

Numerical Study of a Liquid Mixing Device for Electro-osmotic Flow (EOF) Driven Microfluidic Device Using CFD

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ABSTRACT

Microfluidic devices are so small like the micromixers and micropumps that control and mix the fluid inside the device. These devices cannot involve any moving components. Instead, they must take advantage of electro-osmotic flow. Microfluidics deals with controlling and manipulating of fluid flows having length scale on the order of microns and it is a multidisciplinary field which comprises chemistry, physics, mathematics, biotechnology and engineering. Present paper is concerned with the concept of electro osmosis principle, EOF principle. Also analyze the flow pattern for rectangular microchannel using CFD technique.

Keywords—Microfluidic; micropumps; electro-osmotic flow

ARTICLE INFO

Article History

Received: 28th February 2016

Received in revised form :

1st March 2016

Accepted: 3rd March 2016

Published online :

5th March 2016

I. INTRODUCTION

Microfluidics is a multidisciplinary field where researchers combine their efforts to successfully manufacture devices for desired applications. The design of microfluidic devices may require the integration of different physical phenomena and will go through stages such as device analysis, numerical simulations, prototyping, and validation studies before the final micro device is produced.[1]When a gas-liquid or liquid-liquid interface is present, fluid motion can be generated by controlling spatial variations of surface tension. These variations can be created with thermal, chemical, electrical, or light gradients. It is also possible to move liquid/gas or liquid/liquid in channels with partially wetting surfaces by using capillary pressure gradients. Following the Young-Laplace law, the latter can be generated by varying along the channel either wetting properties (contact angle, surface tension) by one of the above mentioned means, or geometrical features (channel diameter). For example, thermal gradients can give capillary pressure motion of droplets, whereas variation of channel width allows liquid motion within a channel without a power supply. [1] Alternatively, electrokinetics is now studied in a variety of forms for controlling microflows. Electro-osmosis, where the fluid moves relative to stationary charged boundaries; dielectrophoresis, which moves an interface (often a particle) in a gradient of electric field; and electrowetting, where the electric field modifies wetting properties, have all been exploited. AC and DC fields can be considered, and the

system response then depends on frequency and amplitude of the field. Both capillary-driven and electrically driven flows offer advantages relative to the more familiar pressure-driven flows as the device scale is reduced. Other means can be used to control flows. In particular, external fields can be used to induce motion of objects embedded in the fluid, or the channel walls can be systematically distorted; magnetic fields can influence flows directly or manipulate dispersed magnetic particles; sound fields can produce acoustic streaming motions, cyclic deformation of a wall etc. For each manner of driving a fluid motion, the surface characteristics of the device can also be exploited to provide additional control. For example, the geometrical, chemical, and mechanical features of the channel and network of channels can be patterned or altered. In addition, the rheology of the fluid can be significant, so both Newtonian and non-Newtonian fluids need consideration. It is then possible to combine the driving forces and the surface characteristics when considering how best to mix, react, detect, analyze, separate and so on in microflows. Microfluidics is the science of manipulating fluid flow through channels having dimensions of less than 1 mm. The flow of a fluid through a microfluidic channel can be characterized by the Reynolds number, and is represented by Eq.(1.1)

$$Re = \frac{LV\rho}{\mu} \text{-----(1.1)}$$

Where L is the length of the channel, V is the average velocity flow, ρ is the density of the fluid, and μ is the viscosity of the fluid. The Reynolds number, which determines the turbulence of flow, is extremely low at small scales, meaning that the fluid flow stays laminar.[2,6]

The study of microfluidics becomes significant because of handling of less amount of fluids, reduction in size, the reduced consumption of chemical reagents, low power consumption, user friendly, portability, reliability, safety

II. PRINCIPLE OF EOF MIXING

When a glass capillary is filled with electrolyte solution and is applied with a high voltage, the solution flows along the capillary channel. This phenomena is called electro-osmotic flow (EOF) The physics behind the phenomena is explained in the following manner and schematically shown in Fig.1: when a metal oxide surface is exposed to electrolyte solution, the solid surface is charged either positively or negatively depending on the combination of the solid surface property and liquid pH .Counter-ions then appear in the electrolyte in the vicinity of the contact surface. When the high voltage is applied, the ions move toward the direction of electric field accompanied by the bulk fluid flow. The velocity of the bulk liquid flow is called EOF velocity and is represented by Eq. (2.1) (Smoluchowski's equation):

