The Optimum Surface Pattern
to Enhance Flow Oscillation in Micro-channel

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Abstract

Mixing of analytes and reagents in microfluidic devices is often crucial to the effective functioning of lab-on-a-chip. It is possible to affect the mixing in microfluidics by intelligently controlling the thermodynamic and chemical properties of the substrate surface. Numerous studies have shown that the phase behavior of mixtures is significantly affected by surface properties of microfluidics. For example, the phase separation between the fluids can be affected by heterogeneous patterns on the substrate. The patterned substrate can offer an effective means to control fluid behavior and in turn to enhance mixing.

In this study, we numerically studied the effect of optimum surface pattern on mixing in a micro channel and found that the flow oscillation was enhanced apparently when the ratio of hydrophobic and hydrophilic boundary follows certain ratios.

1 Introduction

It is well known that the Reynolds number Re is low in typical microfluidic channel, and the flow is laminar under normal conditions, especially for liquids. Therefore in a microchannel the mixing of binary or multicomponent fluid stream is difficult without the turbulence mixing mechanism, and the mixing due to pure molecular diffusion mechanism may take considerably long time. Meanwhile, mixing in lab-on-a-chip or μTAS (micro total analysis system) is responsible for preprocessing, sample dilution, or reactions between samples and reagents in particular ratios [22]. The initial concept of lab-on-a-chip, or "miniaturized total chemical analysis system," has been accredited to Manz *et al.* [19], who proposed the use of integrated microfabricated devices for sample pretreatment, separation, and detection for chemical analysis. Now lab-on-a-chip is becoming an increasingly familiar term used to connote the miniaturization of chemical, biological and biochemical analyses, environmental chemical assays, electrochemistry, thermocapillary pumping, and electro-osmotic flow [1, 8, 9, 20, 32]. The ability to create structures and patterns on micro and smaller length scales has triggered a wide range of scientific investigation, as well as the development of many devices to transport and manipulate fluids and pattern surfaces. Recently studies on patterned surfaces [7, 12, 13, 14, 26] revealed interesting phenomena that can be exploited to control liquid motions in microfluidic devices.

Since Qian *et al*. [23] brought forth the simple lattice Boltzmann equation based on the single relaxation time model for collisions [2], the model has become the most popular, and been successfully applied to various complex physical processes, such as the interfacial dynamics and multiphase flows [10, 25], flows through porous media [3, 24], reaction-diffusion systems, and other complex systems. However, numerical simulation for micro-channel about micro-devices is one of the recent new frontiers of computational fluid dynamics (CFD) and lattice Boltzmann method

(LBM). Meanwhile, studying or simulating the multiphase fluids, multi-component fluids and phase transitions in micro- and nano-channel by LBM has increased significantly in recent years. Many of lattice Boltzmann models for multiphase fluids come forth that based on mean-field interaction, or two-component lattice gas

model, or using the free-energy approach, or using the idea of level-set [10, 11, 27]. In 1998, Chen *et al.* [4], through the comparison with a macroscopic two-phase fluid flow model suggested by Nadiga and Zaleski [21], derived a lattice Boltzmann equation from the continuous Boltzmann Bhatangar-Gross-Krook (BGK) equation with an external force term. Recently, Luo, and Luo and Girimaji [15, 16, 17] have rigorously obtained the LBM model for multicomponent fluids based on kinetic theory by Chapman-Enskog analysis. Verberg *et. al.* [31] used a lattice Boltzmann model to carry out numerical study of the flow pattern of binary fluids confined between rough, chemically heterogeneous surfaces. Chew *et. al.* [6] presented a 3D lattice Boltzmann BGK model for simulation of microflows with heat transfer in a rectangular microchannel.

In this paper, we applied Lou and Girimaji's model [15, 16, 17] to study the optimum surface pattern for binary fluids mixing in a microchannel. The surface is arranged alternatively with either hydrophilic and hydrophobic features. Our work is motivated by the golden mean phenomenon in science, mathematics and nature, and the objective is to investigate the effect of golden mean of micro mixing. In the following, Section II simply states binary-fluid mixing lattice Boltzmann model under the isothermal assumption suggested by Luo and Girimaji [15, 16, 17]. Section III presents the mixing boundary conditions of optimum surface pattern. In section IV, we design a T-type microchannel to enhance fluids mixing effectively. The T-type channel can combine two fluid streams, in which the streams are parallel to each other in the microchennel, and the alternating surface pattern enhances the mixing effectively. Then Section V gives the conclusion.

