Numerical Simulation of Time-Dependent Electro-osmotic Micro-Mixer for Laboratory-On-a-Chip Applications

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Abstract

Design of Laboratory-On-a-Chip (LOC) devices and components such as micro-pump, micro-mixer, micro-separator, and micro-needle are main challenges in chemical and biological micro-engineering process. Due to low Reynolds number in micro-channel we need to perturb the fluid by time-dependent secondary lateral force. In this paper we design a novel miniaturized micro-channel with embedded electrodes in both micro-chamber and micro-channel. Efficient electro-osmotic flows are generated near the electrodes by exciting the electrodes properly. We studied the interaction between the fluids behavior, electric field and convection-diffusion equation in the proposed model. Velocity field and concentration analysis revealed a high performance mixing efficiency (above 96%) for a 130µm long mixer. The exciting parameters such as frequency and voltage effect are discussed to optimize the proposed micro-mixer.

Keywords: Laboratory-On-a-Chip, Low Reynolds number, Chaotic regime, Micro-mixer, electro-osmotic force.

Introduction

Micro process engineering is the science of various physics and applications. In last decades, advances in micro-process engineering have been applied in biological testing and chemical laboratory applications. Laboratory-On-a-Chip (LOC) devices integrate the micro-mixers, micro-pumps, micro-valves, micro-separators, micro-reactors and detectors in a chip and done the whole process with small fluid and sample volume, in short time and low cost. In most processes we need to mix two or multiple fluids (for example: blood solution with particles or biomarkers immersed in a buffer solution) and the mixing efficiency, mixing time and controlling the time is very important. Perform the mixing operation in a micro-channel resulting to low Reynolds number flow (equation-1):

$$ Re = \frac{\rho U d_b}{\mu}. $$

Where, Re is the dimension less Reynolds number, $\rho$ is the fluid density, $U$ is the average flow velocity, $d_b$ is the hydraulic diameter of the channel and $\mu$ is the dynamic viscosity of the liquid. Without external force, the main transport phenomenon in micro-channel is the molecular diffusion, so the mixing performance is poor. Broadly speaking, micro-mixers can be categorized to passive and active types. The passive micro-mixer perturbs the fluid streamlines by complicated channel geometry, such as serial lamination micro-mixer, enhance the mixing process by obstacles. Contrary to the passive mixers, the active mixers achieving a mixing process by using external force to improve the mixing effect, including ultrasonic perturbation, electro-kinetic instability mixer and so on. The chaotic regime is more efficient to generate significant increase in the fluids interfacial contact area and overcome the viscous resistance of the fluid flow. Recently the chaotic mechanism is used to mix low Reynolds number liquids, associated with stretching, folding and breaking process. AC electro-osmotic force shows the potential for application in LOC devices. If a tangential electric field is applied to an electrolyte solution, the charges in the electrical double layer between the electrolyte and the surface experience a significant force. As a result, these double layer charges move, pulling the fluid along the micro-channel, and generating a flow, called electro-osmotic effect. A ring electro-kinetic chaotic micromixer with integrated electrodes was designed by Chen, H. and et al.

This study investigates mixing process in a novel miniaturized micro-chamber and micro-channel. The paper is organized as follows: First, the methods and design of the micro-mixer will be described in Section 2. Second, the micro-mixer design, theory, and the initial/boundary conditions of the proposed micro-mixer will be described in Section 3. Third, a set of simulations will perform to investigate a chaotic regime and corresponding mixing performance in Section 4. The both geometrical and excitation parameters are going to be investigated in this section. Finally, conclusion and comparison with same works will be presented in Section 5.

Material and Methods

In this work, we use the both chamber and channel for high throughput mixing process. Actually, two fluid at nano-liter scale inter the micro-channel (from inlets A and B), we use a miniaturized micro-chamber for premixing process ($L_{\text{Chamber}}$) and the high performance mixing will be occurred in the micro-channel ($L_{\text{Mix}}$). Curvatures ‘r’ at the corners of the model...
enhances generation of electro-osmotic flow (the Coanda effect). The design and the value of geometrical parameters are visualized in figure-1 and the dimensions were assigned in accordance with table-1. Four electrodes are embedded in the chamber and some electrodes are embedded in the long micro-channel (the size and positions of the electrodes are shown in figure-1). We design an AC electro-osmotic micro-pump for Lab-On-a-Chip applications\textsuperscript{12}. So, it assumes the pumping process occurred by AC electro-osmotic pump and we perturb the initial pumped fluid by time-dependent electro-osmotic force.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>W\textsubscript{chamber}</td>
<td>Width of the chamber</td>
<td>40</td>
</tr>
<tr>
<td>W\textsubscript{channel}</td>
<td>Width of the channel</td>
<td>20</td>
</tr>
<tr>
<td>L\textsubscript{elec}</td>
<td>Length of the electrodes</td>
<td>8</td>
</tr>
<tr>
<td>L\textsubscript{interface}</td>
<td>Length between the electrodes in the channel</td>
<td>14</td>
</tr>
<tr>
<td>d</td>
<td>Length between the electrodes in the chamber</td>
<td>3</td>
</tr>
<tr>
<td>L\textsubscript{q}</td>
<td>Length of the channel before the chamber</td>
<td>15</td>
</tr>
<tr>
<td>L\textsubscript{o}</td>
<td>Length of the channel after the last electrode</td>
<td>31</td>
</tr>
<tr>
<td>r</td>
<td>Curvature radius of the chamber</td>
<td>5</td>
</tr>
</tbody>
</table>

