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A comparative numerical simulation of the electrokinetic micromixers

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Abstract

Micromixers have a practical application in analyzing of many biochemical and biologicals detection devices of lab-on-a-chip (LOC). The conventional static micromixers require the channel with more lengths and also require times to reach to complete mixing owing to its dependence on transverse diffusion. However, in the electrokinetic micromixers, as the surface properties of the microchannel run the electro-osmotic flow characteristics, surface heterogeneity (non-uniform zeta potentials) can be seen to make vortices or specific flow structures for better mixing performance. This study aims to use computational fluid dynamics (CFD) to numerically compare the concentration rate of the various electrokinetic micromixers in in the presence of the electric conductor. The results revealed that the off-center microchannel design in a micromixer can augment the rate of concentration. In addition, circular microchannel design showed better mixing compared to the triangular and square designs. These results are useful not only for understanding of the profiles of concentration in the electrokinetic micromixers, but also for providing a comprehensive information on the design of the microchannels, which may result in better mixture in the fluids.

Keywords Micromixer; Lab-on-a-chip; Design; CFD; Concentration.

Introduction

Mixing is a sensitive process in most of microfluidic systems, such as lab-on-a-chip (LOC) devices or micro-total analysis systems. Turbulent flow is the natural driving force of mixing process, however, the microfluidic devices have very small characteristic scale , the fluid flow is assumed as a low Reynolds number regime (Re <<1) [1]. Micromixers are important devices in the bio-microfluidics, where they are used in complex enzyme reactions [2] and biochemical analysis [3]. Low analysis time duration and portability are among the best advantages of these micromixer devices. There are two types of micromixers, active and passive [4] based on their mixing strategy. The mixing performance of electrokinetic passive mixers could be improved by using geometric modifications [5], heterogeneous charged walls/bottom [6], and grooves patterning on channel base [7]. Moreover, such geometric/surface changes can enhance the non-axial flow for

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improved mixing. However, active mixers use external energy - via pressure or electro-kinetic disturbance to induce transverse flows [8].

Electrokinetic methods, including electroosmosis, electrophoresis, and dielectrophoresis, are of high importance in microfluidic devices. These have been extensively used for pumping, mixing, gradient generation, separation, and sorting on LOC devices. Electroosmosis has been applied as a pumping method, as it has significant advantages over the conventional pressure-driven flow, such as plug-like velocity profile, ease to control and switch flow, and no mechanical moving parts. Generally, electrokinetically-driven flows in microchannels are assumed to be laminar because the velocity and the length are not high which lead to low Reynolds numbers. Consequently, mixing in such a laminar flow of parallel streams occurs only by diffusion, which is problematic for situations requiring rapid mixing of different solutions in microchannels. Some electrokinetic mixing devices have been designed for enhancing the mixing efficiency.

One example is T-shaped microchannel mixers, that uses electroosmotic flow to pump liquids from two horizontal channels to the T-intersection and mix liquids in the vertical channel while the liquid flows to downstream. T-shaped mixers have been utilized used in various lab-on-a-chip devices, for example, to dilute sample in a buffer solution and to generate concentration gradients [9]. However, there is still little knowledge about the mixing ability of the micromixers based on their design and the position of the electric conductor in the system. In this research, the main aim has been focused at performing a computational fluid dynamic (CFD) study to calculate the concentration and mixing ability of different microchannels designed in producing homogenous fluid at the outlet.

2. Materials and Methods

2.1. Electrokinetic formulations

According to the equations proposed by [10], for a two-dimensional hollow cylinder the zeta potential can be defined as:

$$\zeta_i = 2\mathrm{Ea}\cos\theta \qquad (1)$$

Since there is no analytical solution for the problem, a numerical approach has been proposed lately as:

$$\zeta_i = -\varphi_e + \frac{\oint \varphi_e dA}{A} \qquad (2)$$

The above equation works as long as the there is no chemical reaction between the fluid and solid phases and Dukhin number (Du) is negligible.

$$Du = -\frac{k^{\sigma}}{k_m a} \qquad (3)$$

where k^{σ} is the surface conductivity, k_m is fluid bulk electrical conductivity, and a is the particle size. This will lead to an electroosmotic flow, which can be defined with the Helmholtz equations:

$$u = -\frac{\varepsilon\varepsilon_0}{\mu} E\zeta_i \qquad (4)$$

2.2. Fluid model

We have used Navier-Stokes equations to present the velocity and pressure of the incompressible flows in dynamic situation [11]:

$$\rho(u.\nabla)u + \nabla p - \nabla.\eta(\nabla u + (\nabla u)^T) = f \qquad (5)$$

$$-\nabla.u = 0 \qquad (6)$$

where u is the velocity of fluid, p is the pressure of flow, ρ is the density, η is the viscosity and f is the body force which is applied on the fluid.

In Navier-Stokes flow, the body force can be presented as [12].

$$f = -\alpha u \qquad (7)$$

where α is the impermeability of a porous medium. It depends on the optimization design variable γ [12].

$$\alpha(\gamma) = \alpha_{min} + (\alpha_{max} - \alpha_{min})\frac{q(1-\gamma)}{q+\gamma} \qquad (8)$$

where $\alpha_{\min}$ and $\alpha_{\max}$ are minimum and maximum values of α , and q is a real and positive parameter used to adjust the convexity of the interpolation function in Eq. (8).

