D$ with $k/(\rho C_p)$ and $C_A$ with $T$ for converting Equation (8) to Equation (9)
Figure 2-8: Variation in heat transfer across a membrane surface with changing viscosity.

Therefore, the heat transfer coefficient calculated for a heat transfer problem can be converted into a mass transfer coefficient.

2.6 Mass Transfer Coefficient Calculation

The procedure for calculating the Sherwood number from the simulation results is described next. The procedure consists of the following steps:

1. Calculate heat transfer rate \( (u) \) to top and bottom membrane surfaces
2. Calculate the average temperature \( (T_{avg}) \) through the fluid domain
3. Calculate the membrane area \( (A) \)
4. Calculate the heat transfer coefficient
h = \frac{u}{A \times LMTD} \quad (10)

LMTD: log mean temperature difference

\[ LMTD = \frac{(T_{in} - T_0) \ln \left( \frac{T_{in} - T_0}{T_{out} - T_0} \right)}{(T_{in} - T_0) - (T_{out} - T_0)} \]

T_0: Membrane temperature

5. Calculate a Nusselt number

\[ Nu = \frac{h \times H}{k_f} \quad (11) \]

k_f: fluid thermal conductivity

H is the height of channel to compare different spacers.

6. Calculate Sherwood number (Sh)

\[ Sh = \frac{k \times H}{D} \quad (12) \]

D: mass diffusivity

k: mass transfer coefficient

We used the mass and heat analogy to replace the mass transfer coefficient (k) with heat transfer coefficient (h) and mass diffusivity with \( \frac{k_f}{\rho \cdot c_p} \).

Sherwood number vs. Graetz number is plotted after the calculation.

2.7 Discretization Schemes and Solution

The finite volume method is used for discretization of conservation equations on a structured mesh for all simulations. To calculate the convective terms in the equation, the second order upwinding scheme was applied. SIMPLEC algorithm was used for pressure-
velocity coupling and liquid phase was assumed as incompressible. The second order implicit method in space was applied to solve the conservation of momentum and continuity equations.

To prevent the “zero normal pressure gradient” assumption near the spacer walls and membrane surfaces, the PRESTO (Pressure Staggering Option) scheme was performed for pressure interpolation. The discrete continuity balance for a “staggered” control volume for volume element face was used to compute the pressure on the face.

The corrected face flux satisfies the discrete continuity equation during each iteration. For cases where the pressure-velocity coupling is one of the solution limiting factors, the SIMPLEC uses the modified correction equations to accelerate convergence. As a result, the calculation must be repeated until the balance is satisfied.

2.7.1 Spatial Discretization

The discrete values of transport quantities (Φ) are stored at the center of each volume element. In the discretized transport equations, the face values of these quantities, |Φ|, are used to calculate the rate of convection of Φ through face “f”. These values are interpolated from the center values using an upwind scheme from the values that lie along the direction of the normal velocity component to each face.

FLUENT offers the following upwind schemes:

1. First-order upwind scheme
2. Second-order upwind scheme
3. Power law scheme
4. QUICK scheme

The second-order upwind scheme is used for this work because it is the most accurate scheme. The second-order scheme uses a multidimensional Taylor series expansion of the solution to obtain the face value from the value at the center of the volume, the centroid value. Truncating the expansion to second-order gives the following equation for $\Phi_f$:

$$
\Phi_{f,SOU} = \Phi + \nabla \Phi \cdot \vec{r}
$$

(13)

$\Phi$: Cell center value

$\nabla \Phi$: Cell center gradient

$\vec{r}$: Displacement vector from upstream cell centroid to the face centroid

This formulation requires the determination of the gradient $\nabla \Phi$ in each cell. Finally, the gradient $\nabla \Phi$ is limited so that no new maxima or minima are introduced. The second-order upwind scheme is available in the pressure-based and density-based solvers.

2.7.2 Second Order Upwind Scheme

In computational fluid dynamics, upwind schemes denote a class of numerical discretization methods for solving hyperbolic partial differential equations. Upwind schemes use an adaptive or solution-sensitive finite difference stencil to numerically simulate the direction of propagation of information in a flow field. The upwind schemes attempt to discretize hyperbolic partial differential equations by using differencing biased in the direction determined by the sign of the characteristic.
At the cell faces, a multidimensional linear reconstruction approach is applied to compute quantities to obtain second order accuracy. Higher-order accuracy is obtained at the cell faces through a Taylor series expansion of the solution about the cell centroid. The face value $\phi_f$ is calculated for second order upwind using equation (14) [17]:

$$
\phi_f = \phi + \nabla \phi \cdot \vec{z} 
$$  \hspace{1cm} (14)

$\phi$ : Cell centered value

$\nabla \phi$ : Cell centered gradient

$\vec{z}$ : Displacement vector from the upstream cell centroid to the face centroid

The calculation of the cell centered gradient for each cell is needed for equation (14) and the divergence theorem is used to calculate the $\nabla \phi$.

$$
\nabla \phi = \frac{1}{V} \sum_{f}^{N_{faces}} \phi_f \cdot \vec{A}
$$  \hspace{1cm} (15)

Where, the face values $\bar{\phi}_f$ are calculated by averaging $\phi$ from the two cells adjacent to the face.
Chapter 3

Validation

3.1 Introduction

Computational Fluid Dynamics (CFD) tools are used widely to simulate transport in diverse applications. The commercial code FLUENT is used here. FLUENT is considered one of most versatile commercial CFD packages. To help establish the validity of a numerical simulation, researchers often simulate a case for which an analytical solution is available or the literature contains results from previous studies. The simulation of transport in a membrane bounded rectangular channel without a spacer is used here to establish the validity of the simulation.

The validation simulation is for mass transfer across a membrane bounded empty channel. Figure 3-1 illustrates the cross sectional area of the channel. The right and left surfaces of the channel are assumed to be symmetric so the shear stresses and normal mass fluxes are zero along the surfaces.
3.2 Geometry and Mesh

SOLIDWORKS is used to create the geometry. Gambit then is used to mesh and assign zone types to the model. Zones are defined as domains (i.e., the faces of a mesh element) for which material properties and boundary conditions are assigned. The mesh file that is generated is imported into FLUENT for definition of the boundary conditions, material properties, and solver specifications before solving the equations.

Figure 3-1: Fully structured meshed static mixing spacer.

A typical meshed domain is shown in Figure 3-1. To enhance the convergence rate and improve convergence, a structured mesh is used. Depending on the quality of the mesh; the number of nodes may vary from 2 million to 4 million. The density of mesh intentionally increases from the center of channel to the membrane surfaces where the concentration gradients are highest.
3.2.1 Boundary Conditions

For the solution domain, the boundary conditions are specified as discussed in the previous chapter and illustrated in Figure 3-2.

1. Inlet: velocity inlet at 310 K
2. Outlet: pressure outlet
3. Membrane: no slip wall at constant temperature of 300 K
4. Left and right sides: symmetry

![Figure 3-2: Empty Channel (Slit) boundary conditions.](image)

The inlet temperature is set to 310K and membrane temperature is set to 300K. This 10 K temperature difference results in heat transfer from the liquid to the membrane. The pressure outlet boundary condition assumes a well-developed velocity field exists at the outlet. The symmetry boundary condition is set for right and left surfaces.
3.3 **Analytical Solution**

We derive the analytical solution for heat and mass transfer to the membrane in two limits:

1. **Well developed limit** in which the mass/heat transfer coefficient reaches a constant value.

2. **Entry level limit** where there is a concentration or temperature boundary layer adjacent to the membrane surface and the local mass/heat transfer coefficient decreases along the length of the channel. The geometry of the slit is illustrated in Figure 3-3.