**Electro-osmotic Theory and Initial/Boundary Conditions:**
As discussed earlier, the initial mixing performance relies on molecular diffusion and is poor, but we can improve it by electro-osmotic force. In order to solve the mixing process, we need to solve the Navier-Stokes equation (equation-2) and continuity equation (equation-3)\textsuperscript{13}.

\[
\rho \frac{\partial \bar{u}}{\partial t} + \bar{u} \nabla \bar{u} = -\nabla p + \mu \nabla^2 \bar{u} + \rho_e \bar{E}. \tag{2}
\]

\[
\nabla \bar{u} = 0. \tag{3}
\]

Where, \( \rho \) is the fluid density, \( \bar{u} \) is the bulk electroosmotic flow velocity, \( p \) is the pressure in the microchannel, \( \mu \) is the fluid viscosity, \( \rho_e \) is the net electric charge density, and \( \bar{E} \) is the local electric field strength. The interaction between electrical double layer (EDL) and excess ions represents the electrical driving force which can be expressed as\textsuperscript{14}:

\[
\bar{E} = -\nabla \varphi.
\tag{4}
\]

Where, \( \varphi \) is the applied electric potential. The charges in the EDL will experience an efficient force by applying a tangential electric field. As a result, the charges move, pulling the fluid along and generating a secondary flow called as electro-osmotic flow. The electroosmotic velocity (\( U_{\text{electro-osmotic}} \)) is approximated by Helmholtz-Smoluchowski equation (equation-5). This approximation is valid only for thin double layer (typically 10 nm)\textsuperscript{14}:

\[
U_{\text{electro-osmotic}} = \frac{2 \epsilon_0 \epsilon \bar{E}}{k_B T}.
\tag{5}
\]

**Figure-1**
Schematic view of geometrical parameters of the miniaturized micro-mixer (including micro-chamber, micro-channel, micro-electrodes, inlets and outlet)
\[ U_{\text{electro-osmotic}} = -\frac{\varepsilon_0 \varepsilon_r \zeta \bar{E}}{\mu}. \]  

(5)

Where \( \varepsilon_0 \) is the dielectric permittivity in a vacuum, \( \varepsilon_r \) is the relative dielectric permittivity of the solution, \( \zeta \) is the electro-osmotic zeta potential, \( \mu \) is the fluid dynamic viscosity and \( \bar{E} \) is the electric field. Another equation required for solving mixing process is Convection-Diffusion equation (equation-6), which solve the concentration field of the solutions. The effect of electroosmotic flow is considered as slip wall boundary condition for fluid motion equation.

\[ \frac{\partial C}{\partial t} + (\bar{u}_{\text{electro-osmotic}} + \bar{u}_{\text{electro-phoretic}}) \nabla C = D \nabla^2 C. \]  

(6)

Where \( C \) is the concentration of species (Species concentration of the fluids A and B are described by 1 and 0 mol.m\(^{-3}\), respectively), \( D \) is the diffusion coefficient of the fluid A and B, \( \bar{u}_{\text{electro-osmotic}} \) is the electroosmotic velocity of the solutions, and \( \bar{u}_{\text{electro-phoretic}} \) is the electrophoretic velocity of the solutions. \( \bar{u}_{\text{electro-phoretic}} \) is negligible in comparison with \( \bar{u}_{\text{electro-osmotic}} \). Material properties of the proposed micro-mixer were assigned in accordance with table-2. Initial and boundary conditions of the micro-mixer are visualized in figure-2. As shown in figure-2, the electrodes are located in the side walls and excited by time-dependent voltages (\( \phi_1(t) \), \( \phi_2(t) \) and \( \phi_3(t) \), \( \phi_4(t) \)). The phase difference between \( \phi_1(t) \) and \( \phi_2(t) \) is 180 degrees (there is similar relation between the \( \phi_3(t) \) and \( \phi_4(t) \)). As discussed earlier, the current simulation model considers the laminar flow due to the small characteristic length scale. It mixes two species in to the micro channel. It assumes the variation in the fluid concentration does not alter the viscosity and density properties of two fluids. The mean velocity of the initial fluid is \( U_0 \) (driven by AC electro osmotic). The pressures at the inlet and outlet of the micro-channel were specified as zero \( (P = 0) \) and also pressure gradient at the micro-channel walls set to be zero, considering no flux across the walls \( (n \nabla P = 0) \).

