Mathematical modeling of magnetohydrodynamic micropumps

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MATHEMATICAL MODELING OF MAGNETOHYRDO_DYNAMIC MICROPUMPS

by

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Entitled
MATHEMATICAL MODELING OF MAGNETOHYDRODYNAMIC MICROPUMPS

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Examination Committee Chair

Dean of the Graduate College

Graduate College Faculty Representative
ABSTRACT

MATHEMATICAL MODELING OF MAGNETOHYDRODYNAMIC MICROPUMPS

By

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A lab-on-a-chip (LOC) system is a minute chemical processing plant consisting of interconnected networks of microchannels and reservoirs operating with small volumes of reagents. In many LOC systems, it is necessary to propel fluids from one part of the device to another, control fluid motion, stir and interact various reagents, and detect the presence of target analytes. In LOC systems, these tasks are far from trivial.

This thesis focuses on fluid propulsion under the action of electric and magnetic fields. Both Non-RedOx and RedOx-based Magneto-hydrodynamic (MHD) micropumps, in which the flow is directed by judicious interplay between electric and magnetic fields, have been modeled. The theoretical predictions agree with the experimental results available in the literature. The developed models can be used to test various operating conditions and assist in the MHD micropumps’ design and optimization.
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Finally I would be amiss for not being grateful to the Supreme Being, my Heavenly Father, and His Only Begotten in the flesh, for the opportunity and mercy I know in my heart I have been given to remain on this earth to learn, discover, and progress. Although I am often burdened with my inadequacies, medical conditions, and
character flaws, I know who to turn to for help in these matters and I hope to do and become as they want me to be.
CHAPTER I

LITERATURE REVIEW

1.1 Lab-on-a-chip technology

In recent years there has been a growing interest in developing lab-on-a-chip (LOC) technology for bio-detection, biotechnology, chemical and biological reactors, medical, pharmaceutical, and environmental monitoring (Jensen, 1999; Jain, 2000; Langer, 2000; Stone and Kim, 2001; Whitesides and Stroock, 2001; Chow, 2002; Verpoorte, 2002; and Huikko et al., 2003). Lab-on-a-chip is a minute chemical processing plant, where common laboratory procedures ranging from filtration and mixing to separation and detection are done on devices no larger than the palm of the hand. This technology has the potential of revolutionizing various bioanalytical applications. The interconnected networks of microchannels and reservoirs with tiny volumes of reagents are well matched with the demands for small volume, low cost, rapid response, massive parallel analyses, automation, and minimal cross-contamination that characterize many applications in biotechnology.

Resembling electronic circuit boards, these integrated LOC devices contain a network of micro conduits, which dilutes the sample, separates it into multiple channels for parallel analysis, mixes the sample with target-specific antibodies or reagents, propels the sample from one part of the device to the other, and detects the presence of chemical and biological targets. All of this is done automatically on a single platform, allowing for
precise and reproducible operations, resulting in high data quality, and reducing the need for trained personnel.

In many LOC systems, it is necessary to propel fluids from one part of the device to another, control fluid motion, enhance mixing, and separate fluids (Terray et al., 2002). Fluid propulsion is one of the central problems facing the designer of LOC systems. Thus, my thesis focuses on the use of magnetic and electrostatic forces to pump fluids in micro-conduits. Below, I provide a brief survey of various means of propelling fluids in lab-on-a-chip.

1.2. Fluid Propulsion in LOC

In recent years, various means for propelling the fluid in networks of microchannels have been proposed. Some of these techniques are summarized below.

a) Pressure-driven Flow (Kopp et al., 1998; Fu et al. 2002; Park et al., 2003)

Pressure-driven flow in LOC can be generated either by external pumps, on chip-integrated pumps, or compressed gas. The advantage of pressure-driven flow is that it has the potential to reach high flow rates in micro-conduits. Many microfluidic systems such as flow cytometry use this flow propulsion method to achieve flow rates in the meter per second range in channels having characteristic length scales ranging from a few to hundreds of micrometers (Fu et al. 2002). The pressure driven flow is Poiseuille flow characterized by a parabolic velocity profile, which also has the disadvantage of dispersion. The interplay of convection and diffusion is crucially important in many applications, especially those involving chemical and biological reactors.

b) Electrokinetically Driven Flow (Probstein, 1994).
There are three kinds of electrokinetically driven flow phenomena associated with the propulsion of fluids: electroosmosis, electrophoresis and dielectrophoresis.

The electroosmotic phenomenon is caused by the formation of a net electric charge on the solid's surface that is in contact with the electrolyte solution and the accumulation of mobile counter ions in a thin liquid (double electric or Debye) layer next to the solid's surface. Away from the solid's surface, the electrolyte is neutral. In the presence of an external (driving) electric field, the counter ions in the Debye layer are attracted to the oppositely charged electrode and drag the liquid along. In other words, the electric field, through its effect on the counter ions, creates a body force that, in turn, induces fluid motion. Since the body force is typically concentrated in a very narrow region next to the solid boundaries, the electroosmotic flow has nearly flat velocity profile. The nearly uniform velocity profile reduces dispersion. Additionally, the flow velocity is conduit’s size invariant as long as the conduit’s size is much larger than the thickness of the electric double layer.

Electrophoresis refers to the movement of charged particles under external applied electric field, and it has been widely used to separate large molecules (such as DNA fragments or proteins) from a mixture of similar molecules. In the presence of electric field, various molecules travel through the medium at different rates, depending on their electrical charge and size. The separation is based on these differences. Agarose and acrylamide gels are commonly used for electrophoresis of proteins and nucleic acids. An uncharged conducting object suspended in a solution subject to electric field is polarized. When the electric field is non-uniform, this results in a dipole moment. Due to the interactions between the electric dipole and the gradient of the electric field, the
object migrates in the solution. This phenomenon is called dielectrophoresis (DEP). DEP has been used to trap cells, beads, nano-tubes or other targets to be selectively manipulated or held in a place when washed (Arai et al., 2001; Wheeler et al., 2003). However, the successful application of DEP to separation problems demands awareness of a number of confounding factors such as the polarization of the double layer, electrode polarization, thermal convection, and wide range of particle characteristics under different AC electric field frequency (Gascoyne and Vykoval, 2002).

The big advantage of electric field induced flows is that they do not require any moving parts. However, electrostatic forces usually induce very low flow rates and require the use of very high electric fields. Another significant drawback is the internal heat generation (commonly referred to as Joule heating) caused by the current flows through the buffer solution in the presence of high electric fields (Erickson et al., 2003).

c) Surface tension-driven Flow (Vladimirova et al., 1999; Zhao et al., 2001; Erickson et al., 2002; Mauri et al., 2003; Stange et al. 2003)

Since the characteristic length scale of microfluidic systems is very small, surface forces play an important role. Some research groups took advantage of the surface forces to drive a liquid droplet by modifying the contact angle of the drop with the solid surface. Contact angle modifications can be achieved through the use of temperature or electric fields normal to the liquid-solid interface (electriwetting). Capillary force can also be used to fill initially dry conduits. For example, lateral flow reactors use this mechanism to move the reagents to the detection site. No external driving force such as pump is required for this propulsion method. It is, however, difficult to control the flow direction and flow rate and the process terminates once the dry conduit is fully saturated.
d) Centrifugally Driven Flow (Johnson et al., 2001; Chen et al., 2004)

When the device is rotated such as in the case of a lab-on-a-CD, one can obtain very high accelerations, and fluid motion results. One can control the flow by adjusting the angular rotation speed and the position of the component within the device. However, fluids can only move in the direction of the centrifugal force.

e) Buoyancy-driven Flow (Krishnan et al., 2002; Chen et al., 2004)

Buoyancy effects are generally very small due to the small length scales and small temperature variations in microfluidic devices. However, certain processes such as thermal Polymerase Chain Reaction (PCR) for DNA amplification requires large temperature variations that are sufficient to induce significant flow velocities even in micron-size conduits. Recently, Krishnan et al. (2002) took advantage of the naturally occurring circulation in a cavity heated from below and cooled from above (the Rayleigh-Benard cell) to circulate reagents between two different temperature zones. Chen et al. (2004) significantly improved this concept by confining the reagents in a closed loop thermosyphon.

f) Magneto-hydrodynamics (MHD) Flow

The application of electromagnetic forces to pump, confine, and control fluids is by no means new. MHD is, however, mostly thought of in the context of highly conducting fluids such as liquid metals and ionized gases (i.e., Woodson and Melcher, 1969; Davidson, 2001). Recently, though, Jang and Lee (2000), Lemoff and Lee (2000), Bau (2001), and Zhong, Yi and Bau (2002), Lemoff and Lee (2003) constructed MHD micro-pumps on silicon, ceramic and plastic substrates and demonstrated that these pumps are able to move liquids around in micro conduits. Bau et al. (2001) and Bau et al.
(2002 and 2003) demonstrated the feasibility of using magnetohydrodynamic (MHD) forces to control fluid flow in microfluidic network. By judicious application of different potential differences to different electrode pairs, one can direct the liquid to flow along any desired path without a need for valves and pumps. West et al. (2002) fabricated a MHD continuous flow microreactor with three thermal zones to facilitate the thermocycling needed for DNA amplification. Bao and Harrison (2003) fabricated an AC MHD pump for tubular liquid chromatography. Eijkel et al. (2003) fabricated a circular AC MHD pump for closed loop liquid chromatography.

