Design of an Electro-osmotic Microfluidic Mixer

Stefan Keilich^{1*}, Tom A. Eppes^{2*}, and Ivana Milanovic^{3*}

1. Dept. of Mechanical Engineering

2. Dept. of Electrical & Computer Engineering

3. Dept. of Mechanical Engineering

* University of Hartford, 200 Bloomfield Ave., West Hartford, CT USA 06117

Abstract: This paper describes the results of a microfluidic mixer design initiative that uses the electro-osmotic effect in which an applied voltage is used to accelerate diffusion and advection of two liquid species. In this effort, a 2D model was developed using the COMSOL® microfluidics module and involved both stationary and time-dependent study steps. Two distinct geometries were analyzed, and a design of experiment (DoE) was performed to evaluate a range of parametric settings. The species concentrations were investigated as well as the mixing efficiency to quantify how well the two fluids were combined at the outlet.

Keywords: microfluidic mixer, electro-osmotic mixer, active mixing.

Introduction

Over the past two decades, 'lab on a chip' devices have attracted much attention. They are currently used in the food, chemical, and biomedical fields to analyze a range of fluid properties and constituents. Their small scale required only small fluid samples and only seconds to obtain accurate readings of such important parameters as glucose level, pathogen presence, and DNA sequencing.

One particular subset involves the electroosmotic effect to increase the rate of mixing between two or more liquid species. This paper presents the results of a design effort that focused on this type of mixer design. The Comsol® microfluidics module was used to create both stationary and time-dependent study steps. The electro-osmotic effect was employed to accelerate the mixing process of two fluids entering the device. Two distinct geometries were investigated as well as two secondary parameters within each physical configuration.

A design of experiment (DoE) approach was used to narrow the solution space to two specific designs. The mixing efficiency (ME) at the outlet as defined by the relative improvement in concentration consistency between the inlet and outlet was the principal measure of performance.

Background

Two comprehensive literature reviews of microfluidic mixer research were published by Lee et al. in 20011 and 2016^{1,2}. These papers covered both active and passive devices. In 2017, Cai et al. provided a survey that focused on recently reported findings³. His paper referenced 149 articles and contains a thorough overview of a wide range of designs and methodologies.

Microscale mixing devices fall into two broad classes: passive and active. Each class has advantages and disadvantages that determine its suitability in any particular application^{4,5,6}. For example, passive devices do not require an external energy source; however, their physical structure tends to be more complicated, and they require more time to produce a result. In general, complex geometries are sued as a means to promote diffusion and chaotic advection. Techniques reported include obstacles, convergent-divergent channels, spirals and unbalanced collisions. Nevertheless, passive deices are fundamentally limited in their equilibration times and consistency.

Active devices utilize moving parts or some form of applied energy to increase the mixing rate. Techniques that have been reported include pressure, thermal, acoustic, and AC/DC electric/magnetic fields. As may be expected, active devices have shorter mixing times and in many cases deliver a more consistent outlet concentration. To quantify how uniformly two fluids are combined, one popular measure in the literature is ME defined as the ratio of the rootmean-square of concentration from the average at both the inlet and outlet ports as expressed in the equation below. $ME = (1 - \{\Gamma_{o}[(c_{o}-c_{avg})^{2}]/\Gamma_{i}[(c_{i}-c_{avg})^{2}]\}^{1/2})*100 (1)$

where $c_o = Concentration across outlet$ $c_i = Concentration across inlet(s)$ $c_{avg} = Mean concentration$ $\Gamma = integral across inlet or outlet$

Ideal mixing and no mixing are then defined by ME = 100% and 0%, respectively. The closer ME comes to 100%, the better the mixing within the device.