$$u = -\frac{\epsilon_r \epsilon_0}{\mu} \xi \cdot E, \text{-----(2.1)}$$

Where ξ is the electrical potential at the slip plane in the electric double layer and called zeta potential. The value of the zeta potential is determined depending on the relation between the channel wall material and the pH of the electrolyte. The zeta potential value becomes zero at certain liquid pH, and this pH value is called isoelectric point, pH_0 . The isoelectric point is therefore a unique property for each metal oxide; for instance, the value of pH_0 is equal to 2 for SiO_2 , 9 for Al_2O_3 , and 10 for NiO . When pH_0 is lower than the electrolyte's pH, the oxide surface charges negatively, while the pH_0 is higher, the surface charges positively. Different value of pH_0 , which means different channel wall material, therefore leads to different EOF velocity. Figure1 shows that how an electroosmotic flow is created in a microchannel with the wall surface negatively charged. Under the external electric field, the movement of counterions (now is the positive ions) and coions (the negative ions) in EDL will drag the water molecules (the neutral particle) to move. Since the concentration of counterions is higher than that of coions in the ionized solution, the overall driving force points to the movement of counterions, thus the fluid has the same flow direction as the movement of counterions [2].

Electroosmotic flow is the bulk liquid motion that results when an externally applied electric field interacts with the net surplus of charged ions in the diffuse part of an electrical double layer. An electrical double layer (EDL) is a very thin region of non-zero net charge density near a two phase interface (for the cases of interest here, typically a solid-liquidinterface) Most solid surfaces acquire a surface electrical charge when brought into contact with an electrolyte liquid. When a polar liquid was placed in contact with another phase (like the wall of the surrounding channel), a potential difference develops at the interface. Molecules of the polar liquid (dipoles) would re-orient

themselves near the phase boundary. Ions or excess electrons present would cause a charge re-distribution at the interface, causing formation of the so-called electrical double layer (EDL). The thickness of electrical double layer was described by several models. An important one was the Debye length, which could be stated as in Eq. (2.2),

$$\Psi = \Psi_0 \exp(-r_{edl} z) \text{-----(2.2)}$$

Where Ψ was the electrical potential, z is the distance from the wall and r_{edl} was identified as the reciprocal of the thickness of the electrical double layer, also commonly referred to as the "Debye length". [3] The first layer, known as the surface charge layer, is made of ions absorbed in the surface due to chemical reactions (negative charges in this case). The second layer, known as the diffusive layer, is made of free ions attracted to the surface due to the influence of electric attraction and thermal motion. This second layer is the surface charge and its net charge is equal to the surface charge, but has the opposite polarity. In the field of microfluidics, the flow is often driven by an electric field. By definition, electroosmosis refers to the motion of a liquid induced by an applied potential across a microchannel. Driving the flow with an electric field allows for the fabrication of pumps and mixers without moving parts.[6]

Governing Equations:

Incompressible fluid flow is governed by the Navier-Stokes (momentum) Eq. (2.3), and continuity equations Eq. (2.4), shown below, [3,6]

$$\rho \left(\frac{\partial v}{\partial t} + v \cdot \nabla v \right) = -\nabla p + \eta \nabla^2 v - \rho e \nabla \Phi \text{-----(2.3)}$$

$$\nabla \cdot v = 0 \text{-----(2.4)}$$

Where v =velocity, t =time, p =pressure, η = viscosity and ρ = density.

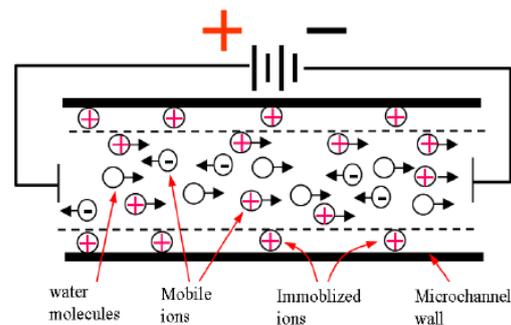


Figure 1: Mechanism of the electro-osmotic flow. [2]

