

LATTICE BOLTZMANN SIMULATIONS OF MIXING ENHANCEMENT BY THE ELECTRO-OSMOTIC FLOW IN MICROCHANNELS

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The Lattice Boltzmann methods are used to study the mixing enhancements by the electro-osmotic flow in microchannel. Three sets of lattice evolution methods are performed for the fluid flow, for the electrical potential distribution, and for the concentration propagation. The simulation results show that the electro-osmotic flow induces y-directional velocity which enhances the mixing in microchannels. The mixing enhancement is related with the surface zeta potential arrangement and the external electric field strength.

Keywords: Lattice Boltzmann method; Mixing enhancement; Electro-osmotic flow

1. Introduction

Obtaining a complete mixing in the microfluidic systems is difficult because the operations are always limited to low Reynolds number regimes characterized by laminar flow. Therefore, many researchers have developed a number of microfluidic mixing-enhancement devices [1,2], which can be broadly classified as either passive or active mixers. The electro-kinetic flow can be used as an active mixer with no mechanically moving parts. It has many promising applications due to its easy control and suitability for integration with M/NEMS devices [3].

Some researchers analyzed the mixing process in electrically driven micro flows using the classical CFD methods [3-5]. Biddiss et al [6] experimentally investigated the heterogeneous surface charge enhanced micromixing for electro-kinetic flows and developed an optimized electrokinetic micromixer applicable to the low Reynolds number regime. Recently, the Lattice Boltzmann method was tried in modeling the mixing in microchannel flows [7]. However, in their work, the one-dimensional linear Poisson was solved for the electric potential and the mixing process was analyzed only by flow stream field. We have developed a Lattice Poisson-Boltzmann method (LPBM) to model the electro-osmotic flow correctly [8]. In LPBM, two sets of lattice evolution equations are used, one for non-linear Poisson equation for electric potential, and the other for the fluid flow driven by the external electrical force. In this paper, another lattice evolution equation is added for the concentration propagation into the LPBM so that the mixing enhancement can be characterized quantitatively. The effect factors are therefore investigated for a better mixing enhancement.

2. Numerical Method

Three sets of lattice evolution methods are used, one for electrical potential propagation, one for fluid flow and the other one for concentration diffusion. The combination of the first two, the Lattice Poisson-Boltzmann method (LPBM), serves as a solver for the electro-osmotic flows. The non-linear Poisson equation can be solved correctly for the electric potential distribution by the Lattice Poisson method (LPM). Then the Lattice Boltzmann method (LBM) solves the Navier-Stokes equation for fluid flows with external force driven. The details can be found in the Ref [8]. After the flow field is solved, another lattice evolution method is used to solve the scalar diffusion equation. Here, the evolution equation for the concentration distribution function in a D2Q4 model [9] can be written as:

$$g_\alpha(\mathbf{r} + e_\alpha \delta_{t,g}, t + \delta_{t,g}) - g_\alpha(\mathbf{r}, t) = -\frac{1}{\tau_d} [g_\alpha(\mathbf{r}, t) - g_\alpha^{eq}(\mathbf{r}, t)], \quad (1)$$

where $g_\alpha(\mathbf{r}, t)$ is the concentration distribution function and $g_\alpha^{eq}(\mathbf{r}, t)$ is the corresponding equilibrium distribution

$$g_\alpha^{eq} = \frac{C}{4} \left[1 + 2 \frac{e_\alpha \cdot \mathbf{U}}{c^2} \right], \quad \alpha = 1, 2, 3, 4 \quad (2)$$

with C is the concentration, \mathbf{U} is the velocity, c is δ_x / δ_t , and τ_d is the relaxation parameter related with the diffusivity D as:

$$\tau_d = \frac{3}{2} \frac{D}{c^2 \delta_t} + 0.5. \quad (3)$$

After evolution, the concentration distribution is obtained by

$$C(\mathbf{r}, t) = \sum_{\alpha=1}^4 g_\alpha(\mathbf{r}, t). \quad (4)$$

3. Results and Discussion

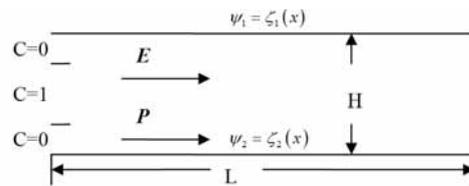


Fig. 1 Boundary conditions for the electro-osmotic flow in a microchannel

The physical model for the electrokinetically enhanced mixing in a 2D microchannel is shown in Fig. 1. The channel is H wide and L long. The channel walls are charged heterogeneously. The fluid is driven fluid by a pressure gradient. The external electric field is used to drive vortices near the wall to enhance the mixing. At the inlet, two kinds of fluids flow into the channel. One is from the center and the other is from the sides. Both the upper and lower sides are $1/4$ the across section area. This structure has applications in Bio-techniques. In current simulations, with $H = 1 \mu\text{m}$ and $L/H = 10$

the diffusivity between species takes $10^{-9} \text{m}^2 \cdot \text{s}$ so that it can be treated completely mixed at the outlet. The properties parameters can be found in reference [8].