![Figure 3-3: Cross section of Slit in well-developed limit.](image)

3.3.1 **Well Developed Limit**

The well-developed axial velocity is determined by solving the $z$-component of the momentum equation by assuming $v_x = v_y = 0$

\[
\rho \left( \frac{DV}{DT} \right) = -\nabla p + \mu \nabla^2 V + \rho g \tag{16}
\]

From velocity boundary conditions,
The species conservation of mass equation for a dilute component is written in terms of a dimensionless length and concentration defined by Equations (19) and (20), respectively.

\[ z^* = \frac{z}{L} \]  
\[ C^* = \frac{C}{C_0} \]

where \( L \) is the length of the channel and \( C_0 \) is the inlet concentration. Substituting the well-developed velocity, which will not change with the transport of a dilute component, yields:

\[ V_x \frac{C_0 \partial C^*}{L \partial z^*} = D \left[ \frac{C_0 \partial^2 C^*}{\partial x^2} - \frac{C_0}{l^2} \frac{\partial^2 C^*}{\partial z^2} \right] \]

Where the x-coordinate is non-dimensionalized with \( \partial \). The thickness of the concentration boundary layer. If the boundary layer is thin relative to the length of the flow channel, i.e.,

\[ \frac{\partial}{L} \ll 1 \]

Then diffusion in the flow direction (z-direction) may be neglected relative to diffusion in the normal direction (x-direction) and convection in the flow direction and may be set to zero as indicated in Equation (23).

\[ \left( \frac{\partial}{L} \right)^2 \frac{\partial^2 C}{\partial z^2} \approx 0 \]

Therefore, the species conservation of mass equation becomes:

\[ V_z \frac{\partial C}{\partial z} = D \frac{\partial^2 C}{\partial x^2} \]
To solve this equation for the concentration, the concentration is assumed to be equal to the product of \( f(z) \) and \( g(x) \):

\[ C = f(z) * g(x) \]  \hspace{1cm} (25)

Substituting Equation (25) in (24) gives Equation (26)

\[ \frac{D}{v_{\text{max}}(1-(\frac{x}{B})^2)} \frac{g''}{g} = \frac{f''}{f} = -\varphi^2 \]  \hspace{1cm} (26)

where \(-\varphi^2\) is a constant representing the Eigen values of the solution which may be calculated to obtain a series solution for the concentration in terms of the associated Eigen-functions. In the well develop limit, only the largest term must be determined.

Equation (26) may be rearranged to obtain:

\[ g'' + \varphi^2 g \frac{v_{\text{max}}}{D} [1 - \left(\frac{x}{B}\right)^2] = 0 \]  \hspace{1cm} (27)

Where the boundary conditions are:

Concentration symmetry:

\[ g'(x = 0) = 0 \]  \hspace{1cm} (28)

and since the wall concentration is 0:

\[ C^*(x = B) = \frac{c}{c_0} = 0 \]  \hspace{1cm} (29)

So

\[ g(x = B) = 0 \]  \hspace{1cm} (30)

Defining

\[ h = g' \]  \hspace{1cm} (31)

Equation (27) becomes:

\[ h' + \varphi^2 g \frac{v_{\text{max}}}{D} [1 - \left(\frac{x}{B}\right)^2] = 0 \]  \hspace{1cm} (32)

Or
\[ \frac{dh}{dx} + \phi^2 g \frac{V_{\text{max}}}{D} \left[ 1 - \left( \frac{x}{B} \right)^2 \right] = 0 \quad (33) \]

From the definition of \( h \):
\[ g' = \frac{dg}{dx} \quad (34) \]

Equations (33) and (34) must be solved simultaneously for \( g \) and \( h \). Defining \( y = \frac{x}{B} \) gives:
\[ \frac{dg}{Bdy} = \frac{dg}{dx} \quad (35) \]
\[ \frac{d^2g}{B^2dy^2} = \frac{d^2g}{dx^2} \quad (36) \]
\[ \frac{d^2g}{dy^2} \frac{1}{(1-y^2)g} = -\phi^2 \frac{V_{\text{max}}}{D} B^2 = -\varphi^2 \quad (37) \]
\[ h' = -\varphi^2 (1 - y^2)g \quad (38) \]
\[ g' = h \quad (39) \]

The boundary conditions for \( h \) and \( g \) in terms of \( y \) are:
\[ h(y = 0) = g'(y = 0) = 0 \quad (40) \]
\[ g(y = 1) = 0 \]

The value of \( g \) at \( y = 0 \) may be set equal to any arbitrary value since the function \( f \) can be scaled to provide the correct value of concentration at the entrance to the flow channel.

Here, the boundary condition is taken to be:
\[ g(0) = 1 \quad (41) \]

This boundary condition allows the determination of \( \varphi \) by the algorithm illustrated in Figure 3-4.
Using this algorithm gives a value of -2.8276 for $-\varphi^2$. Given this value, Equation (26) can be solved for $f$ and substituted into Equation (25). Solving Equation (26) for $f$ and substituting into Equation (25) gives the first term in the series expansion for $C$ as:

$$C = m e^{-\varphi^2 y} g \quad (42)$$

Integrating the product of concentration and velocity along the slit cross-section gives the flow rate of the solute per unit channel width as:

$$\frac{Q_C}{w} = 2 \int_0^B V C \, dx \quad (43)$$

Substituting for $V$ gives:

$$\frac{Q_C}{w} = 2 \int_0^B V_{\text{max}} \left(1 - \left(\frac{x}{B}\right)^2\right) C \, dx \quad (44)$$

Substituting for $C$ gives:
\[ \frac{Q \bar{C}}{w} = 2 \int_0^B V_{max} \left( 1 - \left( \frac{x}{B} \right)^2 \right) me^{-\varphi^2 z} g \, dx \]  \hspace{1cm} (45)

The rate of change of the solute flow rate with respect to flow direction is equal to the rate the solute diffuses across the slit boundary:

\[ \frac{dQ \bar{C}}{dz} = 2wD \frac{dc}{dx} \bigg|_{x=B} \]  \hspace{1cm} (46)

Substituting for \( C \) in the right-hand side gives:

\[ \frac{dQ \bar{C}}{dz} = 2wD me^{-\varphi^2 z} g' \bigg|_{x=B} \]  \hspace{1cm} (47)

Equation (45) also gives:

\[ \frac{dQ \bar{C}}{dz} = 2wV_{max} \left[ \int_0^B \left( 1 - \left( \frac{x}{B} \right)^2 \right) g \, dx \right] me^{-\varphi^2 z} (-\varphi^2) \]  \hspace{1cm} (48)

Equating Equations (47) and (48):

\[ \frac{g' |_{x=B}}{\int_0^B \left( 1 - \left( \frac{x}{B} \right)^2 \right) g \, dx} = \frac{-V_{max} \varphi^2}{D} \]  \hspace{1cm} (49)

The Sherwood number is given by:

\[ Sh = \frac{B \frac{-2D \frac{dc}{dx}}{c}}{D} \]  \hspace{1cm} (50)

Substituting for the concentration gradient and average concentration from the right hand side of Equation (47) and Equation (45), respectively:

\[ Sh = \frac{-B \int_0^B V_{max} \left( \frac{2Dme^{-\varphi^2 z} g}{\int_0^B V_{max} \left( 1 - \left( \frac{x}{B} \right)^2 \right) g \, dx} \right) \, dx}{D \int_0^B V_{max} \left( \frac{1 - \left( \frac{x}{B} \right)^2}{D} \right) \, dx} \]  \hspace{1cm} (51)

Using Equation (49) this simplifies to:

\[ Sh = 2B \frac{V_{max} \varphi^2}{D} \int_0^B \left( \frac{1 - \left( \frac{x}{B} \right)^2}{D} \right) \, dx \]  \hspace{1cm} (52)

Since:

\[ -\varphi^2 = -\varphi^2 \frac{V_{max}}{D} B^2 \]  \hspace{1cm} (53)
Equation (53) can be rewritten as:

\[ Sh = 2\varphi^2 \left[ \int_0^1 (1 - y^2) dy \right] \]  
(54)

\[ Sh = 2\varphi^2 [y - \frac{y^3}{3}]_0^1 \]  
(55)

\[ Sh = \frac{4\varphi^2}{3} \]  
(56)