III. LIQUID FLOWS IN MICROCHANNELS

In a typical microfluidic device, viscosity dominates flow, and as a result, the Reynolds number is low and the flow is laminar. Therefore, the mixing of two or more fluid streams in microfluidic devices is by virtue of diffusion, which is a slow process. On the other hand, for microfluidic applications towards biomedical or chemical diagnostics, such as lab-on-a chip, it was very important to mix two or more reagents and test samples thoroughly before detection can take place. This requires, a) the mixing needs to be done in a confined area; b) The volume of fluids for detection should be adequate and sufficiently mixed. Therefore,

microfluidic mixing is challenging and device design issues need to be solved, and many mixing methods have been developed. Based on the mixing mechanism, micro-mixers have pure molecular diffusion. The molecular structure of the liquid also affects the flow. Molecules with no electrical charge can have a dipole configuration (e.g. water). Pfahler et al (1991) found that the value of the viscosity of polar isopropanol decreases from the nominal value for a channel height smaller than 40 microns and reaches an asymptotic value at a channel height of about 10 microns. It is reasonable that the size effect becomes more pronounced for a narrow channel. Electro osmotic pumping has been demonstrated as a suitable way to drive liquid flows in microchannels. Electroosmosis describes the motion of fluids with respect to a fixed, charged solid surface. If a surface is positively charged, the negative ions in the solution will be attracted by the Coulomb forces toward the solid wall. There is thus a thin solvated layer of negatively charged particles in contact with the solid surface. [4,5]

TABLE I: ELECTRO-OSMOTIC FLOW VARIABLES

Sr. No.	Variables / Parameters	Effect on EOF	Possible Problems
1	Electric Field	Directly proportional	Can cause heating
2	Ionic Strength	Inversely proportional	Sample heating and adsorption
3	Covalent Coating	Dependent on coating	Often unstable
4	pH	Directly proportional	An alter structure and charge of analytic
5	Temperature	Inversely proportional	Changes in viscosity
6	Organic Modifiers	Usually inversely proportional	Can alter selectivity of instrument
7	Hydrophilic Polymer	Usually inversely proportional	Dependent on polymer

Table I gives the various EOF parameters with their effect on flow pattern. Electro-osmotic flow results when an electric field is applied to this electrical double layer that spontaneously forms at the interface between a liquid and solid when they are brought into contact. The most significant disadvantages associated with the use of electro-osmotic flow tend to be related to the relatively high applied potentials that are required to generate significant low velocities.

IV. CFD ANALYSIS

Therefore, to achieve the objective of this work, advanced computational fluid dynamics (CFD) techniques were chosen as the major tools for the investigation. In addition, a simplified experimental method was also setup to validate selected numerical models used in the CFD simulations. By the experimental validation, the numerical models could be verified, and confidence to use CFD for further investigation could be achieved. Experimental and analytical results were used for the validation of simulation results. The methodology for the investigation is described as below by considering a rectangular microchannel only by performing

the analysis using software. Two dimensional domains of 1mm length and 200 μm width is solved using ANSYS CFX. The wall material is either SiO₂ or Al₂O₃ (regular one). The fluid flowing through micro channel is KCL.

Steps for Meshing:

1. Geometry of rectangular cross section microchannel of size 1000 X 200X 20 μm (length along x-axis, width length along y-axis, thickness along z-axis) is created with the help of ANSYS ICEM using create point, Create /Modify curve, sweep surface etc. option.
2. Parts are created for simulation in ANSYS CFX which is useful for giving boundary condition in pre-processing as shown in fig.2 below. Different parts are:
 - Inlet
 - Outlet
 - Side wall
 - Opening
 - Bottom
3. No blocking is required as geometry have regular shape.
4. Number of nodes are changed using Edit Mesh=Pre-Mesh Params option. Nodes are to be changed : 20-nodes along length, 10-nodes along width, 3-nodes along thickness.
5. At last load from blocking option is used for complete meshing. As meshing is shown in fig.2
6. Quality of mesh is checked.