2 Lattice Boltzmann model for binary mixtures

According to the kinetic theory of gas mixture, Luo and Girimaji [15, 16, 17] proposed the LBM with binary fluids. Similar to single component LBM equation, one can derive N simultaneous equations for a system of N species, therefore the Boltzmann equations for a binary species system are:

$$\partial_t f^\sigma + \boldsymbol{\xi} \cdot \nabla f^\sigma + \boldsymbol{a}_\sigma \cdot \nabla_\xi f^\sigma = Q^{\sigma\sigma} + Q^{\sigma\varsigma}, \qquad (1)$$

$$\partial_t f^\varsigma + \boldsymbol{\xi} \cdot \nabla f^\varsigma + \boldsymbol{a}_\varsigma \cdot \nabla_\xi f^\varsigma = Q^{\varsigma\varsigma} + Q^{\varsigma\sigma}, \qquad (2)$$

where f is the probability distribution function, $\boldsymbol{\xi}$ is the particle velocity, σ and ς represent the two species, $Q^{\sigma\varsigma}$ and $Q^{\varsigma\sigma}$ are the collision term due to the interaction between two different species σ and ς, $Q^{\sigma\sigma}$ and $Q^{\varsigma\varsigma}$ are the self-collision term. The lattice Boltzmann equation can be discretized as follows:

$$f_\alpha^\sigma(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta_t, t + \delta_t) - f_\alpha^\sigma(\boldsymbol{x}, t) = J_\alpha^{\sigma\sigma} + J_\alpha^{\sigma\varsigma} - F_\alpha^\sigma \delta_t \quad (3)$$

The self-collision term is derived similarly to single fluid LBM, and also adopts the BGK model. Under the isothermal assumption of the system, the cross-collision is derived a two-fluid theory. At the right-hand-side the terms of the collision equation are:

$$J_\alpha^{\sigma\sigma} = -\frac{1}{\tau_\sigma}[f_\alpha^\sigma - f_\alpha^{\sigma(0)}], \qquad (4)$$

$$J_\alpha^{\sigma\varsigma} = -\frac{1}{\tau_D}\frac{\rho_\varsigma}{\rho}\frac{f^{\sigma(eq)}}{\delta_t c_s^2}(e_\alpha - u)\cdot(u_\sigma - u_\varsigma), \qquad (5)$$

$$F_\alpha^\sigma = -w_\alpha \rho_\sigma \frac{e_\alpha \cdot a_\sigma}{c_s^2}, \qquad (6)$$

F_α^σ represents the forcing term. ρ_σ and ρ_ς, and u_σ and u_ς are the mass densities and flow velocity for species σ and ς, respectively. a_σ is the acceleration set. ρ and u are the density and velocity of the mixture fluid, which are defined as $\rho = \rho_\sigma + \rho_\alpha$ and $\rho u = \rho_\sigma u_\sigma + \rho_\varsigma u_\varsigma$, respectively. In the binary fluid mixing model, the different viscosities of the two components are related to the τ_σ and τ_ς, respectively. The cross-collision term determines how strong the diffusion effect is of the miscible or immiscible mixture, so the miscibility of the mixture can be adjusted easily by adjusting the collision coefficient τ_D. For simulating immiscible mixtures, τ_D should be less than 0.5. On the contrary, for simulating miscible mixtures, τ_D should be more than 0.5. Therefore the viscosity and the diffusion of component fluid mixture are conveniently controlled by the clear physical insight. Zhu *et al.* [34] simulated miscible fluid mixtures successfully using LBM and found that the collision coefficient τ_D has significant effect on the fluid mixtures. When τ_D approximates to 0.5, the obvious contact surface can be identified between the fluids.

The equilibrium distribution function $f_\alpha^{\sigma(0)}$ is defined as

$$f_\alpha^{\sigma(0)} = f_\alpha^{\sigma(eq)}[1 + \frac{1}{c_s^2}(e_\alpha - u)\cdot(u_\sigma - u)], \qquad (7)$$

$$f_\alpha^{\sigma(eq)} = w_\alpha \rho_\sigma [1 + \frac{e_\alpha \cdot u}{c_s^2} + \frac{(e_\alpha \cdot u)^2}{2c_s^4} - \frac{u \cdot u}{c_s^2}]. \qquad (8)$$

For the D_2Q_9 model, e_α is given by

$$e_\alpha = \begin{cases} (0,0), & (\alpha = 0) \\ (\pm 1, 0)c, (0 \pm 1)c, & (\alpha = 1, \cdots, 4) \\ (\pm 1, 1)c, (\mp 1, -1)c, & (\alpha = 5, \cdots, 8) \end{cases} \qquad (9)$$

and $w_0 = 4/9$, $w_{1,2,3,4} = 1/9$, $w_{5,6,7,8} = 1/36$.