MHD driven flow provides an inexpensive means for controlling the flow and stirring liquids in microfluidic systems. MHD driven flow has many advantages over electroosmosis. Magneto-hydrodynamics requires low electrical potentials (<1V) while electroosmotic flows require potentials in the hundreds of volts. Additionally, MHD flow is much faster than electroosmotic flow. Some potential problems of MHD driven flow are bubble formation, electrode corrosion, and migration of analytes in the electric field. Most of these problems can, however, be reduced or eliminated altogether with the appropriate selection of electrolytes, electrode materials, and operating conditions. Bubble formation is not likely to be a problem at sufficiently low potential differences (smaller than the potential needed for the electrolysis of water). With the use of RedOx solutions such as FeCl₂ / FeCl₃, potassium ferrocyanide trihydrate (K₄[Fe(CN)₆]×3H₂O) potassium ferricyanide (K₃[Fe(CN)₆]), and hydroquinone in combination with inert electrodes, one can obtain relatively high current densities without electrode corrosion, bubble formation, and electrolyte depletion.
In addition to the mechanisms described above, some other techniques are available to induce fluid motion such as surface acoustic wave inducing movement in the fluid boundary close to the surface and thus propelling the fluid (Moroney et al., 1991; Zhu and Kim, 1998; Nguyen and White, 1999; Huang and Kim, 2001) and peristalsis (Liu, Enzelberger and Quake, 2002; Bu et al., 2003). Table 1.1 compares the various means for fluid propulsion used in microfluidic systems.

3. Proposed Work

MHD-based LOC market is still in the early stages, and there is a strong need for a design tool to optimize device design and to obtain estimates of the device’s expected performance. This thesis focuses on the theoretical analysis and numerical simulations of the MHD micro-pumps in the absence and presence of RedOx species, and the numerical predictions are validated with the experimental data obtained from the literature.
Table 1.1: Various means to propel fluid in microfluidic systems

<table>
<thead>
<tr>
<th>Means</th>
<th>Description</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>Fluid motion is induced by pressure difference.</td>
<td>High flow rate; No moving parts</td>
<td>Need a mechanical pump; High pressure</td>
</tr>
<tr>
<td>Electroosmosis</td>
<td>Fluid motion is induced by electrostatic force.</td>
<td>Uniform velocity; No moving parts</td>
<td>Low flow rate; High electric field; Depend on the characteristics of the liquid-solid interface.</td>
</tr>
<tr>
<td>Surface tension</td>
<td>Fluid motion is induced by surface tension.</td>
<td>No external driving force; No moving parts</td>
<td>It is difficult to control the flow rate and flow direction; The process terminates once the conduit is filled.</td>
</tr>
<tr>
<td>Centrifugal force</td>
<td>The device is placed on a rotating platform.</td>
<td>High flow rate</td>
<td>Fluids move only in one direction.</td>
</tr>
<tr>
<td>Buoyancy</td>
<td>Fluid motion is induced by the dependence of fluid density on the temperature variations.</td>
<td>Self-actuated; No moving parts; Simple</td>
<td>Large temperature variations are required.</td>
</tr>
<tr>
<td>MHD</td>
<td>The motion is induced by the interactions between electric and magnetic fields.</td>
<td>Low cost; Low electric field; Reasonable flow rates; No moving parts.</td>
<td>Volumetric force does not scale well with size. To avoid problems with electrode erosion and bubble formation, one needs to use RedOx-based electrolytes that may not be compatible with certain biological interactions.</td>
</tr>
</tbody>
</table>
CHAPTER 2

NON-REDOX MHD MICROPUMPS

2.1 Introduction

In recent years, there has been a growing interest in developing LOC systems for bio-detection, biotechnology, chemical reactors, and medical, pharmaceutical, and environmental monitors. In many of these applications, it is necessary to propel fluids and particles from one part of the device to another, control the fluid motion, stir, and separate fluids. In microdevices, these tasks are far from trivial. Magneto-hydrodynamics (MHD) offers a convenient means of performing some of these functions. Within the current decade, Jang and Lee (2000), Lemoff and Lee (2000), and Zhong, Yi, and Bau (2002) have constructed MHD micro-pumps on silicon and ceramic substrates and demonstrated that these pumps are able to move liquids around in micro conduits. Subsequently, Bau et al. (2002) demonstrated the feasibility of using magneto hydrodynamic (MHD) forces to control fluid flow in microfluidic networks. The liquids need to be only slightly conductive—a requirement met by many biological solutions.

The basic building block (branch) of the MHD-based microfluidic network is depicted in Fig. 2.1. The branch consists of a conduit with two electrodes deposited along its two opposing walls. The conduit is filled with an electrolyte solution such as NaCl electrolyte in the absence of RedOx species. Many conduits of the type depicted in Fig. 2.1 can be connected to form a network. The entire device is subjected to a uniform
magnetic field in the z-direction. The magnetic field can be provided by either a permanent magnet or an electromagnet. When a potential difference is applied across the two electrodes, a current density $J$ transmits through the solution. The interaction between the electric current density $J$ and the magnetic field $B$ generates a Lorentz force $J \times B$ which is directed along the conduit’s axis (in the x-direction that is perpendicular to the cross-section of the microchannel) and drives the fluid motion.

![Diagram](image)

Fig. 2.1: Schematics of a three-dimensional, planar microchannel equipped with two electrodes positioned along the opposing walls. The channel is filled with a dilute weakly conductive electrolyte solution such as NaCl and subjected to a uniform magnetic flux density $B$. A potential difference $\Delta V$ is applied across the electrodes resulting in a current density $J$ transmits through the electrolyte solution. The interaction between the current density $J$ and the magnetic field $B$ generates a Lorentz force $J \times B$ which is directed along the conduit’s axis (in the x-direction that is perpendicular to the cross-section of the microchannel) and drives the fluid motion.
density and the magnetic field induces Lorentz forces which pump the fluid from one end of the channel to the other.

The objective of this chapter is to model the MHD micropumps in the absence of RedOx species. We first describe a full mathematical model to model the MHD micropumps. Then, we numerically solve the model with commercial finite element package COMSOL™ (version 3.3b). Subsequently, the theoretical predictions are compared with experimental data obtained from the literature. Finally, based on the obtained results, a closed-form expression for predicting the flow rate of the MHD micropumps is derived.

2.2 Mathematical Model

In this section, we introduce a full 3D mathematical model consisting of the continuity and Navier-Stokes equations for the fluid motion and the Laplace equation for the electric potential in the electrolyte solution. In the current analysis, the electrolyte solution is treated as an Ohmic conductor with a uniform electric conductivity.

Let us consider a planar microchannel with a rectangular cross-section connecting two identical reservoirs on both sides. In the current analysis, we neglect the effects of the two reservoirs on the fluid motion and the ionic mass transport within the microchannel. The length, width, and height of the microchannel are, respectively, \( L, W, \) and \( H \). We use a Cartesian coordinate system with its origin positioned at one of the channel's corners. The coordinates \( x, y, \) and \( z \) are aligned, respectively, along the conduit's length, width, and depth (\( 0 \leq x \leq L, 0 \leq y \leq W, \) and \( 0 \leq z \leq H \)). Two planar electrodes of length \( L_E \) and height \( H \) are deposited along the opposing walls with the leading edge located at a distance \( L_I \) downstream of the conduit's entrance (\( L_I \leq x \leq L + L_E, 0 \leq z \leq H, y = 0 \)).
and \( W \), respectively). The portions of the conduit's walls that are not coated with electrodes are made of dielectric material. Fig. 2.1 schematically depicts the three-dimensional, planar microchannel with two electrodes deposited along the opposing walls. The conduit is filled with a weakly conductive electrolyte solution such as KCl electrolyte.

When a potential difference, \( A V \), is applied across the two electrodes deposited along the opposing walls, a current density \( J \) transmitted through the electrolyte solution results. Hereafter, bold letters denote vectors. We assume that the entire device is positioned under a magnetic field with a uniform magnetic flux density \( B = B \mathbf{e}_z \) directed in the \( z \)-direction. Here \( \mathbf{e}_z \) is a unit vector in the \( z \)-direction. The interaction between the current density \( J \) and the magnetic field \( B \) induces a Lorentz force of density 

\[
F = J \times B = J_y B \mathbf{e}_x - J_x B \mathbf{e}_y + 0 \mathbf{e}_z,
\]

which can be used to manipulate fluids. In the above expression, \( J_x \) and \( J_y \) are, respectively, the \( x \)- and \( y \)-component current densities; \( \mathbf{e}_x \) and \( \mathbf{e}_y \) are, respectively, the unit vectors in the \( x \)- and \( y \)-directions.

2.2.1. The Mathematical Model for the Fluid Motion

We assume that the electrolyte solution is incompressible. Under steady state, the flow driven by both the Lorentz force and the pressure gradient is described with the continuity and Navier-Stokes equations:

\[
\nabla \cdot \mathbf{u} = 0
\]

(1)

and
\[ \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + F_L \]  

(2)

In the above, \( p \) is the pressure; \( \rho \) and \( \mu \) denote, respectively, the electrolyte solution’s density and dynamic viscosity; \( \mathbf{u} = u \mathbf{e}_x + v \mathbf{e}_y + w \mathbf{e}_z \) is the fluid’s velocity in which \( u, v, \) and \( w \) are, respectively, the velocity components in the \( x-, y-, \) and \( z- \) directions; and \( F_L \) is the induced Lorentz force in the electrolyte solution.