Substituting the value of \( \varphi^2 \) into Equation (57) the Sherwood number in the well developed limit is equal to

\[ Sh = 3.77 \]  
(57)

### 3.3.2 Entry Mass Transfer Limit

The Sherwood number in the entry mass transfer limit can be obtained by solving the conservation of mass equation for a dilute solute in the channel:

\[ \nu_z \frac{\partial C}{\partial z} = D \left( \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) \]  
(58)

Equation (58) is rewritten in terms of the distance from the wall by defining the variable \( y \) as:

\[ y = B - x \]  
(59)

Defining the following dimensionless variables:

\[ Z^* = \frac{z}{L} \]  
(60)

\[ C^* = \frac{C}{C_0} \]  
(61)

\[ y^* = \frac{y}{\delta} \]  
(62)

\[ V_{z^*} = \frac{V_z}{V_{max}} \]  
(63)
where \( \partial \) is an estimate of the thickness of the concentration boundary layer. Substituting into the conservation of mass equation, Equation (58), gives:

\[
V^*_z \frac{\partial C^*}{\partial z^*} = \left( \frac{DL}{V_{\text{max}} \partial^2} \right) \left[ \frac{\partial^2 C^*}{\partial y^*^2} + \left( \frac{\partial}{L} \right)^2 \frac{\partial^2 C^*}{\partial z^*^2} \right]
\] (64)

If the concentration boundary layer is much smaller than the channel length then:

\[
\frac{\partial}{L} \ll 1
\]

And

\[
\left( \frac{\partial}{L} \right)^2 \frac{\partial^2 C^*}{\partial z^*^2} \approx 0
\] (65)

so Equation (64) may be rewritten as:

\[
V^*_z \frac{\partial C^*}{\partial z^*} = \left( \frac{DL}{V_{\text{max}} \partial^2} \right) \frac{\partial^2 C^*}{\partial y^*^2}
\] (66)

This simplification results from neglecting diffusion in the flow direction relative to convection in the flow direction and diffusion to the channel wall. The fully developed axial velocity profile will be used to evaluate mass transfer in the entry limit.

\[
V_z = V_{\text{max}} \left( 1 - \left( \frac{x}{B} \right)^2 \right)
\] (67)

Within the concentration boundary layer, the velocity in the flow direction may assume to be linear in \( y \). The velocity gradient adjacent to the wall is given by:

\[
\frac{\partial V_z}{\partial x} = -\frac{2x}{B^2} V_{\text{max}}
\] (68)

so the \( z \)-component of the velocity is given by:

\[
V_z = \left( \frac{2V_{\text{max}}}{B} \right) y
\] (69)

The velocity gradient along the wall will be required later and is given by

\[
\frac{\partial V_z}{\partial y} = \frac{2V_{\text{max}}}{B}
\] (70)
Letting \( \partial^2 = \frac{DL}{v_{max}} \) gives:

\[
V_z^* \frac{\partial c^*}{\partial z^*} = \frac{\partial^2 c^*}{\partial y^2}
\]  
(71)

Substituting for the velocity from Equation (69):

\[
\left( \frac{2v_{max}}{B} \right) y \frac{\partial c}{\partial z} = D \frac{\partial^2 c}{\partial y^2}
\]  
(72)

Within the concentration boundary layer, it is assumed the concentration is a function only of a similarity variable \( \eta \):

\[
C = C(\eta)
\]  
(73)

Where \( \eta \) is defined as:

\[
\eta = yf(z)
\]  
(74)

Derivatives of \( C \) with respect to \( y \) and \( z \) are given in terms of \( \eta \) by:

\[
\frac{\partial c}{\partial z} = \frac{\partial c}{\partial \eta} \frac{\partial \eta}{\partial z} = C' yf'
\]  
(75)

\[
\frac{\partial c}{\partial y} = \frac{\partial c}{\partial \eta} \frac{\partial \eta}{\partial y} = C' f
\]  
(76)

\[
\frac{\partial^2 c}{\partial y^2} = \frac{\partial}{\partial y} \left( \frac{\partial c}{\partial \eta} \frac{\partial \eta}{\partial y} \right) + \frac{\partial c}{\partial \eta} \frac{\partial^2 \eta}{\partial y^2}
\]  
(77)

\[
\frac{\partial^2 c}{\partial y^2} = C'' f^2
\]  
(78)

Substituting Equations (73) – (78) into (72) gives:

\[
\left( \frac{2v_{max}}{BD} \right) f' \frac{f'}{f^4} = \frac{C''}{\eta^2 C'}
\]  
(79)

The term in brackets on the left-hand side of Equation (79) must be equal to a constant if the similarity transform is to be successful since the concentration and its derivatives are functions of \( \eta \) only. Therefore, this term is set equal to an arbitrary value of -3 to simplify the subsequent mathematics:
\[ \left( \frac{2V_{\text{max}}}{BD} \right) \frac{f'}{f^4} = -3 \]  \hspace{1cm} (80)

Since,

\[ f' = \frac{df}{dz} \]  \hspace{1cm} (81)

Equation (80) may be rewritten as:

\[ \frac{df}{f^4} = -3 \left( \frac{DB}{2V_{\text{max}}} \right) dz \]  \hspace{1cm} (82)

Integrating Equation (82) gives:

\[ f^{-3} = -3 \left( \frac{DB}{2V_{\text{max}}} \right) z \]  \hspace{1cm} (83)

Rearranging Equation (83) gives:

\[ f^{-3} = \left( \frac{9DB}{2V_{\text{max}}} \right) z \]  \hspace{1cm} (84)

or:

\[ f = \left( \frac{2V_{\text{max}}}{9DBz} \right)^{\frac{1}{3}} \]  \hspace{1cm} (85)

Since a functional form for \( f \) was found, Equation (79) may be written as:

\[ -3\eta^2 C' = C''' = \frac{dc'}{d\eta} \]  \hspace{1cm} (86)

Upon rearrangement, Equation (86) may be written as:

\[ -3\eta^2 d\eta = \frac{dc'}{c'} \]  \hspace{1cm} (87)

Integrating yields:

\[ -\eta^3 = \ln C' + K_0 \]  \hspace{1cm} (88)

which can be written as:

\[ C' = K_1 e^{-\eta^3} \]  \hspace{1cm} (89)

and integrated to give:
\[ C = K_1 \int_0^\eta e^{-t^3} dt + K_2 \]  

(90)

The boundary conditions for Care

\[ C = C_0 @ y = 0, \eta = 0 \]  

(91)

\[ C = C_1 @ z = 0, y \to \infty, \eta = \infty \]  

(92)

Equation (91) requires:

\[ C_0 = K_2 \]  

(93)

while Equation (92) requires:

\[ C_1 - C_0 = K_1 \int_0^\infty e^{-t^3} dt \]  

(94)

Substituting into Equation (90) gives

\[ \frac{C - C_0}{C_1 - C_0} = \frac{\int_0^\eta e^{-t^3} dt}{\int_0^\infty e^{-t^3} dt} \]  

(95)

which may be written as:

\[ C - C_0 = \frac{C_1 - C_0}{\Gamma(\frac{2}{3})} \int_0^\eta e^{-t^3} dt \]  

(96)

The solute flux to the wall may be calculated from:

\[ j = D \frac{\partial C}{\partial y} = \frac{D(C_1 - C_0)}{\Gamma(\frac{2}{3})} \frac{\partial}{\partial \eta} \left( \int_0^\eta e^{-t^3} dt \right) \frac{\partial \eta}{\partial y} \]  

(97)

Differentiating the integral gives:

\[ j = \frac{D(C_1 - C_0)}{\Gamma(\frac{2}{3})} \left[ \left( \frac{\partial \eta}{\partial \eta} \right) e^{-\eta^4} \right] \left( \frac{2V_{max}}{9DBz} \right)^{\frac{1}{3}} \]  