Theory

The model reported in this paper uses three physics interfaces that are built into the microfluidics module which are solved in the fluid domain: laminar flow, electric currents, and transport of diluted species. The incompressible electro-osmotic flow in the fluid domain has a low Reynold's number (Re < 1) and is described by a coupled system of the Navier–Stokes equations, the conduction equations for the electrical potential in the channel, and the convection–diffusion equation for the concentration of the species in the fluid:

 $\nabla \cdot [pI - \eta (\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathrm{T}})] + \rho \mathbf{u} \cdot \nabla \mathbf{u} = 0$ (2)

$$\nabla \cdot \mathbf{u} = 0 \tag{3}$$

 $\nabla \cdot (\mathbf{\sigma} \mathbf{E}) = 0 \tag{4}$

$$\mathbf{E} = -\nabla \boldsymbol{\varphi} \tag{5}$$

$$\mathbf{u} \cdot \nabla \mathbf{c} = \nabla \cdot (\mathbf{D} \nabla \mathbf{c}) \tag{6}$$

where
$$u$$
 = velocity field (m/s)
 p = pressure field (Pa)
 ρ = density (kg/m³)
 η = dynamic viscosity (Pa-s)
 I = identity tensor
 D = diffusion coefficient (m^2/s)
 c = species concentration (mol/m^3)
 σ = electrical conductivity (S/m)
 ϕ = electric potential (V)
 E = electric field (N/C)

The constraints for the flow equations are:

- Laminar at inlets with a fixed mean velocity
- Zero pressure at outlet with no backflow

The thicknesses of the electric layers adjacent to the charged channel walls are very thin in comparison to the widths of the channels so the Helmholtz-Smoluchowski boundary condition for Newtonian electro-osmotic slip flow is applied on the walls.

The local electric field **E** is calculated from the electric potential φ by $\mathbf{E} = -\nabla \varphi$. The wall condition is then set to the following:

$$\mathbf{u} = \varepsilon \zeta \mathbf{E}_{\mathrm{t}} \tag{7}$$

where $\mathbf{E}_{t} = \text{electric field tangent to wall}$ $\varepsilon = \text{fluid electrical permittivity (F/m)}$ $\zeta = \text{zeta potential (V)}$

The tangential electric field at the walls is computed from the x- and y- components as

$$\mathbf{E}_{t} = \mathbf{E} - (\mathbf{E} \cdot \mathbf{n})\mathbf{n} \tag{8}$$

$$\mathbf{E} = \mathbf{E}_{\mathbf{x}} * \sin(\omega t) \mathbf{i} + \mathbf{E}_{\mathbf{y}} \sin(\omega t) \mathbf{j}$$
(9)

where $E_x = x$ -component of E $E_y = y$ -component of E $\omega = voltage$ frequency (rad/s) i,j = unit Cartesian vectors

For the conduction equations, all walls except on electrodes, inlet and outlet, are electrically insulating. A fixed amplitude voltage signal is applied to each pair of electrodes.

The constraints for the convection–diffusion equation are as follows. One inlet has a uniform concentration of 0 while the other is set to 1. The outlet is designated as an outflow, and all walls have a no flux condition.

Geometric Design

The results presented here stem from two distinct 2D geometric designs. Both incorporate some passive design features as well as electrodes to capitalize on the electro-osmotic effect to enhance mixing. Each design has two inlets on the left of the device and one outlet on the right each with a width of 25μ m. Two fluid species enter the mixer via a designated inlet. A sinusoidal AC voltage potential is applied to several pairs of electrodes, and each pair has a

positive terminal (0^0 phase angle) and a negative terminal (180^0 phase angle).

Fig. 1 shows the physical structure of Geometry 1. It contains an open middle area with three pairs of electrodes on the walls. Mixing is primarily depends on the electro-osmotic effect. Fig. 1 also shows a surface plot of the electric potential based obtained in a stationary study.