In order to solve the equations (1) and (2), appropriate boundary conditions are required. A non-slip boundary condition is specified at the solid walls of the microchannel:

\[
\mathbf{u}(x, 0, z) = \mathbf{u}(x, W, z) = 0 \\
\mathbf{u}(x, y, 0) = \mathbf{u}(x, y, H) = 0
\]

(3)

(4)

In other words, all the velocity components along the solid walls of the microchannel are zero. Normal pressure boundary conditions are used at the entrance \((x=0)\) and exit \((x=L)\) of the microchannel:

\[
p(0, y, z) = P_1 \\
t \cdot \mathbf{u}(0, y, z) = 0 \\
p(L, y, z) = P_2 \\
t \cdot \mathbf{u}(L, y, z) = 0,
\]

(5)

(6)

(7)

(8)

where \( t \) is the unit vector tangent to the planes \( x = 0 \) in (6) and \( x = L \) in (8). The externally applied pressure gradient is \( \Delta p/L \) with \( \Delta p = P_1 - P_2 \). In the absence of the externally applied pressure gradient across the microchannel, \( P_1 = P_2 = 0 \).
To numerically solve the flow field from the equation (1) and the set of the
equations (2) subjected to the boundary conditions (3)-(8), the spatial distribution of the
current density, \( \mathbf{J} = J_x \mathbf{e}_x + J_y \mathbf{e}_y + J_z \mathbf{e}_z \), within the electrolyte solution is required, and is
developed in the next section.

2.2.2. The Mathematical Model for the Current Density

According to Ohm's law for a moving conductor of conductivity \( \sigma \) in a
magnetic field, the potential difference \( \Delta V = V_1 - V_2 \) induces a current of density:

\[
\mathbf{J} = \sigma \left( -\nabla V + \mathbf{u} \times \mathbf{B} \right).
\]  \( \text{(9)} \)

In the above, \( \mathbf{u} \times \mathbf{B} \) is the induction term. Typically, in microfluidic systems,
\( ||\mathbf{u}|| < 10^2 \text{m/s}, ||\mathbf{B}|| < 1 \text{T}, ||\nabla V|| > 10^3 \text{V/m}, ||\mathbf{u} \times \mathbf{B} / \nabla V|| < 10^{-5} \), thus allowing the induction
term to be neglected. Therefore, one can calculate the current density \( \mathbf{J} \) with

\[
\mathbf{J} = -\sigma \nabla V
\]  \( \text{(10)} \)

The electric potential \( V \) satisfies the Laplace equation:

\[
\nabla^2 V = 0
\]  \( \text{(11)} \)

We use insulating boundary conditions at all dielectric surfaces:

\[
\mathbf{n} \cdot \nabla V (0 < x < L, y = 0, 0 < z < H) = 0
\]  \( \text{(12)} \)

\[
\mathbf{n} \cdot \nabla V (0 < x < L, y = W, 0 < z < H) = 0
\]  \( \text{(13)} \)

\[
\mathbf{n} \cdot \nabla V (L_x < x < L, y = 0, 0 < z < H) = 0
\]  \( \text{(14)} \)

\[
\mathbf{n} \cdot \nabla V (L_x < x < L, y = W, 0 < z < H) = 0
\]  \( \text{(15)} \)
\[ \mathbf{n} \cdot \nabla V(0 < x < L, 0 < y < W, z = 0) = 0 \]  \hspace{1cm} (16) \\
\[ \mathbf{n} \cdot \nabla V(0 < x < L, 0 < y < W, z = H) = 0 \]  \hspace{1cm} (17)

At the entrance and exit cross sections of the microchannel, we assume that the electric fields are zero:

\[ \mathbf{n} \cdot \nabla V(0, 0 < y < W, 0 < z < H) = 0, \]  \hspace{1cm} (18) \\
\[ \mathbf{n} \cdot \nabla V(L, 0 < y < W, 0 < z < H) = 0, \]  \hspace{1cm} (19)

When a potential difference is applied to the electrodes positioned along the opposing walls, we specify the potentials on the surface of the anode and cathode:

\[ V(L_1 \leq x < L_1 + L_{e}, y = 0, 0 < z < H) = U_{an}, \]  \hspace{1cm} (20)

and

\[ V(L_1 \leq x < L_1 + L_{e}, y = W, 0 < z < H) = 0. \]  \hspace{1cm} (21)

In expression (20), \( U_{an} \) is the potential difference applied to the anode, and the cathode connects to the ground of a power supply.

When the total current, \( I \), instead of a potential difference is applied, the potential difference \( U_{an} \) is unknown and it is a part of the solution. \( U_{an} \) will be determined from the following surface integration along the anode:

\[ I = -\sigma \int_{S} \nabla V(L_1 \leq x < L_1 + L_{e}, y = 0, 0 \leq z \leq H) dS, \]  \hspace{1cm} (22)

where \( S \) is the surface area of the anode.
2.3. Solver Validation

To numerically solve the three-dimensional system, we used the commercial finite element package COMSOL (version 3.3b, www.femlab.com) operating with a 64-bit dual-processor workstation of 32GB RAM (www.polywell.com). The 3D computational domain was discretized into quadratic tetrahedral elements. We employed non-uniform elements with a larger number of elements next to the inlet and outlet cross-sections, as well as along the surfaces of the electrodes where the Lorentz force occur. We compared the solutions obtained for different mesh sizes to ensure that the numerical solutions are convergent, independent of the size of the finite elements, and satisfy the various conservation laws.

Since the MHD flow is similar to pressure-driven flow, to verify the code, we simulated the pressure-driven flow in a 3D microchannel and compared the numerical predictions of the fully developed pressure-driven flow with the analytical solutions available in the literature (White, 2006, Page 112-113):

\[
u(y, z) = a \sum_{n=1,3,5,\ldots}^{\infty} \frac{(-1)^{n+1}}{2a} \left[ \cosh \left( \frac{i \pi (z - b)}{2a} \right) \cos \left( \frac{i \pi (y - a)}{2a} \right) \right] \frac{\cosh \left( \frac{i \pi b}{2a} \right)}{i^3}.
\]

In equation (23),

\[
A = \frac{48U}{\pi^3 \left[ 1 - \frac{192a}{\pi^2 b} \sum_{j=1,3,5,\ldots}^{\infty} \frac{\tanh(j \pi b / 2a)}{j^5} \right]},
\]

\[a = W/2, \text{ and } b = H/2.\]
\( \bar{U} \) is the average velocity. The numerical solution favorably agrees with the analytical solution mentioned above (results are not shown here).

### 2.4 Results and Discussion

We first simulated the MHD flows in 3D planar channels with \( L=18 \text{ mm} \) in length, \( H=7 \text{ mm} \) in depth, and various widths when the magnetic field \( B=0.02T \) and the total current \( I=0.7A \). The electrodes cover the entire side walls (i.e., \( L_e=L \), and \( L_f=0 \) in Fig.2.1). The electrolyte solution is saline solution. The channel geometry and the experimental conditions are exactly the same as those used in the experiments conducted by Ho (2006). Fig.2.2 depicts the flow rate as a function of the width of the channel. The solid line and the circles in Fig.2.2 represent, respectively, our numerical predictions obtained from the model described in section 2.2 and the experimental data obtained by Ho (2006). The predictions agree with the experimental data. Under the studied conditions, the flow rate nonlinearly increases as the width of the channel increases.
Fig. 2.2: The flow rate as a function of the width of the channel for a saline solution when $B=0.02$ T, $L=80$ mm, $H=7$ mm, and the externally applied current $I=0.7$ A. The line and symbols represent, respectively, the numerical predictions and the experimental data obtained from the literature.

Figure 2.3 depicts the average velocity of the MHD flow in a planar conduit as a function of the applied current when $B=0.02$T and $L_E=L$. The length, width, and height of the channel are, respectively, $L=80$ mm, $W=3$ mm, and $H=7$ mm. The electrolyte solution present in the solution is saline solution. The line and symbols in Fig. 2.3 represent, respectively, the numerical predictions and the experimental data obtained from Ho (2006). The numerical predictions agree with the experimental data when the current is low. The deviation between the prediction and the experimental data increases as the current increases. In the experiments, since there is no RedOx species present in the

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solution, there are significant bubble formations under high current conditions. The formed bubbles slow down the fluid motion which explains why our predictions are higher than the experimental data when the current is high. The average velocity (or flow rate) linearly increases with the applied current.

![Graph](image)

Fig. 2.3: The average velocity as a function of the externally applied current for a saline solution when \( B = 0.02 \) T, \( L = 80 \) mm, \( W = 3 \) mm, and \( H = 7 \) mm. The line and symbols represent, respectively, the numerical predictions and the experimental data obtained from the literature.

In most regions of the planar microchannel, the current density \( J \) is directed nearly normal to the electrodes’ surfaces, and the induced Lorentz force \( J \times B \) is thus directed along the \( x \)-direction. Consequently, the velocity components in the \( y \)- and \( z \)-directions are at least two orders of magnitude lower than the velocity component in the
The $x$-component velocity is nearly independent of the coordinate $x$, and its profile looks like a paraboloid, as shown in Fig.2.4.

Fig.2.4: The spatial distribution of the $x$-component velocity for a saline solution when $B=0.02$ T, $L=80$ mm, $W=3$ mm, and $H=7$ mm. The applied current $I=0.1$ A. The electrolyte is 1 M NaCl solution.