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>Density of fluid</td>
<td>1 \times 10^3 [kg.m(^{-3})]</td>
</tr>
<tr>
<td>( \mu )</td>
<td>Viscosity of fluid</td>
<td>1 \times 10^{-3} [N.s.m(^{-2})]</td>
</tr>
<tr>
<td>( \varepsilon_0 )</td>
<td>Vacuum permittivity</td>
<td>8.854 \times 10^{-12} [F.m(^{-1})]</td>
</tr>
<tr>
<td>( \varepsilon_r )</td>
<td>Dielectric constant</td>
<td>80.2</td>
</tr>
<tr>
<td>( \bar{u}_{\text{in}} )</td>
<td>Mean input velocity</td>
<td>0.1 mm.s(^{-1})</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>Zeta Potential for Si or Glass channels</td>
<td>-80 [mVolt]</td>
</tr>
<tr>
<td>( \phi_1 )</td>
<td>Amplitude of electric potential ( \phi_2(t) ) and ( \phi_3(t) )</td>
<td>150 [mVolt]</td>
</tr>
<tr>
<td>( \phi_4 )</td>
<td>Amplitude of electric potential ( \phi_5(t) ) and ( \phi_6(t) )</td>
<td>100 [mVolt]</td>
</tr>
<tr>
<td>( f )</td>
<td>Excitation frequency</td>
<td>4 [Hz]</td>
</tr>
<tr>
<td>( D )</td>
<td>Diffusion coefficient</td>
<td>1 \times 10^{-11} [m(^2).s(^{-1})]</td>
</tr>
</tbody>
</table>

**Table-2**

**Fluid material properties, excitation and related diffusion parameters of the mixing process**

**Figure-2**

Boundary conditions; fluids A and B are taken into the channel with different concentration and the micro-electrodes are placed in the side walls of the micro-chamber and micro-channel to mix them. The inlets, outlet and black boundary lines are electrical insulation. The side walls, except the surface of the electrodes (shown with the black lines) have slip velocity condition corresponding with \( U = -\varepsilon \bar{E}/\mu \).
As shown in figure-2, the electrodes in the side walls are excited by applying $\phi(t)$ and insulation conditions $\frac{\partial \phi}{\partial y} = 0$ were applied at other boundary conditions. We can solve the transverse electric potential by Laplace equation ($\nabla^2 \phi = 0$) and subject to the boundary conditions shown in Figure-2. The $\xi$ potential effect determines by slip boundary conditions, so, we apply $u_x = -\varepsilon \frac{\xi E_x}{\mu}$ and $u_y = -\varepsilon \frac{\xi E_y}{\mu}$ at the micro-channel walls, $\frac{\partial u_x}{\partial x} = 0$ and $\frac{\partial u_y}{\partial x} = 0$ at the inlet and outlet of the micro-channel. The electrodes are excited and all the three, incompressible Navier-Stokes equation, Convection-Diffusion of species equation and electric field are solved with finite element method.

Results and Discussion

A set of numerical simulations were performed to evaluate the proposed high throughput micro-mixer. Secondary flow streamlines are generated in different times by applying efficient electric potential to the electrodes. Velocity field streamlines and electric potential during a period of the sinusoidal wave are illustrated in figure-3.

Resulting, time-varying flow patterns will generate by interaction between the primary steady flow and oscillatory external electric field. When the electrodes are excited, different flow patterns are generated by interacting between the initially pumped fluid and secondary oscillating electric field. These secondary flow streamlines cause chaotic regime in the micro-channel and resulting high performance mixing process. We generate flow patterns in the micro-chamber stronger than that of in the micro-channel. So called, the electro-osmotic flows are time-dependent with the frequency of $f$. Resulting, we can see rotation effects near the electrodes. Actually, we stretch, fold and break the two fluids up (solute and solvent) sufficiently in the micro-chamber by applying sinusoidal wave ($\phi(t)$ and $\phi(t)$), which increase the interfacial area between the fluids. Pre-mixed fluid in the micro-chamber, will be thoroughly mixed by applying a set of sinusoidal waves ($\phi(t)$ and $\phi(t)$) in the micro-channel. Figure-4 illustrates the species concentration distribution caused by electro-osmotic flow.
Species concentration distribution, two fluids are taken into the channel with different concentration \( C = 1 \) and \( 0 \) [mol/m\(^3\)]. The generated ac electro-osmotic flows cause repeatedly stretching and folding actions, resulting a high performance mixing process (\( C \) is about \( 0.5 \) [mol/m\(^3\)] at the outlet).