(98)

which evaluated at the channel wall gives:

\[ j = \frac{D(C_1 - C_0)}{\Gamma(\frac{2}{3})} \left( \frac{2V_{max}}{9DBz} \right)^{\frac{1}{3}} \]  

(99)

The local mass transfer coefficient is given by:

\[ h = \frac{j_{total}}{(C_1 - C_0)A} \]  

(100)
and the total flux to the wall is given by:

\[ I_{total} = \int_{0}^{L} j \, dA \]  \hspace{1cm} (101)

Substituting the local flux expression, Equation (99), gives:

\[ I_{total} = \frac{D(C_{1} - C_{0})}{\Gamma(\frac{2}{3})} \left( \frac{2V_{\text{max}}}{9DB} \right)^{\frac{1}{3}} \int_{0}^{L} z^{-\frac{1}{3}} W \, dL \]  \hspace{1cm} (102)

The Sherwood number is given by:

\[ Sh = \frac{h \times B}{D} \]  \hspace{1cm} (103)

Where the average mass transfer coefficient can be calculated from:

\[ \frac{I_{\text{total}}}{(C_{1} - C_{0}) \times (LW)} = h = \frac{D}{\Gamma(\frac{2}{3})} \left( \frac{2V_{\text{max}}}{9DB} \right)^{\frac{1}{3}} \times \frac{2}{3} z^{\frac{2}{3}} \bigg|_{0}^{L} \frac{W}{W} \]  \hspace{1cm} (104)

Substituting into the Sherwood number definition, Equation (103):

\[ Sh = \frac{h \times B}{D} = \left( \frac{3}{2} \right)^{\frac{1}{3}} \left( \frac{B V_{\text{max}}}{D} \right) \times \left( \frac{v}{D} \right) \times \left( \frac{B}{2L} \right) \]  \hspace{1cm} (105)

This may be rewritten as:

\[ Sh = \left( \frac{3}{2} \right)^{\frac{1}{3}} \left( \frac{B V_{\text{max}}}{D} \right) \times \left( \frac{B^2}{2L} \right) \]  \hspace{1cm} (106)

The numerical pre-factor can be explicitly determined to yield the following expression for the average Sh:

\[ Sh = 1.284 \times [Gz]^{\frac{1}{3}} \]  \hspace{1cm} (107)

Where the Graetz number is given by:

\[ Gz = \left( \frac{BV_{\text{max}}}{v} \right) \times \left( \frac{v}{B} \right) \times \left( \frac{B}{2L} \right) = Re \, Sc \left( \frac{B}{2L} \right) \]  \hspace{1cm} (108)

Where \( Re \) and \( Sc \) are the Reynolds and Schmidt numbers, respectively.
3.4 Grid Independence

The dependency of the result on the mesh used can be evaluated through the use of progressively more refined meshes. As explained in the previous chapter, a more accurate solution is obtained with a finer mesh. The most common method to examine grid convergence is to begin with a coarse mesh and continuously refine the mesh by increasing number of geometry elements. This process is continued until the change in the results is less than some desired limit (error).

The required computational effort for very fine meshes is significant and can limit the ability to assess the solution accuracy. For example, the computational effort increases by a factor of eight if the average element size is halved. However, grid convergence is the only method to demonstrate the solution is independent of the mesh size.

![Graph showing measured heat flux versus number of elements](image)

Figure 3-5: Measured heat flux versus number of elements used in the domain.
Figure 3-5 illustrates the results of a mesh refinement study. The numbers 1-4 designate the four mesh sizes used to assess the effect of increasing refinement. The difference indicated is the percent difference in the computed heat flux between two meshes of increasing refinement can be calculated from Figure 3-5. For example, the heat flux computed with mesh 2 is 0.12% larger than that computed with mesh 1. Clearly the difference decreases as the mesh is refined.

3.5 Comparison of Analytical Results with Simulation Results

Figure 3-6: Comparison of the simulated with analytical results.

Figure 3-6 compares the simulated results and the analytical results. The Graetz number was varied from 1 to 10000. Analytical results are expressed in two parts; Entry limit (red
line) and well developed limit (green line). The simulations results are represented by the blue line.

Comparison of the results for short and long slit simulation the short slit is defined for slit with length of single static mixer element where $\frac{d}{L} < 1$ and the long slit is defined for a slit assuming $\frac{d}{L} \ll 1$ and analytical solution shows that both short and long slit give the same slope in the Entry limit region. The slope is within 10% of the analytical value which is the approximate error of the results based on mesh refinement studies. The long slit gives an accurate value in the well developed limit because the aspect ratio of $\frac{d}{L} \ll 1$ is much closer to the analytical solution.
Chapter 4

Simulation of Static Mixing Spacer

4.1 Introduction

As discussed in the previous chapter, SOLIDWORKS is used to create the static mixing geometry, GAMBIT to mesh the geometry and define boundary conditions and FLUENT to solve the governing equations for the model. The performance of the static mixing spacer is studied for boundary conditions defined next.

4.2 Boundary Conditions

The following boundary conditions were specified for the solution domain:

1. Inlet: velocity inlet with 310K temperature for simulations of a single static mixing unit and 350K for simulations of multiple units in series. A higher inlet temperature is used for simulations of multiple units because the increased heat transfer that occurs decreases the temperature more rapidly and calculated outlet temperatures using an inlet temperature of 310 quickly approach the boundary value of 300 as the Graetz number decreases.
2. Outlet: pressure outlet
3. Top and bottom membranes: no slip wall with 300 K
4. Right and Left boundaries: Symmetry
5. Spacer wall: No slip wall with zero heat flux

We used the same inlet, outlet, right and left boundary conditions as for the validation case of an empty channel.

The boundary conditions for solution domain are illustrated in Figure 4-1.

![Figure 4-1: Boundary conditions for Static Mixer spacer simulations.](image)

4.3 **Grid Size Independence Test**

As discussed in Chapter 3, the dependence of the solution on mesh refinement was examined to determine the refinement necessary to obtain a grid-independent solution to within 5% accuracy. The number of elements needed to solve the solution changed for each static mixing spacer configuration. Therefore the optimal mesh changed
for each configuration. The optimal grid size was verified for each case by using the grid convergence method before each case was simulated. The optimal number of elements varied between 1-2.3 million.

4.4 Performance of the Spacer Dimensions

A preliminary study of the effect of spacer dimensions was performed to identify promising configurations for more detailed calculations and experimental evaluation. The range of dimensions that can be considered is limited by the ability to manufacture spacer samples. Stereo-lithography is used here and is capable of producing pieces with a minimum dimension of 1 mm. Therefore, the spacer study focuses on the ratio of dimensions rather than specific values. The design dimensions are illustrated in Figure 4-2 where the spacer thickness is given by the dimension $D$.

![Figure 4-2: Dimension analysis sketch](image)

Figure 4-2: Dimension analysis sketch
Values for the design dimensions considered in the preliminary assessment are tabulated in Table 4-1 in which the dimensions represent:

A: width of flow opening through spacer
B: length of flow opening through spacer
C: length of leading and trailing divider
D: thickness solid regions
F: total length of each element
E: total width of element
G: gap between spacers.

If the spacer wall thickness is set to 1mm because of manufacturing limitations, the minimum height of the spacer, and channel that it can fill, is 3mm. The spacer elements
in Table 4-2 are simulated in a preliminary evaluation of performance to determine which dimensions appear to offer superior performance.

The growth of the concentration boundary layer in the upper and lower halves of the fluid domain is shown in two cross sections in the x-y plane for a spacer 2 element in Figure 4-3.

![Figure 4-3: Concentration field in x-y plane [FLUENT]](image)

Figure 4-3 illustrates the changes in concentration boundary layer that accompany the fluid movement from the upper to the lower half of the flow channel (upper) and vice versa (middle). Concentration decreases as the color changes from red to blue. Flow is from right to left through the flow channel. The red color indicates higher concentration and changing color from red to blue means the decreasing the bulk concentration. As you can see concentration decreases from the right to the left by passing the static mixing spacer which indicates mixing helps to reduce concentration boundary layers and increasing permeation through the top and bottom membranes.
The concentration boundary layer (thickness of blue region) gradually builds up and increases adjacent to the membrane surface until the fluid encounters the spacer. The spacer forces the fluid adjacent to the membrane towards the center of the channel and the fluid in the center of channel towards the membrane surface.