Since the induced Lorentz force is a body force, the induced MHD flow is similar to a fully developed pressure-driven flow in a three-dimensional microchannel. The $x$-component velocity can be approximated with that of a fully developed duct flow with a rectangular cross-section, as shown in the expression (23). By substituting the velocity profile (23) into the $x$-component momentum equation and integrating that equation in the entire domain, the average velocity (flow rate) in terms of a series form can be obtained. However, the obtained expression for the average velocity (flow rate) in terms

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of a series solution is not always practical for applications such as the inverse problems including the optimization of the channel’s dimensions and the determination of the currents or voltages needed to achieve the desired flow rates and flow patterns in MHD microfluidic networks. Therefore, we derive a closed form approximation for the average velocity (flow rate) which will be useful for solving the inverse problems in MHD networks.

The velocity profile (23) can be approximated with the following closed form approximation with an error less than 1% (Natarajan and Lakshmanan, 1972):

$$u(y,z) = \bar{U} \left( \frac{m+1}{m} \right) \left( \frac{n+1}{n} \right) \left[ 1 - \left( \frac{y-a}{a} \right)^m \right] \left[ 1 - \left( \frac{z-b}{b} \right)^n \right],$$  (24)

with

$$m = 1.7 + 0.5 \left( \frac{b}{a} \right)^{-1.4} \quad \text{and} \quad n = \begin{cases} 2 & \text{for } \frac{b}{a} \leq \frac{1}{3} \\ 2 + 0.3 \left( \frac{b}{a} - \frac{1}{3} \right) & \text{for } \frac{b}{a} \geq \frac{1}{3} \end{cases}.$$  (25)

The steady x-component momentum equation can be approximated by:

$$-\frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + J_x B = 0.$$  (26)

The equation (26) represents a balance between the pressure force, the viscous force, and the Lorentz force. Substituting (24) into (26), and taking volume integration of the equation (26), the average velocity becomes
\[
\overline{U} = \frac{BIH - (P_2 - P_1)H^2}{4\mu L \left[ (n+1)\frac{H^2}{W^2} + (m+1) \right]} = G_1 I + G_2 \Delta p.
\] (27)

In the above, \(\Delta p = P_1 - P_2\); \(G_1 = \partial \overline{U} / \partial \eta\) and \(G_2 = \partial \overline{U} / \partial \Delta p\) are, respectively, the electrical and hydraulic transport coefficients. As compared to the expression for the average velocity (flow rate) in terms of a series solution, the obtained closed form approximation (27) will be more practical to compute the flow rates in MHD networks and to solve the control (inverse) problem of determining the magnitudes and polarities of the applied currents of individually controlled branches in the MHD networks so as to achieve the desired flow patterns and flow rates. In the absence of the pressure difference between the conduit’s inlet and exit (i.e., \(P_1 = P_2\)), the average velocity is

\[
\overline{U} = \frac{BIH}{4\mu L \left[ (n+1)\frac{H^2}{W^2} + (m+1) \right]} = G_1 I .
\] (28)

In the absence of the applied pressure gradient (i.e., \(\Delta p = P_1 - P_2 = 0\)), Fig.2.5 depicts the average velocity as a function of the applied current when \(B=0.02\) T, \(L=80\) mm, \(W=2.88\) mm, and \(H=7\) mm. The solid line and circles in Fig.2.5 represent, respectively, the predictions obtained from the 3D full mathematical model and the approximation (28), and they are in good agreement. Therefore, one can use the closed form approximation to estimate the performance of the MHD micropumps without solving 3D PDEs.
Fig.2.5: The average velocity as a function of the externally applied current for a saline solution when $B=0.02$ T, $L=80$ mm, $W=3$ mm, and $H=7$ mm. The line and symbols represent, respectively, the numerical predictions from 3D full mathematical model and the closed form approximation (27) in the absence of the applied pressure gradient.
Fig. 2.6: The average velocity as functions of the height and width of the microchannel with magnetic flux density $B=0.44$ T, applied current $I=0.15$ mA, and length of the conduit $L=18$ mm.

The closed form approximation (27) can also be used to optimize the channel's dimensions and to determine the currents needed to achieve the desired flow patterns and flow rates in complex MHD networks. Fig. 2.6 depicts the average velocity as functions of the height and width of the conduit when its length $L=18$ mm, the magnetic flux density $B=0.44$ T, the current $I=0.15$ mA, and $\Delta p = 0$. When the channel is very shallow, the average velocity increases with the width of the channel. This, however, is not true for a wider channel. Once the width exceeds a certain value, the average velocity peaks and then declines with the increase in the channel's width. For a deep channel, the average velocity increases with the width of the channel. When the area of the cross-section in the $y$-$z$ plane and the length of the channel are fixed, there are optimal values for the height and width of the channel under which the flow rate is the maximum. Using
the closed form approximation (27) when \( \Delta p = 0 \), the optimal height of the channel derived from \( \frac{d\bar{U}}{dH} = 0 \) is governed by the solution of the following equation:

\[
1.5 H^6 / A^3 + 5.7 H^4 / A^2 - 1.9 A^{14} / H^{28} - 2.7 = 0 ,
\]

(29)

where \( A \) is the area of the cross-section in the \( y-z \) plane of the channel. The optimal width of the channel is then \( W=\bar{A} / H \). Fig.2.7 depicts the flow rate, \( Q = \bar{U} A \), as a function of the height of the channel when the cross-section area \( A=0.2211 \text{ mm}^2 \), and all other conditions are the same as those in Fig.2.6. The predefined cross-sectional area and length are the same as those of the channel used in the experiments by Aguilar et al. (2006). When the channel is shallow, the flow rate increases as the height increases. When the height of the channel is larger than a threshold value, the flow rate reaches the maximum and then declines with the height. The maximum flow rate occurs in a channel with \( H \approx 410 \) \( \mu \text{m} \) which corresponds to the solution of the equation (29).
Fig. 2.7: The flow rate as a function of the height of the microchannel when the magnetic flux density $B=0.44$ T, the applied current $I=0.15$ mA, the length of the conduit $L=18$ mm, and the cross-section area in the y-z plane is $0.2211 \text{ mm}^2$. 

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Fig. 2.8: The flow rate as a function of the magnetic field under various currents. The length, width, and height of the channel are, respectively, L=80 mm, W=3 mm, and H=7 mm. L_i=22.5 mm, L_e=35 mm. The electrolyte is 1 M NaCl solution.

Figure 2.8 depicts the flow rate as a function of the strength of the magnetic field when the externally applied current I=0.1A (dotted line), 0.2 A (dashed line), and 0.1 A (solid line). The length, width, and height of the channel are, respectively, 80 mm, 2.88 mm, and 7 mm. For a given current, the flow rate nearly linearly increases as the strength of the magnetic field increases. As the current increases, the effects of the strength of the magnetic field on the flow rate increases.
Fig. 2.9: The flow rate as a function of the applied potential difference. The length, width, and height of the channel are, respectively, $L=80$ mm, $W=3$ mm, and $H=7$ mm. $L_i=22.5$ mm, $L_e=35$ mm, $B=0.044$, and the electrolyte is $1$ M NaCl.

When a potential difference instead of a current is specified, Fig. 2.9 depicts the flow rate as a function of the externally applied potential difference when $B=0.044$ T, $L=80$ mm, $W=2.88$ mm, $H=7$ mm, $L_i=22.5$ mm, $L_e=80$ mm. The electrolyte solution is $1$ M NaCl. The flow rate linearly increases as the potential difference increases. However, the applied potential difference could not exceed the voltage under which the electrolysis occurs. Fig. 2.10 depicts the flow rate as a function of the strength of the magnetic field when the potential differences are $1.2$ V (solid line) and $0.8$ V (dashed line). The other conditions are the same as those used in Fig. 2.9. Similar to the case when the current instead of potential difference is applied, the flow rate nearly linearly increases as the magnetic field increases. The slope $dQ/dB$ increases as the potential difference increases.
Magneto-hydrodynamic (MHD) flow of a weakly conductive electrolyte solution in the absence of RedOx species has been investigated theoretically. Inert electrodes are deposited along segments of the opposing walls of a microconduit that is filled with a Non-RedOx electrolyte solution. The conduit is positioned in a uniform magnetic field. When a potential difference is applied across the opposing electrodes, the resulting current interacts with the magnetic field to induce Lorentz forces, which, in turn, pump the fluid from one end of the channel to the other. A mathematical model including the
Navier-Stokes equations for the flow field and Laplace equation for the electric potential in the electrolyte solution has been developed. The numerical predictions are compared with the experimental data obtained from the literature, and they are in qualitative agreement. When the current instead of the voltage is applied, a closed form expression for estimating the flow rate has been derived, which can be used to estimate the flow rate, and to optimize the channel’s aspect ratio.
CHAPTER 3

REDOX MHD MICROPUMPS

3.1 Introduction

Lab-on-a-chip (LOC) is a minute chemical processing plant, where common laboratory procedures ranging from filtration and mixing to separation and detection are done on devices that are no larger than the palm of the hand. This technology has the potential of revolutionizing various bioanalytical applications. The interconnected networks of microchannels and reservoirs with tiny volumes of reagents are well matched with the demands for small volume, low cost, rapid response, massive parallel analyses, automation, and minimal cross-contamination that characterize many applications in biotechnology. Fluid manipulation such as fluid propulsion and mixing is one of the central problems facing the designer of such LOC devices.