Figure 1. Geometry 1 and electrode placement

Fig. 2 shows the physical structure of Geometry 2. Mixing occurs by a combination of diffusion, advection, and the electro-osmotic effect. This design contains a middle section that features two convergent-divergent zones and center dividers for electrode placement. A final zone is open with a single pair of electrodes. A total of eight pairs of electrodes are located on various walls. Four pairs are placed on the center dividers, and the other four pairs are situated on the outside walls near the convergent portions of the middle zones. Fig. 2 also shows a surface plot of the voltage potential and polarities.



Figure 2. Geometry 2 and electrode placement

Model Parameters

Four global parameters are used in the model and are shown in Table 1 along with their initial values. A parametric study was performed on the voltage amplitude and frequency as part of the DoE. The fluid properties remained constant for all studies and assigned the values shown in Table 2.

Tuble 1. Global parameters		
Parameter	Value	
Mean inlet velocity of fluid	0.1[mm/s]	
Zeta potential	-0.1[V]	
Amplitude of voltage signal	0.1[V]	
Frequency of voltage signal	8[Hz]	
Diffusion coefficient of fluids	1e-11[m^2/s]	
Conductivity of fluids	0.11845[S/m]	

Table 1: Global parameters

Table 2: Fluid properties		
Material property	Value	
Density	1e+3[kg/m^3]	
Dynamic viscosity	1e-3[Pa*s]	
Electrical conductivity	0.11845[S/m]	
Relative permittivity	80.2	

The mesh for both designs consisted of primarily triangular elements and was physics-controlled with a setting of extra-fine. Geometry 1 had a total of 1,906 elements with an average quality of 0.89. For Geometry 2, the number of elements was 3,636 with an average quality of 0.85. Fig. 3 shows the mesh for Geometry 2 and illustrates the clustering of smaller element sizes near each electrode.



Figure 3. Mesh for Geometry 2

Results

Each study consisted of two steps with the first being a stationary analysis that included the simultaneous solution of all three physics. The second step was a time dependent analysis; however, the stationary results for the electric potential from the first step were used. The second step had a start time of 0s and was stopped at 4s when equilibration is expected.

A series of studies were performed as part of the DoE. The purpose was to gather a broad set of results at a few selected points for three key parameters: geometry type, voltage amplitude, and voltage frequency. Table 3 shows the value combinations used hence a total of eight studies were done. As expected, a wide range of results were obtained.

Table 3: DoE parameters & values

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Parameter	Values		
Geometry type	1	2	
Voltage Amplitude	0.15[V]	0.3[V]	
Voltage frequency	4[Hz]	8[Hz]	

Using the concentration at the outlet as the measure of performance, with 0.5 being ideal, revealed the best combination to be Geometry 1 with a frequency of 4Hz and an amplitude of 0.3V. For this study, Fig. 2 shows how the concentration varies across the outlet at five points in time. At t = 0s, the results represent the initial condition which is highly unmixed. By t = 1s, mixing is well underway and is mostly complete by the 2s mark. The time required to reach complete stability is around 4s.



Figure 4. Concentration across outlet, 0s to 4s

Fig. 5 illustrates for this best case study the streamline velocity field and concentration

within the device at t = 4s. Most of the mixing occurs in the first two chambers although the third chamber acts as a finishing agent. ME was also calculated for this study and is shown in Fig. 6. It reveals a high efficiency at t = 2s and reaches 99.8% at 4s. Animations were also useful in examining the mixing process and recirculation zones within each chamber. A sensitivity and optimization study around this best DoE point could provide further performance improvements.



Figure 5. Concentration and streamlines at t=4s



Figure 6. Mixing efficiency at outlet vs. time

Conclusions

This paper presents the results of an electroosmotic microfluidic mixer design and modeling effort. Two different geometries and combinations of voltage amplitude and frequency were investigated. A DoE was conducted to identify the best combination of parametric values. The specific results for this case were presented which shows high level of mixing efficiency (>90%) in a short period of time (t = 2s). Additional improvement may be possible by further refining the values for amplitude and frequency.

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