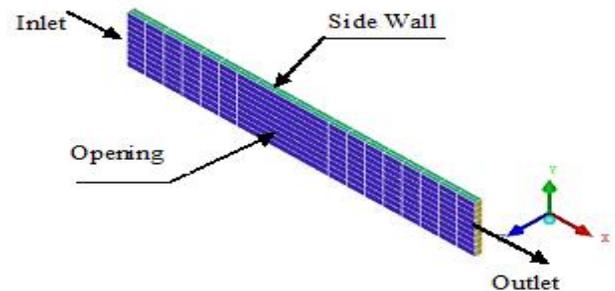
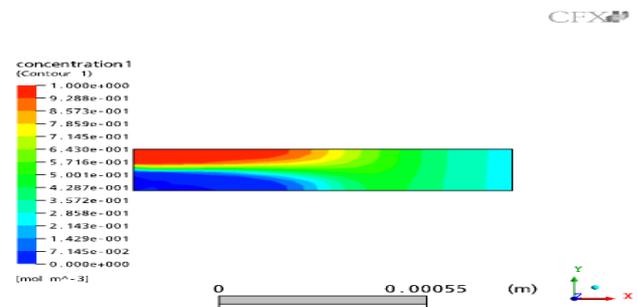


Fig2. Meshing of microchannel showing all parts (Isometric view)

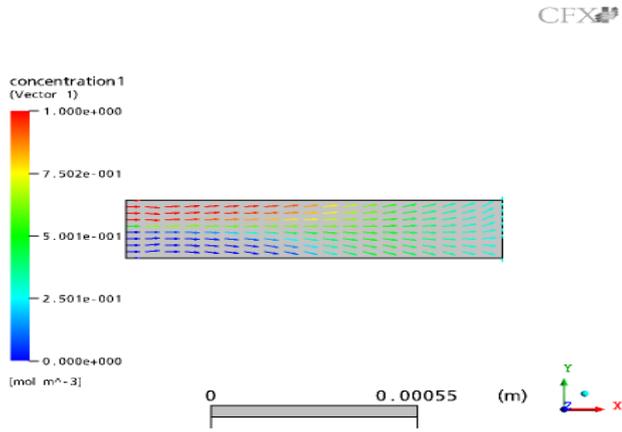
V. RESULT AND DISCUSSION

Simulated Results for 100 V

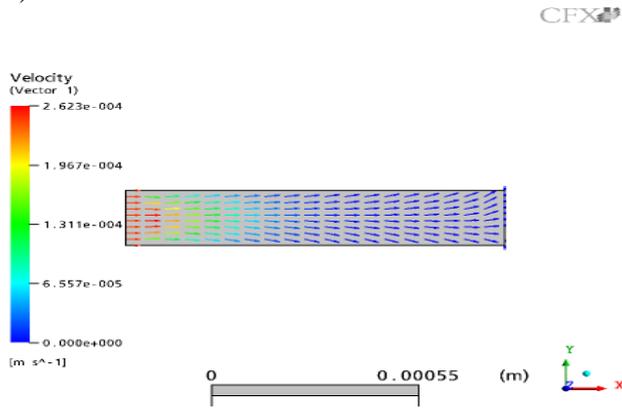
A] Flow Pattern



a) Contour Plot



b) Concentration Vector Plot

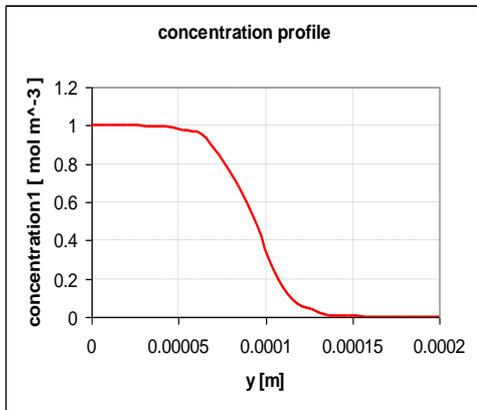


c) Velocity Vector Plot

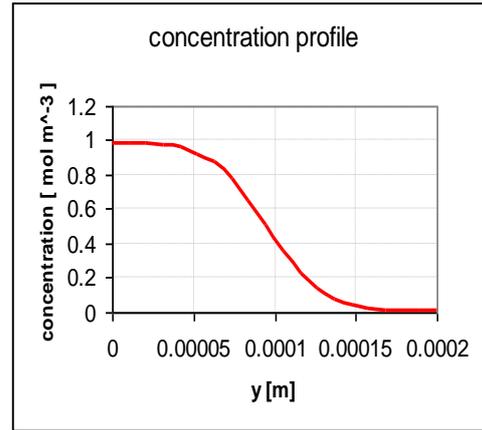
Fig 3 Contour Plot / Vector Plot for 100V

Fig 3 (a) shows the contour plot for concentration, values vary from 0.0 mol/m^3 to 1.00024 mol/m^3 within domain. Fig 3(b) shows the vector plot for concentration and fig 3 (c) shows the vector plot for velocity, values vary from 0.0 m/s to 0.000247 m/s within domain. The dark red area represents higher concentration of reagent, and the dark blue area does lower value. The arrows in the computational domain represent the flow vector, and scale represents the concentration. After CDF simulation we can easily find out any property at any location. So for this case I took six locations from inlet of channel.