In recent years, various means for propelling the fluid in networks of microchannels have been proposed, such as pressure-driven flow, electrokinetically driven flow (electroosmosis, electrophoresis, and dielectrophoresis), surface tension driven flow, centrifugally driven flow, buoyancy-driven flow, and MHD flow, to cite only a few of them. Relative to other methods for manipulating fluids for various microfluidic applications, the MHD-based LOC devices can be operated at very low voltages and with no moving parts. In addition, MHD propulsion is one of the few methods that allow pumping of weakly conductive liquids such as buffer solutions along a closed loop,
thereby forming a conduit with an “infinite length.” Up to now, various MHD micropumps (Jang et al., 2000; Davidson et al., 2001; and Woodson et al., 2006) operating under either AC or DC electric fields have been designed, modeled, constructed, and tested for various applications. The use of AC electric fields usually induces inductive eddy current with significant energy dissipation and heating. By using DC fields, the serious heating problems resulting from the induced eddy currents can be solved. However, two problems which have hindered the practical application of DC MHD microfluidics are short electrode lifetime and bubble generation due to electrolysis. The introduction of RedOx species into the liquid is a potential solution to the problems associated with the DC MHD microfluidics (Leventis et al., 1999; Clark et al., 2004; and Arumugam et al., 2004). RedOx-based DC MHD has several benefits. For example, the electric potential applied across the electrodes can be very low (several mV to ~1V), which eliminates the bubble generation problem. In addition, the electrode lifetime is longer because electrode oxidation does not occur in the presence of the electroactive RedOx species.

There are a large number of factors that affect the operation and performance of RedOx-based MHD devices: the concentrations of the electroactive and supporting electrolyte, the type of the RedOx species, the aspect ratio of the microchannel’s cross-section, the configuration of the electrodes, the externally applied electric potential or electric current, and the strength of the magnetic field. To achieve the desired flow rates and flow patterns in the RedOx-based MHD microfluidics, theoretical analysis of RedOx-based MHD flow in planar conduits will be conducted in this chapter. The rest of this chapter is organized as follows: Section 2 introduces the mathematical model for the
conjugate problem of MHD flow, electron transfer, and ionic mass transport of both electroactive and inert species. Section 3 describes the code validation by comparing our numerical predictions with a few special cases reported in the literature. Section 4 provides the RedOx-based MHD flow in 3D planar conduits. Section 5 concludes.

3.2 Mathematical Model

In this section, we introduce a full 3D mathematical model consisting of the Navier-Stokes equations for the fluid motion, the Nernst-Planck equations for the concentrations of both the electroactive and inert species, and the local electroneutrality condition for the electric potential in the electrolyte solution. This model accounts for the quasi-reversible oxidation and reduction reactions at the electrodes' surfaces and the convection induced by the Lorentz force through the interaction between the Faradaic current and the external magnetic field which can be provided by either a permanent magnet or an electromagnet.

Let us consider a planar microchannel with a rectangular cross-section connecting two identical reservoirs on either side. In the current analysis, we neglect the effects of the two reservoirs on the fluid motion and the ionic mass transport within the microchannel. The length, width, and height of the microchannel are, respectively, \( L \), \( W \), and \( H \). We use a Cartesian coordinate system with its origin positioned at one of the channel's corners. The coordinates \( x \), \( y \), and \( z \) are aligned, respectively, along the conduit's length, width, and depth (\( 0 \leq x \leq L \), \( 0 \leq y \leq W \), and \( 0 \leq z \leq H \)). Two planar electrodes of length \( L_E \) and height \( H \) are deposited along the opposing walls with the leading edge located at a distance \( L_f \) downstream of the conduit's entrance (\( L_f \leq x \leq L_f + L_E \), \( 0 \leq z \leq H \), \( y = 0 \) and \( W \), respectively). The portions of the conduit's walls that are not coated with
electrodes are made of dielectric material. Figure 3.1 schematically depicts the three-dimensional, planar microchannel with two electrodes deposited along the opposing walls. The conduit is filled with a dilute quasi-reversible RedOx electrolyte solution such as the mixture of $K_4[Fe(CN)_6]$ and $K_3[Fe(CN)_6]$.

Fig.3.1: Schematic of a three-dimensional, planar microchannel equipped with two electrodes positioned along the opposing walls. The channel is filled with a dilute RedOx electrolyte solution and subjected to a uniform magnetic flux density $B$. A potential difference $\Delta V$ is applied across the electrodes resulting in a current density $J$ transmits through the electrolyte solution. The interaction between the current density and the magnetic field induces Lorentz forces which pump the fluid from one end of the channel to the other.
When a potential difference, $\Delta V$, is applied across the two electrodes deposited along the opposing walls, a current density $J$ transmitted through the electrolyte solution results. We assume that the entire device is positioned under a magnetic field with a uniform magnetic flux density $B = B \hat{e}_z$ directed in the $z$-direction. Here $\hat{e}_z$ is a unit vector in the $z$-direction. The interaction between the current density $J$ and the magnetic field $B$ induces a Lorentz force of density $F = J \times B = J_x B \hat{e}_x - J_y B \hat{e}_y + 0 \hat{e}_z$, which can be used to manipulate fluids. In the above expression, $J_x$ and $J_y$ are, respectively, the $x$- and $y$-component current densities; $\hat{e}_x$ and $\hat{e}_y$ are, respectively, the unit vectors in the $x$- and $y$-directions.

3.2.1. The Mathematical Model for the Fluid Motion

We assume that the electrolyte solution is incompressible. Under steady state, the flow driven by both the Lorentz force and the pressure gradient is described with the continuity and Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \quad (30)$$

and

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F}_L \quad (31)$$

Above, $p$ is the pressure; $\rho$ and $\mu$ denote, respectively, the electrolyte solution's density and dynamic viscosity; $\mathbf{u} = u \hat{e}_x + v \hat{e}_y + w \hat{e}_z$ is the fluid's velocity in which $u$, $v$, and $w$ are, respectively, the velocity components in the $x$-, $y$-, and $z$-directions; and $\mathbf{F}_L$ is the induced Lorentz force in the electrolyte solution, $\mathbf{F}_L = J \times \mathbf{B} = J_x B \hat{e}_x - J_y B \hat{e}_y + 0 \hat{e}_z$. In the current work, we neglect (i) the natural
convection induced by the density variations due to the electrochemical reactions on the surfaces of the electrodes (Qian et al., 2006), (ii) the paramagnetic forces induced by the concentration gradients of the paramagnetic species (Aguilar et al., 2006), and (iii) the induced magnetic field due to small Reynolds numbers of the MHD flows in microchannels.

In order to solve the equations (1) and (2), appropriate boundary conditions are required. A non-slip boundary condition is specified at the solid walls of the microchannel:

\[
\mathbf{u}(x,0,z) = \mathbf{u}(x,W,z) = 0 \tag{32}
\]

\[
\mathbf{u}(x,y,0) = \mathbf{u}(x,y,H) = 0 \tag{33}
\]

In other words, all the velocity components along the solid walls of the microchannel are zero. Normal pressure boundary conditions are used at the entrance \((x=0)\) and exit \((x=L)\) of the microchannel:

\[
p(0,y,z) = P_1 \tag{34}
\]

\[
t \cdot \mathbf{u}(0,y,z) = 0 \tag{35}
\]

\[
p(L,y,z) = P_2 \tag{36}
\]

\[
t \cdot \mathbf{u}(L,y,z) = 0 \tag{37}
\]

where \(t\) is the unit vector tangent to the planes \(x=0\) in (6) and \(x=L\) in (8). The externally applied pressure gradient is \(\Delta p/L\) with \(\Delta p = P_1 - P_2\). In the absence of the externally applied pressure gradient across the microchannel, \(P_1=P_2=0\).
To numerically solve the flow field from the equation (1) and the set of the
equations (2) subjected to the boundary conditions (3)-(8), the spatial distribution of the
current density, \( \mathbf{J} = J_x \mathbf{e}_x + J_y \mathbf{e}_y + J_z \mathbf{e}_z \), within the electrolyte solution is required, and is
developed in the next section.

3.2.2. The Mathematical Model for Multi-Ion Mass Transport

In this section, we present a more general multi-ion mass transport model which
includes the Nernst-Planck equation for the concentration of each ionic species and the
local electroneutrality condition for the electric potential in the solution. In comparison to
the previous analysis in chapter 2 in which the electrolyte was simply treated as a
conductor with a uniform electric conductivity, the ionic mass transport is taken into
account in the current analysis.

We assume that the electrolyte solution contains \( K \) dissolved ionic species
\((k=1,\ldots, K)\). The flux density of each aqueous species due to convection, diffusion, and
migration is given by
\[
\mathbf{N}_k = \mathbf{u} c_k - D_k \nabla c_k - z_k m_k F c_k \nabla V , \quad k=1, \ldots, K. \quad (38)
\]

In the above, \( c_k \) is the molar concentration; \( D_k \) is the diffusion coefficient; \( z_k \) is
the valence; and \( m_k \) is the mobility of the \( k^{th} \) ionic species. The fluid velocity \( \mathbf{u} \) is
determined from the model for the fluid motion described in section 3.2.1; \( F \) is the
Faraday’s constant \((F=96484.6 \text{ C/mol})\); and \( V \) is the electric potential in the electrolyte
solution. According to the Nernst-Einstein relation, the mobility of the \( k^{th} \) ionic species is
\[
m_k = \frac{D_k}{RT} , \quad k=1, \ldots, K. \quad (39)
\]

with \( R \) the universal gas constant and \( T \) the absolute temperature of the electrolyte
solution.