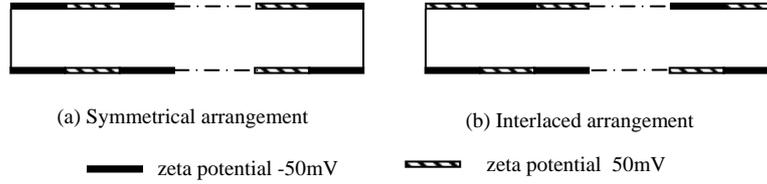


Fig. 2 Two typical charge arrangements of the zeta potential

First, we compared two typical zeta potential arrangements on the wall surfaces: the symmetrical arrangement (see Fig. 2a) and the interlaced arrangement (see Fig. 2b). Each wall is divided into n parts, with each part charged a 50 mV or a -50 mV zeta potential. When n is 4, with the ion concentration of the electrolyte solution at $10^{-5} M$, the external electric field strength at 500 V/m and the pressure gradient at 1×10^6 Pa/m, the concentration contour results are shown in Fig. 3. Comparing with the non-ionic fluid case (Fig. 3a), both arrangements can obtain a mixing enhancement due to the vortices induced by the electrical force in EDL.

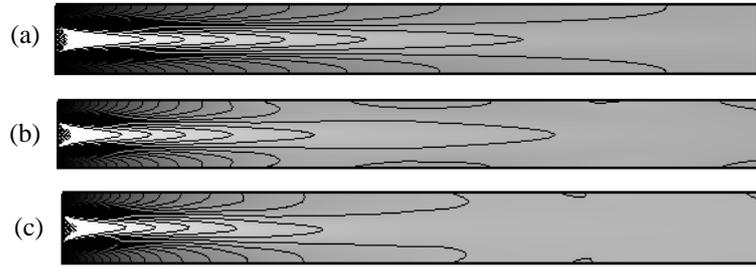


Fig 3 Concentration contours at $n=4$

To quantify the mixing enhancement, the mixing length is introduced, which is defined as the length before fully mixing. The calculation of the mixing length takes the method from Ref. [10], with a criterion value at 3%. For the cases in Fig. 3, the mixing length is $8.13 \mu\text{m}$ for non-EDL case, $6.9 \mu\text{m}$ for the symmetrical arrangement case, and $5.1 \mu\text{m}$ for the interlaced arrangement case. The mixing enhancement effect for the interlaced arrangement is 35% higher than for the symmetrical arrangement.

Fig. 4 shows the mixing lengths versus the external electric field strength when the zeta potential is divided into 4 parts. The stronger the electric field, the better the mixing enhancement effect. This results from a larger electric field drives stronger vortices and y-direction velocity, which enhance the mixing.

At a given electric field strength, the mixing length varies non-monotonically with the parts number, as shown in Fig. 5. There is an optimal part length that reaches the best mixing effect for a certain electric field. If the external electric field is able drive vortices near the wall, when the part length is big enough, increasing the part number (decreasing

the part length) will enhance the mixing; however when the part length is smaller than some critical value, increasing the part number more will restrain the vortices and weaken the mixing enhancement.

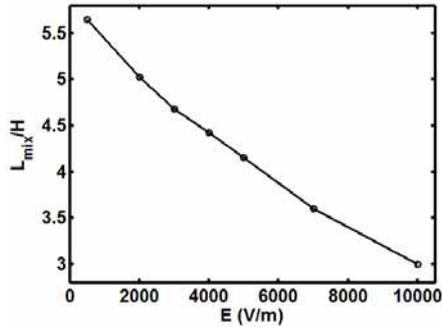


Fig. 4 Mixing length for different electrical field strength

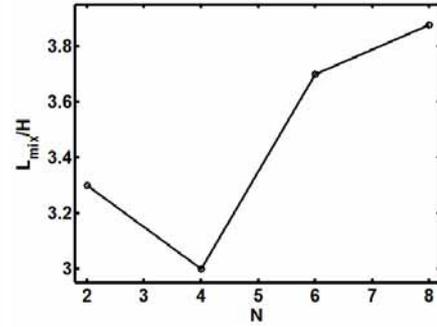


Fig. 5 Mixing length for different part number at $E_x=10^4$ V/m

4. Conclusion

Three sets of lattice evolution methods were used to model the mixing enhancement by the electro-osmotic flows in microchannels. After the lattice Poisson-Boltzmann method solved out the flow field of the EOF, another lattice Boltzmann method in D2Q4 model was used to solve the concentration convection-diffusion equation. The mixing enhancement effect for the interlaced arrangement was higher than that for the symmetrical arrangement. A stronger external electric field led to a better mixing enhancement. There was an optimal part length that made the mixing effect best for a certain electric field.

Acknowledgments

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