Figure 4-4: Concentration field in the x-z plane that lies in the middle of the flow channel. Flow is from bottom to the top.

Figure 4-4 illustrates how the concentration field changes in the x-z plane that lies along the middle of the flow channel. The movement of fluid containing the concentration boundary layer is forced to the downstream side of the opening where it will exit along the center of the flow channel. The red color means higher concentration and the concentration reduction shows by changing color from red to blue.
4.5 Static Mixing Spacer Arrangements

Two promising designs identified by preliminary simulations of the spacer elements in Table 4-2 are selected for more in-depth studies of the effect of spacing between spacer elements. The results of this preliminary evaluation are presented in the next chapter.

For the selected designs, the effect of changing the number of spacer elements, or equivalently the spacing between elements is examined by placing multiple spacer elements in the solution domain. Figures 4-5 through 4-7 illustrate the solution domain for 1, 5, and 13 elements for Spacer 2 while Figures 4-8 through 4-10 illustrate the solution domain for 1, 6, and 12 elements for Spacer 8; Spacers 2 and 8 were selected for this study based on the results presented in the next chapter.

Figure 4-5: Spacer 2 Arrangement, single unit.
Figure 4-6: Spacer 2 Arrangement, med number of repeating units (intermediate).

Figure 4-7: Spacer 2 Arrangement, max number of repeating units.
Figure 4-8: Spacer 8 Arrangement, single unit.

Figure 4-9: Spacer 8 Arrangement, med number of repeating units (intermediate).
The temperature distribution through the spacer filled channel was compared with an empty channel to study the effect of static mixing spacer on the heat transfer rate in Figures 4-11 and 4-12 for spacer 2 and 8, respectively. The temperatures in these Figures represent the velocity weighted average (i.e., mixing cup) temperature for a cross-section normal to the flow direction.
Figure 4-11: Temperature distribution for maximum inlet velocity (Spacer 2) with different number of spacer elements.

Figure 4-12: Temperature distribution for maximum inlet velocity (Spacer 8) with different number of spacer elements.
The results for both Figures indicate a smooth decrease in temperature for the empty channel (i.e., slit). However, the curves for spacer filled channels possess noticeable step changes between smoother regions; these drops are most noticeable for the single spacer filled channels but can be discerned in all cases. These drops correspond to the location of spacer elements and represent the enhancement in mass transfer that accompanies fluid mixing. This mixing eliminates the boundary layer adjacent to the membrane surface and allows it to redevelop which increases the rate of transport. Figures 4-13 to 4-15 illustrate how the temperature or concentration field changes with flow direction within selected cross-sections of the flow channel for spacer 2; Figures 4-16 to 4-18 illustrate the changes for spacer 8. A greater change in temperature is evident as the number of elements increases.

Figure 4-13: Temperature distribution for max number of repeating units (Spacer 2).
As you can see reducing number of elements decreases heat transfer rate through the spacer filled channel. Figure 4-13 indicates higher heat transfer rate by having maximum number of elements.
Figure 4-16: Temperature distribution for max number of repeat units (Spacer 8).

Figure 4-17: Temperature distribution for med number of repeating repeat units (Spacer 8).
The experimental procedure used to evaluate spacer performance, is described in the next chapter. The simulations reported in this chapter do not correspond directly to the experiments since the simulations assume the spacer contacts membranes along both the upper and lower bounding surfaces—the spacer is bounded by an impermeable surface along one boundary and a membrane along the other in the experimental test cell. Therefore, additional simulations were performed with the same boundary conditions as provided by the test cell. The results of these simulations for spacer 2 are provided in Chapter 6. Previous simulations with the flow channel bounded by membranes on both sides demonstrate that spacer 2 provides the highest mass transfer coefficients but also the highest pressure drops.

In this work, the characteristic length used to correlate mass transfer coefficients is taken as the channel height to facilitate comparisons between an empty channel and channels containing spacers of different number of repeating units. The use of other characteristic lengths, such as hydraulic diameter, complicates comparisons as
differences in Sherwood number between channels filled with different spacers may arise from either a change in mass transfer coefficient or a change in the characteristic length.

Theoretical and experimental evaluations of Sherwood number are reported as a function of the Schmidt (Sc) number, Reynolds number (Re), and the channel height-to-length ratio ($H/L$) where the Schmidt number is defined by Equation (109):

$$Sc = \frac{v}{D}$$  \hspace{1cm} (109)

The Reynolds number is defined by Equation (110):

$$Re = \frac{H v_b}{\nu}$$  \hspace{1cm} (110)

Where, $\nu$ is the fluid kinematic viscosity, and $v_b$ is the bulk fluid velocity (the ratio of the flow rate to the superficial flow cross-sectional area normal to the nominal flow direction.

Past analyses of convective mass transfer suggest that the dependence of Sherwood number on the Reynolds (Re) and Schmidt (Sc) number should be given by equation (111) as

$$Sh = \frac{hH}{D} = \alpha \left(\frac{H v_b}{\nu}\right)^a \left(\frac{\nu}{D}\right)^b \left(\frac{d_e}{L}\right)^c = aRe^aSc^b\left(\frac{H}{L}\right)^c$$ \hspace{1cm} (111)

Where, $a$, $b$ and $c$ are geometry dependent constants. The analytical solution for empty channels suggests that Sherwood number should be proportional to the Graetz number raised to the 1/3rd power where the Graetz number is defined by equation (112)

$$Gz = Re Sc \left(\frac{H}{L}\right)$$ \hspace{1cm} (112)

Which follows from equation (111) by setting $a=b=c=1/3$. The analytical results also suggest that Sherwood number approaches a constant value in the well-developed mass transfer limit. Based on these observations, simulation results are presented as dependence of Sherwood number on Graetz number.
The calculated pressure drop is non-dimensionalized by calculating the friction factor defined by equation (113)

\[ f = \frac{2H\Delta p}{\rho L v_b} \quad (113) \]

The relationships between channel pressure drop \( \Delta p \) (or friction factor \( f \)) and flow velocity can be expressed as a function of the Reynolds number:

\[ f = \beta Re^e \quad (114) \]

where \( \beta \) and \( e \) are geometry dependent [1]. Simulation results are presented as the dependence of friction factor on Reynolds number.

The spacer increases mass transfer coefficients at the expense of increased pressure drop. The literature suggests plotting Sherwood number versus the Power number defined by equation (115) [2] to evaluate transport performance at a constant power input:

\[ Pn = fRe^3 \quad (115) \]

The exponent of the dependence of power number on Reynolds number appears to be fairly independent of the geometric parameters [2].
Chapter 5

Materials and Methods

5.1 Introduction

Samples of spacer 2 manufactured by Harvest Technologies were used to perform the experiments. Figure 5-1 illustrates the spacer elements that were produced while Figure 5-2 illustrates the frame used to hold the elements in the filtration cell.

![Figure 5-1: CAD drawing of spacer element.](image)

The frame consists of a series of opposing notches spaced evenly along the flow direction. A spacer element may be placed in each pair of notches. The number and spacing of elements is controlled by the number of notches that are filled. The frame in Figure 5-2 can hold up to 10 elements but additional frames were made that can hold up to 13.
The spacer frame is designed to fit in the permeate channel of an Osmotic Sepa CF II cell as illustrated in Figure 5-3.
5.2 Cross-Flow Filtration Experiments

Polyethersulone ultrafiltration membranes with a molecular cut-off of 5000 Daltons (GE) were used for cross-flow filtration. Cross-flow experiments were run using the polyethersulfoune membrane with length of 19 cm and width of 14 cm mounted in the Osmonics cell with an effective membrane area of 144 cm$^2$.