Under steady state, the concentration of each ionic species is governed by the
following Nernst-Planck equation:
\[ \nabla \cdot \mathbf{N}_k = \frac{\partial N_{kx}}{\partial x} + \frac{\partial N_{ky}}{\partial y} + \frac{\partial N_{kz}}{\partial z} = 0, \quad k=1, \ldots, K. \quad (40) \]

In the above, \( N_{kx}, N_{ky}, \) and \( N_{kz} \) are, respectively, the \( x-, y-, \) and \( z\)-components of the flux density of the \( k^{th} \) species. The set of the equations (11) consist of \((K+1)\) unknown variables: the concentrations of \( K \) ionic species and the electric potential in the electrolyte solution, \( V \). The local electroneutrality condition provides the \((K+1)\) equation:

\[ \sum_{i=1}^{K} z_i c_i = 0. \quad (41) \]

In the equation (12), we neglect the electrical double layers formed in the vicinity of the electrodes since the width of the microconduit is much larger than the thickness of the electrical double layer.

The current density \( \mathbf{J} \) in the electrolyte solution due to convection, diffusion, and migration is given by

\[ \mathbf{J} = F \sum_{k=1}^{K} z_k \mathbf{N}_k. \quad (42) \]

The Nernst-Planck equations (11) and the local electroneutrality condition (12) constitute a well-understood and widely accepted approximation for electrochemical transport phenomenon. In order to numerically solve them, appropriate boundary conditions for the concentration of each ionic species and the electric potential in the electrolyte solution are required.

Since the walls of the microchannel are impervious to inert species (no electrochemical reactions occur for that species), the net ionic fluxes of the inert species such as the ions \( K^+ \) normal to the walls of the microchannel are zero:

\[ \mathbf{n} \cdot \mathbf{N}_k = 0, \quad \text{for the inert species } k \text{ on all solid walls} \quad (43) \]

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In the above, \( \mathbf{n} \) is the unit vector normal to the corresponding surface.

Similarly, the net flux densities of the electroactive species such as \([\text{Fe(CN)}_6]^{3-}\) and \([\text{Fe(CN)}_6]^{4+}\) normal to the dielectric walls where no electrochemical reactions occur are also zero:

\[
\mathbf{n} \cdot \mathbf{N}_k = 0, \quad \text{for the electroactive species } k \text{ on dielectric walls} \quad (44)
\]

On the surface of the electrodes deposited along the opposing walls \((L_i \leq x \leq L_i + L_e, 0 \leq z \leq H, y = 0 \text{ and } W)\), oxidation and reduction reactions occur, respectively, at the surfaces of the anode and cathode:

\[
\text{Ox} + ne^- \leftrightarrow \text{Red} \quad (45)
\]

When the RedOx solution is a mixture of \(K_4[\text{Fe(CN)}_6]\) and \(K_3[\text{Fe(CN)}_6]\), the species Ox and Red in the above electrochemical reaction correspond, respectively, to the ions \([\text{Fe(CN)}_6]^{3-}\) and \([\text{Fe(CN)}_6]^{4+}\), and the number of electrons exchanged in the electrochemical reaction (16) is \(n=1\). Usually, the Butler-Volmer equation is used to describe the kinetics of the electrochemical reaction (Qian et al., 2005 and Arumugam et al., 2006)

\[
\mathbf{n} \cdot \mathbf{N}_{\text{Red}} = -\mathbf{n} \cdot \mathbf{N}_{\text{Ox}} = k_0 \left( c_{\text{Ox}} e^{-\frac{\alpha n F}{RT} \eta} - c_{\text{Red}} e^{-\frac{(1-\alpha)nF}{RT} \eta} \right), \quad (46)
\]

where \(c_{\text{Ox}}\) and \(c_{\text{Red}}\) are, respectively, the concentrations of the electroactive species Ox and Red that are involved in the electrochemical reaction (16) at the edge of the electric double layer; \(\alpha\) is the charge transfer coefficient for the cathodic reaction, usually ranging
from 0.0 to 1.0; $n$ represents the number of electrons exchanged in the reaction; $k_0$ is the reaction rate constant; and

$$\eta = \begin{cases} (U_{an} - V), & \text{along the surface of anode} \\ (U_{ca} - V), & \text{along the surface of cathode} \end{cases},$$

where $U_{an}$ and $U_{ca}$ are, respectively, the externally imposed potential on the anode and cathode, and $\Delta V = U_{an} - U_{ca}$ represents the potential difference applied across the opposing electrodes. Notice that the first and second terms in the RHS of the expression (17) represent, respectively, the forward and backward reaction rates which depend on the concentrations of the reactive species at the electrode's surface (i.e., $c_{ox}$ and $c_{red}$) and on $\eta$, the electric potential drop across the electric double layer formed next to the electrode.

At the inlet cross-section ($x=0$) of the microchannel, we assume that the concentration of each species is determined from the bulk concentration of the electrolyte solution in the left reservoir:

$$c_i(0,y,z) = c_{k0}, \quad k=1,\ldots,K,$$

and obeys the electroneutrality condition $\sum_{k=1}^K z_k c_{k0} = 0$.

At the exit cross-section of the microchannel ($x=L$), the transport of all species is dominated by the convective flux due to sufficiently large Péclet numbers in the MHD flows (Qian et al., 2006):

$$n \cdot N_k = n \cdot (c_i u), \quad k=1,\ldots,K.$$
Similarly, appropriate boundary conditions for the electric potential are also required prior to solving the coupled PDEs (11) and the algebraic equation (12). At the inlet and exit cross-sections of the microchannel, we assume that the $x$-component electric field is zero:

$$
n \cdot \nabla V(0,y,z) = n \cdot \nabla V(L,y,z) = 0.
$$  (50)

Along the dielectric walls of the channel, the electric fields normal to the walls are zero:

$$
n \cdot \nabla V(x,y,z) = 0, \text{ along the dielectric walls.}
$$  (51)

Along the surfaces of the electrodes, note that the potentials of the electrolyte immediately adjacent to the electric double layers are different from the potentials applied on the anode and cathode, and there is a potential drop across the electric double layer. Using the expressions (13), (17), and (18), the potentials of the electrolyte at the edge of the electric double layers adjacent to the anode and cathode can be implicitly calculated from

$$
n \cdot J = n F k_0 \left( c_{\text{on}} e^{\frac{a n F}{R T} \eta} - c_{\text{red}} e^{\frac{(1-a)n F}{R T} \eta} \right),
$$  (52)

Observe that the models for the fluid motion and the ionic mass transport are strongly coupled. The flow field affects the mass transport due to the contribution of the convective flux in the expression (9). On the other hand, the ionic mass transport affects the current density $J$, which, in turn, affects the flow field through the Lorentz force $J \times B$. Therefore, one has to simultaneously solve the full 3D mathematical model which consists of the continuity and Navier-Stokes equations (1)-(2), the set of the Nernst-
Planck equations (11), and the local electroneutrality condition (12) for the flow field, the ionic species' concentrations, and the potential of the electrolyte solution.

3.3. Solver Validation

To numerically solve the strongly coupled three-dimensional system, we used the commercial finite element package COMSOL (version 3.3, www.femlab.com) operating with a 64-bit dual-processor workstation of 32GB RAM (www.polywell.com). The 3D computational domain was discretized into quadratic triangular elements. We employed non-uniform elements with a larger number of elements next to the inlet and outlet cross-sections, as well as along the surfaces of the electrodes where the electrochemical reactions occur. We compared the solutions obtained for different mesh sizes to ensure that the numerical solutions are convergent, independent of the size of the finite elements, and satisfy the various conservation laws. To verify the code, we compared the numerical predictions with solutions available in the literature for special cases such as an electrochemical reactor with known flow field and the two-dimensional RedOx-based MHD flow in the presence of abundant supporting electrolyte under limiting current conditions.

We simulated the 2D parallel-plate electrochemical reactor (PPER) described in Georgiadou (2003). The PPER geometry is similar to the configuration depicted in Fig. 3.1 when \( H >> W \). The computational domain consists of an upstream region, a downstream region, and the region between two parallel electrodes positioned along the opposing walls (Fig. 3.1). In contrast to the MHD problem, in the PPER reactor, a parabolic flow field is specified. In other words, one only needs to solve the Nernst-Planck equations (11) using the prescribed velocity profile and the equation (12) in 2D.
Our finite element results are in excellent agreement with the finite difference results of Georgiadou (2003) (the results are not shown here).

We also simulated 2D RedOx-based MHD flow in the presence of abundant supporting electrolyte such as KCl. The RedOx species is a couple of FeCl_3/FeCl_2. Fig.3.2 depicts the concentration distributions of the active ions Fe^{3+} (dashed line and Δ) and Fe^{2+} (solid line and o) as functions of y at the cross section x=L/2. The lines correspond to the analytical solution derived with boundary layer theory (Qian and Bau, 2005), and the symbols correspond to the numerical results. Fig.3.3 depicts the dimensionless current density in the x-direction along the surface of the anode (the current density is normalized by $FD_0 C_o / W$ and $D_0 = \frac{D_{Fe^{3+}} + D_{Fe^{2+}}}{2}$). The solid line and circles correspond, respectively, the analytical solution and the numerical solution. Our numerical solutions favorably agrees with the analytical solutions.