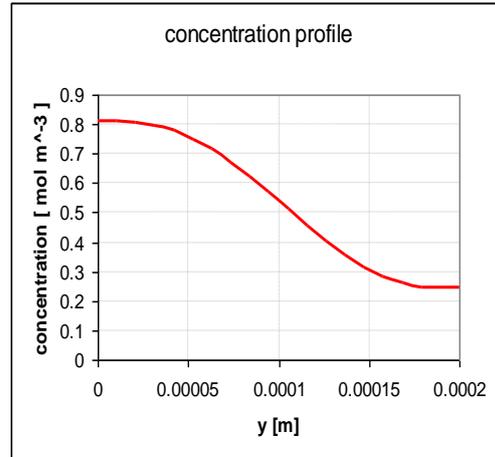
B) Concentration Profile at different location:



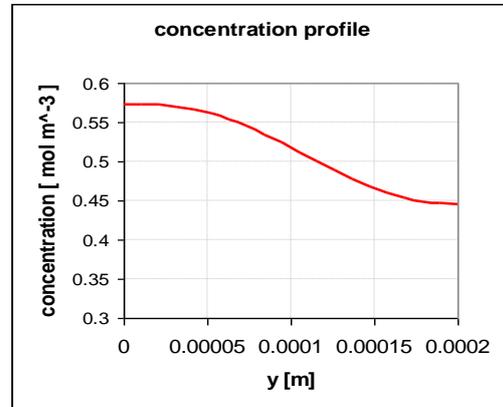
at 150 micron from inlet



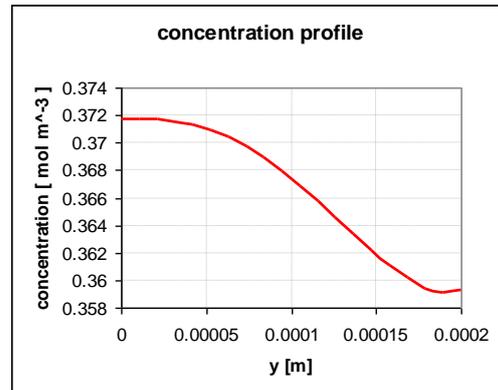
at 300 micron from inlet



at 500 micron from inlet



at 650 micron from inlet



at 815 micron from inlet

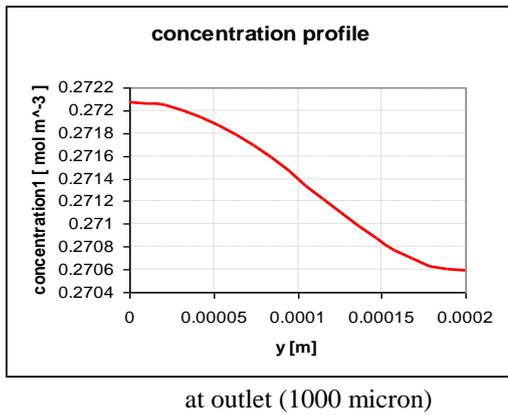


Fig 4 Concentration profile

Fig 4 shows the concentration profile of reagent at different six locations with width of channel (y) in meter along x-axis and concentration (mol/m^3) along y-axis. Without mixing, the profile is a step function: $c=1.0 \times 10^{-5}$ below $y \leq 100 \mu\text{m}$, and $c=0$ below $y \geq 100 \mu\text{m}$. As the mixing proceeds, the profile gradient decreases, and the concentration profile finally reaches a flat line where $c=0.5 \times 10^{-5}$.

VI. CONCLUSION

In a typical microfluidic device, viscosity dominates flow, and as a result, the Reynolds number is low and the flow is laminar. Therefore, the mixing of two or more fluid streams in microfluidic devices is by virtue of diffusion, which is a slow process. On the other hand, for microfluidic applications towards biomedical or chemical diagnostics, such as lab-on-a chip, it was very important to mix two or more reagents and test samples thoroughly before detection can take place. This requires the mixing needs to be done in a confined area and the volume of fluids for detection should be adequate and sufficiently mixed.

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