The Sepa CF II membrane system is a laboratory scale cross-flow membrane filtration unit with a maximum operating pressure of 1000 psig. This membrane system can be used for ultra filtration, nanofiltration and reverse osmosis cross flow applications. Benefits and features of the Sepa CF II system:

1. Compatible with all flat sheet membranes
2. Accepts different spacers to maximize the membrane efficiency during filtration.
3. Stainless steel cell with Viton O-ring to prevent distribution of solutions to the outer part of effective membrane area
4. Withstands pressures up to 1000 psig

The channel width is 165 mm and length is 213 mm and accommodates membrane with length of 190 mm and width of 140 mm. The effective membrane area is 144 cm$^2$. The SepaCFII system has a stainless steel 316 cell body with an anodized aluminum cell holder.

The experimental set-up used to evaluate mass transfer performance is illustrated in Figure 5-4. The Osmonics Sepa CF II filtration cell consists of two 316 stainless steel blocks machined to create flow channels and fluid entry and exit ports. The two halves are held together in operation by an anodized aluminum cell holder that is pressurized using an external hydraulic hand pump.
The retentate and permeate flow channels are 165 mm wide and 213 mm long. The cell requires membranes of 190 mm by 140 mm for sealing with Viton O-rings between the two flow channels. The cell is assembled by placing a permeate spacer in the one cell half (permeate flow channel), a membrane on the permeate spacer, a feed spacer on the membrane, and the second cell half (feed flow channel) on the feed spacer to complete the assembly. The assembled cell is slid into the cell holder and the holder pressurized before conducting experiments. A schematic diagram of the membrane filtration system is provided in Figure 5-4.

![Diagram](image)

Figure 5-4: Experimental set-up used to evaluate mass transfer performance.
The feed solution was circulated using a ISMATEC MV gear pump. The valve V-1 allows adjustment of the differential pressure through the feed channel. Valve V-2 is a three way valve that allows control of the permeate outlet to either the sample collection container or back to the feed tank. Figure 5-5 illustrates how the positions of the three-way valve permits control of flow direction.

Figure 5-5: Schematic of three way valve.

Two digital pressure (Cole-Parmer) indicators were used for the cell holder and retentate. Before each experiment, the cross flow filtration unit was cleaned by recirculating 0.015 (V/V) micro liquid laboratory cleaner (International Products Corp.). After cleaning, the cell was washed for 15 minutes by flushing with de-ionized water.

After assembling the cell with the desired feed and permeate spacers and membrane, de-ionized water was circulated from the feed tank to the cell membrane and both the concentrate and permeate outlets were recycled to the feed tank for two hours. The membrane permeability, \( L_p \), was determined using de-ionized water for each experiment. The membrane was pre-compact ed by permeating de-ionized water for 3 hours for all membranes before starting the cross flow experiments.
After membrane pre-compaction, the de-ionized water was flushed out and a Dextran solution with concentration of 5g/L was circulated for two hours to ensure steady state and uniform concentration throughout the system. The first permeate sample was measured after two hours and was collected every half-hour thereafter. For each sample, 10 ml of permeate was collected and weighted. The Dextran solution was flushed out and the system flushed with de-ionized water for half an hour when an experiment was complete.

Proton NMR (Nuclear Magnetic Resonance) was used to check the permeate for Dextran and demonstrate only water permeates through the membrane. The permeate and the feed solutions were examined.

Figure 5-6 illustrates the 5 peaks for the feed Dextran solution. However, no peaks were observed for the permeate as illustrated in Figure 5-7 indicating the permeate did not contain a detectable amount of Dextran.

![Figure 5-6: NMR test for Dextran Solution.](image)
The experimental data is used to calculate the mass transfer coefficient through the membrane. As explained in previous chapters, the measured values are non-dimensionalized as Sherwood numbers. Values for the diffusion coefficient as a function of Dextran concentration are taken from Wijmans and Nako who report the following relationship for Dextran T 500 diffusion in water [18].

\[ D = (0.1204 + 2.614C_1 - 4.167C_1^2 + 2.132C_1^3) \times 10^{-10} \]  

\[ C_1: C_w \times 10^{-3} \]  

Where \( C_w \) is the concentration in units of Kg/m\(^3\).

Wijmans and Nako obtained Equation (116) by a least square fit to their experimental data, which was correlated by Equation (117)

\[ D = \frac{S_0(A_1+2A_2C_1+3A_3C_1^2)}{(1-\frac{PL}{V_0})(1+k_1C_1+k_2C_1^2)} \]  

Where
A_i: Coefficient equation, i=1, 2, 3 (Pa·ml/g^i)

S_0: S at infinite dilution (sec)

S: Sedimentation coefficient of the solute (sec)

v_0: partial specific volume of the solvent (ml/g)

v_1: partial specific volume of the solute (ml/g)

They performed osmosis and sedimentation experiments from which they calculated diffusion coefficients using the Svedberg equation combined with equations (118) [19], (119)[20] and (120):

\[
D = \frac{S}{(1 - \frac{v_1}{v_0})} \times \frac{d\pi}{dC_1} \quad (118)
\]

Where the osmotic pressure over a wide concentration range is given by Equation (119)

\[
\Delta\pi = A_1C_1 + A_2C_1^2 + A_3C_1^3 \quad (119)
\]

and the sedimentation coefficient is given by:

\[
\frac{1}{S} = \frac{1}{S_0} (1 + k_1C_1 + k_2C_1^2) \quad (120)
\]

The film model is used to calculate the mass transfer coefficient (k) from experimental measurements of permeate flux [21, 22] the calculation procedure is outlined next. First, the trans-membrane pressure is calculated as:

\[
\Delta P_{TM} = \left(\frac{P_{Feed} + P_{Retentate}}{2}\right) - P_{atm} \quad (121)
\]

where the \( P_{Feed} \) and \( P_{Retentate} \) are absolute pressures. Second, the measured permeate flux is used to calculate the trans-membrane osmotic pressure difference from:

\[
J = L_p (\Delta P_{TM} - \Delta\pi_W) \quad (122)
\]
Where the units of the permeate flux \( J \) are \( \text{m}.\text{sec}^{-1} \) and the units of the membrane permeability \( L_p \) are \( \text{m}.\text{Pa}^{-1}.\text{sec}^{-1} \). The osmotic pressure difference is used to calculate the average wall Dextran concentration from:

\[
\Delta \pi_W = 37.5C_W + 0.75C_W^2 + 0.00764C_W^3
\]

(123)

Where the unit of the wall concentration is \( \text{kg}.\text{m}^{-3} \). This calculation assumes the permeate is Dextran free as confirmed experimentally. Finally, the mass transfer coefficient is calculated from the film model using:

\[
J = k\ln\left(\frac{C_W}{C_b}\right)
\]

(124)

where the bulk concentration \( C_b \) has the same units as the wall concentration \( \text{kg}.\text{m}^{-3} \).

To calculate the Reynolds and Schmidt numbers, the following correlations for viscosity and density of Dextran-water solutions are used [23]:

\[
\mu = 0.0019 \exp(0.0245C_1)
\]

(125)

\[
\rho = 1013 + 0.33C_1
\]

(126)

Where \( C_1 = C_w \times 10^{-3} \) as defined previously.

For all experiments, the height of the channel was 3 mm.
Figure 5-8: Comparison between the static mixing spacer, commercial spacer & Slit.

Figure 5-9: Comparison between the static mixing spacer, commercial spacer & Slit in term of frication factor vs Reynolds number.
Typical experimental measurements for mass transfer coefficient and pressure drop are illustrated in Figures 5-8 and 5-9.

Use of the commercial spacer increases the mass transfer coefficient marginally. However, use of the static mixing spacer increases the mass transfer coefficient by a factor of four. Similarly, the commercial spacer increases pressure drops marginally but the static mixing spacer can increase pressure drops by almost a factor of 10.
Chapter 6

Results

6.1 Introduction

Simulation and experimental results for the static mixing spacer are presented in this chapter and future lines of research are proposed. Theoretical results for different spacer geometries are presented first. Then results are presented for two promising geometries and the results compared to experiment for different numbers of elements in the flow channel.