As discussed earlier, when the electrodes are not excited, the mixing process is based on molecular diffusion (figure-4(a)). But, when the electrodes are excited, chaotic perturbation associated with stretching, folding and breaking the fluids up will occur repeatedly. Concentration profiles at the outlet of the mixer are shown for various times (\( t = 0, 0.25, 0.6875 \) and \( 1 \) second) as a function of channel width in Figure-5. As shown in the figure, without the electro-osmotic flow the concentration profile has smooth profile.

**Mixing Quality:** For a certain application, different mixers quality can be compared by mixing time, mixing efficiency, energy consumption, size of the mixer and some others. In order to estimate mixing process, obviously, the mixing efficiency \( Q \) at any cross-section of the channel can be quantified by the equation-13:

\[
Q = \left[ 1 - \frac{\int[C - C_\infty] dA}{\int[C_0 - C_\infty] dA} \right] \times 100 \%
\]  

(13)

Where, \( C \) is the species concentration across the width of the channel, \( C_\infty \) is the species concentration in the completely mixed state (\( C_\infty = 0.5 \)), and \( C_0 \) is species concentration in the perfectly unmixed condition (\( C_0 = 0 \) or \( 1 \)). Figure-6 visualize mixing quality for miniaturized micro-mixer. Mixing efficiency of the proposed mixer is over 96% in a one second. Therefore, it is very efficient for Lab-On-a-Chip applications.

**Optimization Parameters:** The most important parameters for enhance the mixer yield, are frequency and voltage of the applied sinusoidal wave. We can control the electro-osmotic flow intensity by frequency and voltage of the excitation. As shown in Figure-7 by increasing the frequency, electro-osmotic flow intensity decreases because it has not sufficient time to overcome the primary flow. Frequency range of \([3 \text{Hz}]\) to \([8 \text{Hz}]\) is effective for mixing process. Using high voltage amplitudes cause intensive electro-osmotic flow. But on the other hand, high voltage amplitude leads to high electric field and resulting, damage the fluid or samples. Broadly speaking, the frequency effect is more significant than amplitude.
**Figure-5**
Concentration C versus channel width W_{Channel} at the outlet of the mixer; the concentration profile is shown for different times, (as shown in figure legend). It should be noted that t = 0 sec is corresponds to lack of excitation.

**Figure-6**
Mixing quality; the micro-mixer efficiency over the channel width in different times as shown in the figure legend (a). Concentration plot (b)
Figure-7
Frequency and voltage amplitude effect on mixing efficiency; this profile are plotted for two different cases of voltages, as shown in legend

Conclusion

In this paper a novel miniaturized micro-mixer was designed and investigated numerically. We drive ac electro-osmotic flow by interaction between the initial pumped fluid and time-dependent electric field which applied to the electrodes embedded in the side walls of the channel. These flows generate intensive perturbation effects associated with stretching, folding and breaking the fluid up actions. Numerical results revealed high mixing process with efficiency of over 96% for a 130µm long channel. Since the high electric field will damage the medium fluid and cells, we use below the 0.15 Volt for voltage excitation amplitude. The frequency variation revealed the proposed mixer works efficiently at low frequencies. The mixer is compared with same type of the other mixers in accordance with table-3.

Acknowledgement

The authors would like to thank Ahar Branch, Islamic Azad University for the financial support of this research.

Table-3
Comparison Table

<table>
<thead>
<tr>
<th>Reference</th>
<th>Mixing Type</th>
<th>Channel width</th>
<th>Using chamber</th>
<th>Velocity [mm/s]</th>
<th>Frequency [Hz]</th>
<th>Mixing Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>Passive-parallel</td>
<td>85 [µm]</td>
<td>Without chamber</td>
<td>0.7</td>
<td>-</td>
<td>Not reported</td>
</tr>
<tr>
<td>24</td>
<td>Chaotic-patterned wall</td>
<td>200 [µm]</td>
<td>Without chamber</td>
<td>0.01-0.09</td>
<td>-</td>
<td>90 %</td>
</tr>
<tr>
<td>25</td>
<td>Dielectrophoretic</td>
<td>50 [µm]</td>
<td>Without chamber</td>
<td>0.5</td>
<td>1</td>
<td>Not reported</td>
</tr>
<tr>
<td>11</td>
<td>AC-Electroosmotic</td>
<td>10 [µm]</td>
<td>With Circular chamber</td>
<td>0.1</td>
<td>8</td>
<td>75 %</td>
</tr>
<tr>
<td>This paper</td>
<td>Electro-osmotic</td>
<td>20 [µm]</td>
<td>With chamber</td>
<td>0.1</td>
<td>4</td>
<td>96 %</td>
</tr>
</tbody>
</table>

References