The good agreement of our computational results with the results obtained with different computational techniques as well as other comparisons with specialized solutions for the RedOx-based MHD flow give us confidence in our computational results.
Fig. 3.2: The concentration distributions of the active ions Fe$^{3+}$ (dashed line and △) and Fe$^{2+}$ (solid line and ○) as functions of $y$ at cross-section $x=L/2$ in the presence of abundant supporting electrolyte and under limiting current. The lines and symbols correspond, respectively, to the analytic boundary layer approximations and the numerical simulation.
Fig. 3.3: The dimensionless limiting current flux as a function of $x$ along the anode in the presence of abundant supporting electrolyte solution and under limiting current conditions. The line and circles represent, respectively, the limiting current flux obtained with the analytic boundary layer approximation and the numerical simulation.

### 3.4. Results and Discussion

We first simulated the RedOx-based MHD flow in a 3D planar microchannel of 18 mm in length, 330 μm in width, and 670 μm in depth. The electrodes cover the entire side walls of the microchannel (i.e., $L_j=0$, and $L_k=L$). The RedOx electrolyte solution is a mixture of $K_4[Fe(CN)_6]$ and $K_3[Fe(CN)_6]$ in the absence of a supporting electrolyte. The simulation conditions are the same as those used in the experiments conducted by Aguilar et al. (2006). The electrolyte solution contains three ionic species $K^+$, $Fe(CN)_6^{3-}$, and
Fe(CN)\_6^{4^-} with charges $z_1=1$, $z_2=-3$, and $z_3=-4$, respectively. The diffusion coefficients at room temperature of the species K\(^+\), Fe(CN)\(_6\)^{3^-}, and Fe(CN)\(_6\)^{4^-} are, respectively, $1.957 \times 10^9$ m\(^2\)/s, $0.896 \times 10^9$ m\(^2\)/s, and $0.735 \times 10^9$ m\(^2\)/s. For the electrochemical reaction, Fe(CN)\(_6\)^{3^-} + e\(^-\) $\leftrightarrow$ Fe(CN)\(_6\)^{4^-}, the reaction rate constant and the charge transfer coefficient are, respectively, $k_0=1.0 \times 10^{-3}$ M/s and $\alpha=0.5$. Since the ferricyanide and ferrocyanide system has a very high reaction rate constant, the obtained results are not sensitive to the values of $k_0$ and $\alpha$. Since the RedOx electrolyte solution is very dilute, the density and dynamic viscosity of the RedOx electrolyte solution are assumed to be the same as those of water ($\rho \approx 1000$ kg/m\(^3\) and $\mu \approx 10^{-3}$ Pa\(\cdot\)s). In all our computations, the temperature $T=298$ K, and the bulk concentrations of both $K_4[Fe(CN)_6]$ and $K_3[Fe(CN)_6]$ in the left reservoir are taken to be equal. We also assume that there is no externally applied pressure difference between the conduit’s inlet and exit (i.e., $P_1=P_2$).
Fig. 3.4: The resulting current as a function of the applied potential difference in the presence ($B=0.44$ T) and absence ($B=0$) of a magnetic field. The symbols represent the experimental data obtained from the literature. The dash-dotted and solid lines represent, respectively, the resulting currents obtained from the full 3D model when $B=0.44$ T and $B=0$. The dotted and dashed lines represent, respectively, the currents obtained from the 2D model when $B=0.44$ T and $B=0$. The concentration of the RedOx species $K_4[Fe(CN)_6]/K_3[Fe(CN)_6]$ $C_0=0.25$ M, $L=18$ mm, $W=330 \mu$m, and $H=670 \mu$m.

The steady flow field and ionic concentration field under various potential differences ($\Delta V$), bulk concentrations of the RedOx couple in the left reservoir ($C_0$), and magnetic flux densities ($B$) are obtained by simultaneously solving the coupled full 3D mathematical model described in section 3.2. Here I present the results of my numerical computations and compare them with the experimental data obtained by Aguilar et al.

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Figure 3.4 depicts the steady-state current transmitted through the electrolyte solution as a function of the externally applied potential difference, $\Delta V$, across the electrodes in the absence ($B=0$) and presence ($B=0.44$ T) of a magnetic field when the inlet bulk concentrations of $K_4[Fe(CN)_6]$ and $K_3[Fe(CN)_6]$ are $C_0=0.25$ M. In other words, the effects of the magnetic field on the resulting current are studied for two different magnetic flux densities, one at $B=0$ and the other at $B=0.44$ T under different potential differences. The circles (●) and triangles (▲) represent, respectively, the experimental data obtained from Aguilar et al. (2006) for $B=0$ and $B=0.44$ T. The dash-dotted and solid lines in Fig.3.4 represent, respectively, the currents obtained from the 3D model at $B=0$ and $B=0.44$ T. The dashed and dotted lines represent, respectively, the predicted currents from the 2D model at $B=0$ and $B=0.44$ T with the assumption of $H \gg W$. The current nonlinearly increases with the applied potential difference, and the theoretical predictions of the 3D model qualitatively agree with the experimental data.

The discrepancies between the theoretical predictions and the experimental data may be due to the differences between the actual and assumed diffusion coefficients of the electroactive species. In the presence of a magnetic field, the interaction between the current density and the magnetic field induces a Lorenz force which pumps the fluid from the reservoir located at the left end ($x=0$) to the reservoir positioned at the right end ($x=L$) of the channel. The induced fluid motion reduces the thicknesses of the concentration boundary layers formed next to the surfaces of the electrodes which, in turn, leads to an increase in the concentration gradient and current density along the surfaces of the electrodes. Consequently, the total current in the presence of a magnetic field is higher than that in the absence of a magnetic field in which there is no fluid.
motion. However, the effects of the magnetic field on the resulting current are not very significant under the above conditions. As expected, the currents obtained from the 2D model are higher than those obtained from the 3D model since the effects of the boundaries \( z=0 \) and \( z=H \) on the fluid motion and the ionic mass transport are neglected in the 2D case. The 2D approximation is valid only when the aspect ratio \( H/W \gg 1 \), and is not appropriate for the experimental microchannel with the aspect ratio \( H/W \approx 2 \). Comparing to the resulting currents obtained from the 2D model, the currents obtained from the 3D model are closer to the experimental data.

Similar to the MHD flow in the absence of the RedOx species (Chapter 2), the RedOx-based MHD flow can be approximated with a fully developed duct flow with a rectangular cross-section. The velocity profile can be approximated with the closed form expression (24), and the average velocity can be estimated with the expression (27) in Chapter 2. Using the predefined velocity profile (24) in Chapter 2, one can easily simplify the coupled full mathematical model without solving the continuity and Navier-Stokes equations. In the 3D approximation model, one only needs to solve the mass transport equations (11)-(12) to determine the concentration field and the current density. Subsequently, the total current, \( I \), can be obtained by integrating the current density along the surface of the anode. The average velocity and velocity profile can then be obtained from the expressions (24) and (27) in Chapter 2, respectively.
Fig. 3.5: The average velocity as a function of the applied potential difference for concentrations of the RedOx species $K_4[Fe(CN)_6]/K_3[Fe(CN)_6]$ $C_0=0.1$ M and 0.25 M when $B=0.44$ T. The solid, dash-dotted, and dashed lines represent, respectively, the results obtained from the full 3D model, the full 2D model, and the 3D approximation model using the predefined velocity profile. The triangles and circles represent the experimental data obtained from the literature for $C_0=0.1$ M and 0.25 M, respectively. All other conditions are the same as Fig. 3.4.

Next, we compare the average velocities obtained from the 2D model, the full 3D model, and the 3D approximation model with the experimental data obtained from the literature. Figure 3.5 depicts the average velocity, $\bar{U}$, as a function of the applied potential difference for various bulk concentrations of the RedOx electrolyte when

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$B=0.44 \, T$. The triangles (▲) and circles (●) represent the experimental data obtained from Aguilar et al. (2006) for the RedOx concentrations $C_q=0.1 \, M$ and $C_o=0.25 \, M$, respectively. The solid, dashed, and dash-dotted lines in Fig.3.5 represent, respectively, the predictions obtained from the full 3D mathematical model, the 3D approximation model using the velocity profile (24) and the expression (27) in Chapter 2, and the full 2D mathematical model. The predictions obtained from the full 3D mathematical model (solid lines) and from the 3D approximation model (dashed lines) are in good agreement. The average velocity nonlinearly increases with the potential difference. This behavior is attributed to the nonlinear relationship between the current and the applied potential difference as depicted in Fig.3.4 since the average velocity is proportional to the current as shown in the closed form approximation (27) in Chapter 2. The predictions obtained from the full 3D mathematical model and from the 3D approximation model are over predicting the experimental data, especially for the case with a higher bulk concentration ($C_o=0.25 \, M$). The experiments were conducted by tracing a dye placed on one end of the channel (i.e., $x=0$) which then was observed on the other end of the channel (i.e., $x=L$) after a certain time interval $\Delta t$. The average velocity is estimated as the ratio $L/\Delta t$. We would suspect that the measured velocities would appear to be slower than they really are because the dye can be seen on the exit reservoir only when its concentration is sufficiently high enough. The average velocities obtained from the 2D model (dash-dotted lines) are higher than those obtained from the 3D models due to the neglect of the boundary effects arising from the bottom ($z=0$) and top ($z=H$) walls in the 2D case. As compared to the deviations between the experimental data and the average velocities.
obtained from the 3D model, larger deviations between the experimental data and the average velocities predicted from the 2D model are obtained.