6.2 Initial Results

The simulation results for the spacer bounded by two membranes are provided in Table 6.1 as the values of $\alpha$, $a$, $\beta$ and $e$ obtained that best fit the form of Equation (111). Note that the values for $\alpha$ and $a$ in Equation (6.4) were obtained from results for the highest Graetz number (i.e. the entry mass transfer limit) where a log-log plot yielded a linear relationship between $Sh$ and $Gz$; the constants $b$ and $c$ were assumed to be equal to $a$ as expected in the entry mass transfer limit.
Table 6.1: Simulation values for $\alpha$, $a$, $\beta$ and $e$

<table>
<thead>
<tr>
<th>Spacer</th>
<th>$\alpha$</th>
<th>$a$</th>
<th>$\beta$</th>
<th>$e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.14</td>
<td>0.321</td>
<td>194</td>
<td>-0.988</td>
</tr>
<tr>
<td>2</td>
<td>2.25</td>
<td>0.32</td>
<td>267</td>
<td>-0.988</td>
</tr>
<tr>
<td>3</td>
<td>1.96</td>
<td>0.328</td>
<td>181</td>
<td>-0.991</td>
</tr>
<tr>
<td>4</td>
<td>1.9</td>
<td>0.326</td>
<td>190</td>
<td>-0.986</td>
</tr>
<tr>
<td>5</td>
<td>2.16</td>
<td>0.314</td>
<td>171</td>
<td>-0.989</td>
</tr>
<tr>
<td>6</td>
<td>2.08</td>
<td>0.316</td>
<td>140</td>
<td>-0.987</td>
</tr>
<tr>
<td>7</td>
<td>1.86</td>
<td>0.332</td>
<td>157</td>
<td>-0.988</td>
</tr>
<tr>
<td>8</td>
<td>1.82</td>
<td>0.332</td>
<td>130</td>
<td>-0.991</td>
</tr>
<tr>
<td>Slit</td>
<td>1.52</td>
<td>0.333</td>
<td>24</td>
<td>-1</td>
</tr>
</tbody>
</table>

The values for the slit are in excellent agreement with the analytical solution. The results indicate that Spacer 2 gives the highest mass transfer coefficient in the entry mass transfer limit but also possesses the highest pressure drop. Spacer 8 gives the lowest mass transfer coefficient and pressure drop. All spacers give higher mass transfer coefficients than an empty channel.

Figure 6.1 compares the simulations results for spacer 2 and 8 as well as an empty slit for a broad range of Graetz numbers that extend beyond the entry mass transfer limit. The results indicate that the static mixing spacer gives higher mass transfer coefficients from the entry to the well-developed mass transfer limits.
Figure 6-1: Sherwood number dependence on Graetz number for spacers 2 and 8 and empty slit.

The friction factor dependence on Reynolds number is illustrated in Figure 6-2. Over the range shown, the friction factor is inversely proportional to Reynolds number as expected for laminar flow. Additionally, pressure drop through the spacer filled channels can be up to an order of magnitude greater than the pressure drop through an empty channel.
Figure 6-2: Friction factor dependence on Reynolds number for spacer 2 and 8 and empty slit.

Sherwood number dependence on Power number is illustrated in Figure 6.3. Sherwood number is scaled by the product of Schmidt and channel height-to-length ratio raised to the one-third power to yield a value that is dependent only on Reynolds number in the entry mass transfer limit based on the results presented in Table 6-1. Therefore, the curves in Figure 6-3 are dependent only on the Reynolds number.

Figure 6-3 indicates that the spacers and slit give comparable performance in the entry mass transfer region (i.e. high Reynolds or Power number) since for a given power
input; mass transfer coefficients are nearly identical. However, as the transition to the well-developed mass transfer limit occurs, the spacers give better performance.

![Figure 6-3: Sherwood number dependence on Power number for spacer 2 and 8 and an empty slit.](image)

We believe that the lack of improvement in spacer performance in the entry limit is due to the length of the flow channels considered. Simulations were limited to flow channels that contained only a single spacer element and the result were compared to the empty channel of approximately one half length.

If the flow channel length between spacer elements is similar to the empty channel length, the boundary layers that develop will be of comparable thickness. This is the case for the results presented here since the spacer divided the channel into two sections each of which was approximately the same length as the empty channel. To observe mass
transfer performance enhancement, flow channels that contain multiple spacer elements must be compared to empty channels of the same length. This would be the case in reverse osmosis and ultrafiltration spiral wound applications.

6.3 Spacer Arrangement Result

As explained in Chapter 4, the effect of increasing the number of static mixing elements for Spacers 2 and 8 was examined. The simulation results are presented in terms of the Sherwood number dependence on Graetz number and the friction factor on Reynolds number. The results indicate that although the mass transfer coefficient increases by adding more static mixing elements, the friction factor also increases as illustrated in Figures 6-4 through 6-7.

For a single static mixing element, Spacers 2 and 8 gave mass transfer coefficients comparable to that for an empty slit. Adding additional static mixing elements reduces the concentration boundary and increase mass transfer coefficients by a factor of 2 as illustrated in Figures 6-4 and 6-5.

This increase in mass transfer coefficient is accompanied by an increase in pressure drop as illustrated in Figures 6-5 and 6-7. The pressure drop can increase by an order of magnitude relative to an empty channel. However, the increase in pressure drop is smaller when increasing the number of elements from the intermediate value to the maximum value than from a single element to the intermediate number of elements.
Figure 6-4: Sherwood number dependence on Graetz number for Spacer 2 arrangements and empty slit.

Figure 6-5: Sherwood number dependence on Graetz number for Spacer 8 arrangements and an empty slit.
Figure 6-6: Friction factor dependence on Reynolds number for Spacer 2 arrangements and slit.

Figure 6-7: Friction factor dependence on Reynolds number for Spacer 8 arrangements and slit.
Figure 6-8 illustrates the dependence of Sherwood number on Power number for the two spacers considered. The results indicate that for the range of Power number considered both spacer geometries give higher mass transfer coefficients than an empty channel for the same nominal power input.

6.4 **Optimal Parameters to Compare Simulation with Experiment**

As discussed previously, the spacer contacts a single membrane and an impermeable wall in the experimental apparatus. Therefore, simulations were conducted
using the boundary conditions illustrated in Figure 6-9 for comparison with experimental results.

![Diagram](image.png)

Figure 6-9: Boundary conditions corresponding to experimental apparatus.

These boundary conditions were used to simulate Spacer 2 and an empty channel for which experiments were conducted.

### 6.5 Comparison of Experimental Result and Simulation Results

Figure 6-10 illustrates the wall concentration obtained from the experimental results for an empty channel (slit), the commercial spacer supplied with the Sepa cell, and the static mixing spacer with 13 elements. The lower wall concentration of static mixer is indicative of better performance. The lower value of wall concentration indicates that the static mixer mixes fluid in the concentration boundary layer and thereby mitigates concentration polarization as desired.
Figure 6-10: Wall concentration on Reynolds number.

Figure 6-11 illustrates the theoretical predictions obtained from the simulations of the experimental apparatus.

Figure 6-11: Non-dimensionalized Sherwood number depends on \((Reynolds\ number)^{1/3}\)
Although the experimental and theoretical results for the empty channel span different Reynolds number ranges, the two lines appear to lie along a common curve. This is in contrast to the results for the static mixing spacer. The experimental results indicate a significantly higher mass transfer coefficient than predicted by the simulation. The Reynolds number is so low because of wall concentration which indicated in Figure 6-10.