γ could be between zero and one, where $\gamma = 0$ relates to an artificial solid domain and $\gamma = 1$ to a fluidic domain, respectively. Normally, $\alpha_{\min}$ is selected as 0, and $\alpha_{\max}$ is selected as a high finite number to ensure that the optimization is numerically stable and a solid with negligible permeability [13].

The model has three parts: the inlet, the design area and the outlet. Moreover, the body force, f, for inlet and the outlet (non-design area) is set to zero in the Navier-Stokes equations where f can be defined as follows:

$$f = \begin{cases} -\alpha u, & in\ \Omega_D \\ 0, & in\ \Omega_N \end{cases} \qquad (9)$$

Ω_D is the design area and Ω_N is the non-design area.

Based on what mentioned above, optimization problem of the model can be shown as follows:

$$min\phi(u,\gamma) \qquad (10)$$

$$s.t\ \rho(u.\nabla)u = -\nabla p + \nabla.\eta(\nabla u + (\nabla u)^T) - \alpha(\gamma)u, \ \ in\ \Omega$$

$$-\nabla.u = 0, \ \ in\ \Omega$$

$$u = u_0, \qquad at\ \Gamma_{inlet}$$

$$u = 0, \qquad at\ \Gamma_{wall}$$

$$p = 0,$$

$$\eta(\nabla u + \nabla u^T)n = 0, \ \ at\ \Gamma_{outlet}$$

$$0 \le \gamma \le 1$$

where u_0 is the inlet velocity [14].

Da is the penetration ability of a porous medium and *Re* (Reynolds number) is the ratio of inertia force and viscous force. They are defined as:

$$Da = \frac{\eta}{\alpha_{max} \times L^2} \qquad (11)$$

$$Re = \frac{uL_\rho}{\eta} \qquad (12)$$

where *L* refers to the length, characteristic, of the fluid. For non-circular pipes, *L* refers to hydraulic diameter. η is coefficient of kinematic viscosity.

Mixing efficiency of the species is obtained as follows [15]:

$$M = 1 - \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{c_i - \bar{c}}{\bar{c}}\right)^2} \qquad (13)$$

M is the efficiency of mixing, *N* is the total number for sampling points, c_i is normalized concentration and c^{-} desired normalized concentration. Mixing efficiency varies from 0 (0%, not mixing) to 1 (100%, full mixed) [14].

The velocity field in the micromixers were calculated as following:

$$u_x = \frac{-\varepsilon\varepsilon_0\zeta}{\mu}E_x \qquad (14)$$

$$u_y = \frac{-\varepsilon\varepsilon_0\zeta}{\mu}E_y \qquad (15)$$

The velocity field in the micromixer wall can be defined as:

$$u_x = \frac{-\varepsilon\varepsilon_0\zeta_i}{\mu}E_x \qquad (16)$$

$$u_y = \frac{-\varepsilon\varepsilon_0\zeta_i}{\mu}E_y \qquad (17)$$

where Ex and Ey are the electrical fields in the X and Y directions, respectively.

The structure of the micromixer as well as the electrical field in the system are displayed in Figs. 1a and 1b, respectively. The flow under the velocity of 1 cm/s was considered in the models with different designs from the left inlet. We considered no-slip boundary condition for interaction of solid and fluid domains. The parameters of the modeling are listed in Table 1.

3. Results and Discussion

The profiles of the concentration in the micromixer with the circular microchannel structure are shown in Fig. 2. When there is no electric conductor in the microchannel the results showed that the concentration is not changed following by an inappropriate mixing (Fig. 2a). However, the presence of the electric conductor in the center of the micromixer results in a vortex formation not only at the inlet but also the outlet of the micromixer (Fig. 2b). To understand the role of the location of the electric conductor in the micromixer, the off-center design was also simulated and the results showed a higher mixing rate at both the inlet and outlet sides of the micromixer (Fig. 2c). Therefore, it is stemmed that the presence as well as the location of the electric conductor in the micromixer have a considerable impact on the mixing ability of the micromixer.

The design of the microchannels in the electrokinetic micromixers in the presence of the electric conductor was also investigated. The profiles of the concentration in the square, triangular, and circular design of the microchannels in the micromixers are displayed in Fig. 3. The results revealed a higher mixing ability for the circular design as the flow can go through the channels easily and well mixed up and, as a result, the out flow will be homogeneous, which is desired. In the square and triangular designs, two vortexes were occurred at the outlet which augment the mixing rate of the fluid. However, the mixing rate was still However, the most suitable concentration rate was observed in the circular design.

4. Conclusions

This study was aimed at employing CFD to investigate the mixing ability of the electrokinetic micromixers in the presence of an electric conductor. Three different designs, including the square, triangle, and circular, were established and the results in terms of the mixing ability was compared. The circular microchannel design showed higher mixing ability compared to other designs. In addition, the off-center electric conductor design revealed a better mixing rate compared to the center design. These findings provide a comprehensive knowledge on design of the microchannels of the electrokinetic micromixers.

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Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Competing interests

The authors declare that they have no competing interests.

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