Fig. 3.6: The maximum velocity as a function of the current for the RedOx Nitrobenzene with concentrations $C_0=0.1$ M (dashed line and circles) and $C_0=0.25$ M (solid line and triangles) when $B=0.41$ T, $L=18$ mm, $W=270$ μm, and $H=640$ μm. The lines and symbols represent, respectively, the predictions of the closed form approximation and the experimental data obtained from the literature.

The closed form approximation is validated by comparing its predictions with the experimental data obtained from the literature. Figure 3.6 depicts the maximum velocity, $U_{\text{max}}$, as a function of the current for $C_0=0.1$ M (dashed line and circles) and 0.25 M (solid line and triangles) Nitrobenzene (NB) species in a planar conduit of 18 mm in length, 270 μm in width, and 640 μm in height when the magnetic flux density $B=0.41$ T. Using the measured currents from the experiments, we estimated the average velocity.
\( \bar{U} \), with the closed form approximation (27) in the absence of the externally applied pressure gradient. According to the expression (24), the maximum velocity is 

\[
U_{\text{max}} = \frac{(m+1)(n+1)}{mm} \bar{U}.
\]

The lines and symbols in Fig.3.6 represent, respectively, the predictions of the closed form approximation (27) and the experimental data obtained from Arumugam et al. (2004). The predictions qualitatively agree with the experimental observations. The deviation between the solid and dashed lines is basically due to the difference in the dynamic viscosities of 0.1 M and 0.25 M NB RedOx electrolyte solution. The dynamic viscosities for \( C_0=0.1 \) M and 0.25 M NB electrolyte solution are, respectively, 0.00038 Pa\( \cdot \)s and 0.00043 Pa\( \cdot \)s, which explains the slope for \( C_0=0.25 \) M NB solution is smaller than that of \( C_0=0.1 \) M NB electrolyte solution.

To validate further the 3D approximation model using the velocity profile (24), Figure 3.7 depicts the resulting current as a function of the applied potential difference across the two opposing electrodes for the RedOx species K\(_4\)[Fe(CN)]\(_6\) and K\(_3\)[Fe(CN)]\(_6\) with concentrations \( C_0=0.05 \) M, 0.1 M, and 0.25 M. The lines and symbols represent, respectively, the solutions of the full 3D mathematical model and the 3D approximation model using the predefined velocity profile (24) without solving the continuity and Navier-Stokes equations. The other conditions are the same as those in Fig.3.4. The results from both models are in good agreement which makes us more confident in applying the 3D approximation model. The resulting current increases as the bulk concentration of the RedOx species increases.
Fig. 3.7: The resulting current as a function of the externally applied potential difference for various concentrations of the RedOx species $K_{2}[\text{Fe(CN)}_6]/K_{3}[\text{Fe(CN)}_6]$. The Lines and symbols represent, respectively, the predictions obtained from the full 3D model and from the 3D approximation model using the predefined velocity profile. All other conditions are the same as Fig. 3.4.

Next, we check the relationship between the resulting average velocity, $\bar{U}$, and the resulting current for various concentrations of the RedOx species under different potential differences. Figure 3.8 depicts the resulting average velocity, $\bar{U}$, as a function of the resulting current for various concentrations of the RedOx species. The resulting currents (x-axis) in Fig. 3.8 are the currents obtained from the full 3D model under various voltages and RedOx concentrations as shown in Fig. 3.7. The symbols (♦), (▲), and (●) in
Fig.3.8 represent the resulting average velocities and currents obtained from the full 3D mathematical model for the RedOx species $K_4[Fe(CN)_6]$ and $K_3[Fe(CN)_6]$ with the concentrations $C_0=0.05\text{ M}$, 0.1 M, and 0.25 M when the applied voltages vary from 0 to 0.4 V. All other conditions are the same as those in Fig. 3.7. The solid line in Fig.3.8 represents the prediction obtained from the closed form approximation (27) in Chapter 2. It is clearly shown that resulting average velocity, $\bar{U}$, is linearly proportional to the resulting current, $I$, for various concentrations of the RedOx species and different applied voltages. The predictions obtained from the full 3D mathematical model (symbols in Fig.3.8) favorably agree with those obtained from the closed form approximation (solid line).

![Figure 3.8: The average velocity as a function of the resulting current for the RedOx species $K_4[Fe(CN)_6]/K_3[Fe(CN)_6]$ with concentrations $C_0=0.05\text{ M (♦), 0.1 M (▲), and 0.25 M (●)}$. The symbols and solid line represent, respectively, the predictions obtained from the](image-url)
full 3D model and from the closed form approximation. All other conditions are the same as Fig.3.7.

A full 3D mathematical model consisting of the coupled Nernst-Planck equations for the concentration fields of the ionic species in solution, the generalized Butler-Volmer equation for the electron transfer, and the Navier-Stokes equations is introduced for the flow field to investigate the performance of RedOx-based MHD microfluidic devices under various operating conditions. The model presented here will be useful for the design and optimization of RedOx-based MHD microfluidic devices. Moreover, the model allows one to test rapidly and inexpensively the effects of various parameters and operating conditions on the device's performances. The major conclusions are:

(i) The resulting current transmitted through the electrolyte solution nonlinearly increases with the externally applied potential difference. The theoretical predictions obtained from the 3D mathematical model agree with the experimental data obtained from the literature. However, the 2D model overpredicts the current and the average velocity (flow rate) since the effects of the top and bottom dielectric walls on the flow and mass transport have not been taken into account.

In planar microconduits, a 3D approximation model was introduced where the velocity profile is approximated by that of a fully developed duct flow with a rectangular cross-section. Upon doing so, one only needs to solve the Nernst-Planck and the local electroneutrality equations without solving the continuity and Navier-Stokes equations. The results obtained from the full 3D model and from the 3D approximation model are in excellent agreement.

The average velocities obtained from the full 3D model, the 3D approximation model, and the closed form approximation are in good agreement and qualitatively agree
with the experimental observations obtained from the literature. The closed form approximation described in Chapter 2 can be used to optimize the dimensions of the channel and to solve the control (inverse) problems in MHD networks so as to achieve the desired flow patterns and flow rates.

The average velocity (flow rate) linearly increases with the increase in the current for different concentrations of the RedOx species, various magnetic flux densities, and dimensions of the channel.
CHAPTER 4

CONCLUSIONS

Microfluidics is a key component toward developing the lab-on-a-chip technology, which has the promise to revolutionize chemical analysis and medical diagnostics. In microfluidic devices, it is necessary to propel fluids from one part of the device to another, control fluid motion, stir reagents, monitor biological interactions, and detect the presence of biological and chemical agents. This thesis theoretically studied fluid manipulation under the action of electric and magnetic fields in microfluidic systems. More specifically, we focused on the propulsion of fluids in micro-conduits using the Lorenz forces resulting from the interactions between electric and magnetic fields. The main results of this work are summarized below.

1) The MHD micropump in the absence of RedOx species has been modeled with the Navier-Stokes equations for the flow field and the Laplace equation for the electric potential. In the analysis, the electrolyte solution was treated as a conductor with a uniform electric conductivity. The theoretical predictions agree with the experimental data obtained from the literature.

a) A closed form approximation for the average velocity (flow rate) has been derived in terms of the current, applied pressure difference, the strength of the magnetic flux density, viscosity of the fluid, and the dimensions of the channel. The predictions of the closed form approximation agree with the experimental data.
b) obtained from the literature. The closed form approximation can be used to optimize the dimensions of the channel and to solve the control (inverse) problems in MHD networks so as to achieve the desired flow patterns and flow rates.

c) The flow rate linearly increases with the applied current.

d) The flow rate nearly linearly increases with the applied voltage.

e) The flow rate nearly linearly increases with the strength of the magnetic field.

2) The MHD micropump in the presence of RedOx species has been modeled with the Navier-Stokes equations for the flow field, the Nernst-Planck equations for the ionic mass transport, the local electroneutrality condition for the electric potential in the electrolyte, and the Butler-Volmer equation for the electrochemical reaction.

(ii) The resulting current transmitted through the electrolyte solution nonlinearly increases with the externally applied potential difference. The theoretical predictions obtained from the 3D mathematical model agree with the experimental data obtained from the literature. However, the 2D model overpredicts the current and the average velocity (flow rate) since the effects of the top and bottom dielectric walls on the flow and mass transport have not been taken into account.

(iii) In planar microconduits, a 3D approximation model has been introduced where the velocity profile is approximated by that of a fully developed duct flow with a rectangular cross-section. Upon doing so, one only needs to solve the Nernst-Planck and the local electroneutrality equations without solving the continuity and Navier-Stokes equations. The results obtained from the full 3D model and
from the 3D approximation model are in excellent agreement.

(iv) The average velocities (or flow rates) obtained from the full 3D model, the 3D approximation model, and the closed form approximation are in good agreement and qualitatively agree with the experimental observations obtained from the literature.

(v) The average velocity (flow rate) linearly increases with the increase in the current for different concentrations of the RedOx species, various magnetic flux densities, and dimensions of the channel.
BIBLIOGRAPHY


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