The difference between experimental and theoretical mass transfer coefficients for the static mixing spacer is attributed primarily to the strong dependence of fluid properties, in particular viscosity and diffusivity, on Dextran concentration. The theoretical predictions assume constant physical properties and do not account for this dependence. While simulations can be performed that account for specific physical property variations, the results will be difficult to generalize and apply to other systems. Consequently, the literature commonly assumes theoretical results obtained in the absence of physical property variations can be used if physical properties are evaluated at the concentration of the fluid adjacent to the membrane. Experimental results are non-dimensionalized and reported in Figure 6-11 based on this assumption.

The good agreement between theoretical and experimental results for the empty channel (and the poorer agreement for the static mixing spacer) suggests the effect of material property variations is greater for high mass transfer rates where the concentration boundary layer is thinner. As the boundary layer becomes thinner, concentration gradients become larger.

Figure 6-12 compares theoretical predictions and experimental measurements of the friction factor as a function of Reynolds number. In all cases, the experimental
measurements are significantly higher than the theoretical predictions. These differences also are attributed to the strong dependence of viscosity on concentration.

Figure 6-12: Friction factor dependence on Reynolds number (experiment and simulation).

Figure 6-13: Sherwood number dependence on Power number (experiment and simulation).
Figure 6-13 compares theoretical predictions and experimental measurements of the mass transfer coefficient as a function of Power number. The results indicate that the static mixing spacer gives significantly better performance at comparable power inputs. While the dimensions of the spacer have not been optimized, this improvement suggests the static mixing spacer concept may be of commercial value.
Chapter 7

Conclusion and Future Work

7.1 Conclusion

A static mixing spacer for planar flow channels has been developed. The spacer moves fluid from the upper part of the flow channel to the lower part and vice versa. Streamlines that lie along the external boundaries are moved to the middle of the flow channel and replaced by streamlines from the middle of the flow channel. This mixing disrupts the growth of concentration and temperature boundary layers without the use of eddies or turbulence. Moreover, this mixing fundamentally differs from that produced by static mixing elements for tubular flow channels which do not move surface streamlines to the center of the flow channel.

Preliminary evaluations of mass transfer using a single static mixing element were performed using computational fluid dynamics. The calculations examined the effect of spacer dimensions on mass transfer and pressure drop. In addition, the flow behavior through the solid surface of static mixer was studied to understand how concentration and temperature boundary layer were mixed passing through the static mixer.

The computational results indicated mass transfer coefficients increased dramatically with the static mixing element. However, this performance enhancement came at the cost of increased pressure drop. More pump power needs to provide same
flow rate in an empty channel. This means more utility cost however the main goal for
the static mixer spacer design is to increase the mass transfer coefficients.

The preliminary calculations were used to identify configurations that gave the
highest mass transfer coefficient and highest pressure drop as well as the lowest mass
transfer coefficient and lowest pressure drop. The effect of using multiple spacer
elements in a flow channel was determined for the two configurations. Multiple elements
further increased both mass transfer coefficients and pressure drops. Studying different
spacer arrangement with variation number of elements brought an idea which increasing
the gap length between two elements bring tendency to increasing the potential of the
concentration boundary layer growth at the membrane surface.

Samples of the best performing configuration were fabricated using
stereolithography. Experimental measurements of mass transfer coefficients and pressure
drops were obtained for filtration of Dextran solutions. The experimental measurements
confirm the significant enhancement in mass transfer achieved with the static mixing
spacer.

Experimental results were compared for an empty channel, a commercial spacer,
and the new static mixing spacer as a function of power input by plotting the Sherwood
number versus the Power number. The comparison clearly indicates the ability of the
static mixing spacer to increase mass transfer coefficients significantly, by a factor of
four, for a fixed power input.

Theoretical predictions of mass transfer coefficients and pressure drops are in fair
agreement with experimental measurements for an empty channel but poorer agreement
for the static mixing spacer. The differences are attributed to the following factors:
1. Concentration dependent material properties, especially viscosity and diffusivity

2. A constant temperature boundary condition was used in the simulations while the experiments correspond to a specified wall permeance boundary condition

3. Potential non-uniform flow distribution in the experimental test cell; fluid distribution from the distribution slit into the flow channel was not characterized

7.2 Future Work

While this work demonstrates the potential for the static mixing spacer concept, Future work could improve our understanding of the physics of operation by

1. Performing simulations that account for variability of material properties to determine their influence on mass transfer rates

2. Performing simulations using a constant wall permeance (hydraulic permeability) boundary condition

3. Performing experiments to determine the uniformity of flow distribution in the experimental test cell

4. Performing heat transfer experiments to measure heat transfer coefficients and the ability of the static mixing element to enhance heat transfer; such measurements could be compared directly to the FLUENT simulations
5. Performing experiments and simulations over a broader Reynolds number range to enhance the comparison of experiment and theory, especially in the turbulent flow region.

It also would be of interest to simulate other commercial spacers. Most of the previous work has simulated one or two spacer elements. The lack of simulation results for multiple elements represents an opportunity for additional work to improve our understanding of spacer performance.

Methods to mass produce sheets of the spacer also should be explored. Economical manufacture of the spacer and incorporation in commercial spiral wound modules should be pursued.
References


15. FLUENT USER GUIDE, Chapter 23.3.4 Momentum Equation.

16. FLUENT USER GUIDE, Chapter 23.3.5 Energy Equation.

17. FLUENT USER GUIDE, Chapter 25.3.1 Spatial Discretization.


26. Synderfiltration, degrees of filtration separation

27. Spectrumlabs, filtration

28. Environmental expert, result each product.
Appendix

The procedure to calculate mass transfer coefficients from experimental data is presented in this Appendix for one set of experiment data.

To calculate membrane permeability ($L_p$) the DI water flux is divided by the transmembrane pressure differential.

$$L_p = \frac{J}{\Delta P_{TM}} \tag{1}$$

$\Delta P_{TM}$ : trans membrane pressure

$$\Delta P_{TM} = 52400 \text{ pa} \tag{2}$$

$J$ : permeate flux

$$J = 2.416E - 6 \text{ m/Sec} \tag{3}$$

$$L_p = \frac{2.416E-6}{52400} \tag{4}$$

$$L_p = 4.61078E - 11 \frac{m}{\text{pa \ sec}} \tag{5}$$

The osmotic pressure at the wall ($\Delta \pi_W$) is calculated from the water flux measured during dextran filtration as follows.

$$\Delta \pi_W = \Delta P_{TM} - \frac{J}{L_p} \tag{6}$$

$$\Delta P_{TM} = 54430 \text{ pa} \tag{7}$$

$$J = 2.3924E - 6 \text{ m/Sec} \tag{8}$$

$$\Delta \pi_W = 54430 - \frac{2.3924E-6}{4.61078E-11} \tag{9}$$

$$\Delta \pi_W = 2541 \text{ pa} \tag{10}$$

$$\Delta \pi_W = 37.5C_W + 0.75C_W^2 + 0.00764C_W^3 \tag{11}$$
\[ C_w = 34.86 \text{ kg/m}^3 \text{ and } C_b = 5 \text{ kg/m}^3 \] (12)

The mass transfer coefficient is calculated from the wall concentration based on film theory.

\[ k: \text{ Mass transfer coefficient} \]

\[ k = J/\ln\left(\frac{C_w}{C_b}\right) \] (13)

\[ k = 2.3924E - 6/\ln\left(\frac{34.86}{5}\right) \] (14)

\[ k = 1.232E - 6 \text{ m/sec} \] (15)

The diffusion coefficient is evaluated using the calculated wall concentration.

\[ D: \text{ Diffusion coefficient} \]

\[ D = (0.1204 + 2.614C_1 - 4.167C_1^2 + 2.132C_1^3) \times 10^{-10} \] (16)

\[ C_1: C_w \times 10^{-3} \] (18)

\[ D = 2.0655E - 11 \text{ m}^2/\text{sec} \] (17)

\[ Sh = \frac{kH}{D} \] (18)

\[ H = 0.003 \text{ m} \] (19)

\[ Sh = \frac{1.232E - 6 \times 0.003H}{2.0655E - 11} \] (20)

\[ Sh = 178.94 \] (21)