3 Boundary conditions for the system

In this study, we simulate micro-channel fluid, in which the slip and no-slip boundary is used alternately. That means the concurrence of hydrophilic and hydrophobic wall, named composite boundary. The hydrophilic wall is bounce back and the other is specular reflection boundary [28, 29, 30, 33]. As shown in Figure 1, node A indicates the bounce back condition, the f_4, f_7, f_8 are reflected to f_2, f_5, f_6, respectively. Node C indicates the reflection condition, the f_4, f_7, f_8 become f_2, f_6, f_5, respectively. That means the angle of incidence is equal to the angle of reflection. This case is for perfect slip at the wall that no shear forces will be transmitted and their tangential momentum will be conserved. Node B is the joint node between hydrophilic and hydrophobic boundary conditions. The left side of node B is the bounce back boundary condition and the right side is the specular reflection boundary condition.
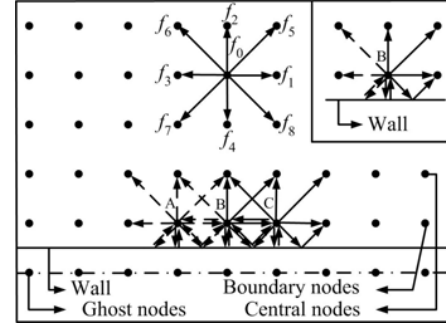

Figure 1. Boundary conditions for the distribution function.

The outflow boundary condition is applied at the outlet and the velocity boundary condition is applied at the inlet. The inlet boundary conditions for binary fluid model can be derived according to the methods of Chen *et al.* [5], Maier *el al.* [18], and Zou *et al.* [34]:

$$f_1 = f_3 + (f_1^{(eq)} - f_3^{(eq)}), \qquad (10a)$$

$$f_5 = f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{2}(\rho_{in} u_x - f_1^{(eq)} + f_3^{(eq)}), \qquad (10b)$$

$$f_8 = f_6 + \frac{1}{2}(f_2 - f_4) + \frac{1}{2}(\rho_{in} u_x - f_1^{(eq)} + f_3^{(eq)}), \qquad (10c)$$

$$\rho_{in} = \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{1 - u_x}. \qquad (10d)$$

4 Results and Discussion

In this study we use two-dimensional binary-fluid lattice Boltzmann model to examine the effect of boundary pattern on the mixing behavior of two partially immiscible fluids, A and B, which pass through a T-type microchannel as shown in Figure 2. The width of the mixing microchannel is h_3 and the length of the main channel is L. The ratio of the width h_3 to the length L is 1:20. Figure 2 shows the schematic view of the micro channel. The h_1 denotes the length of the hydrophobic boundary and h_2 indicates the length of the hydrophilic boundary. The inlet velocity profile is parabolic and the maximum velocity is the same (i.e., $U_{max} = 0.01$) for the two fluids at their entrance, respectively. The collision coefficient, τ_D, of the binary-fluid mixing lattice Boltzmann model is defined as 0.49999 for simulating immiscible fluids mixing, and the viscosities of the two different species fluids are 1.5 and 1.5001, respectively. These parameters can satisfy the immiscible requirement and make an obvious contact surface between fluids. The viscosity of the species is equal to $c_s^2(\tau - 1/2)\Delta t$, where $c_s = c/\sqrt{3}$; and the Re is defined as $\mathrm{Re} = (U_0 L)/v$. The gravity force constant is zero.
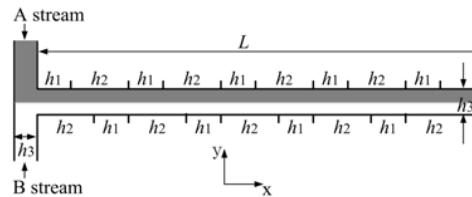

Figure 2. Schematic illustration of elementary models with distribution of hydrophobic boundary length h_1 and hydrophilic boundary length h_2.

Figure 3 shows the comparison of streamlines and density contours between no-slip boundary and composite boundary conditions. It indicates clearly that the combined surface pattern can enhance the mixing behavior significantly. For no-slip boundary condition, the streamlines and density contours are typically stratified, indicating the diffusion is dominant in the micro channel. When the surface is patterned by hydrophilic and hydrophobic boundaries, the flow is obviously oscillating which would enhance the mixing definitely.
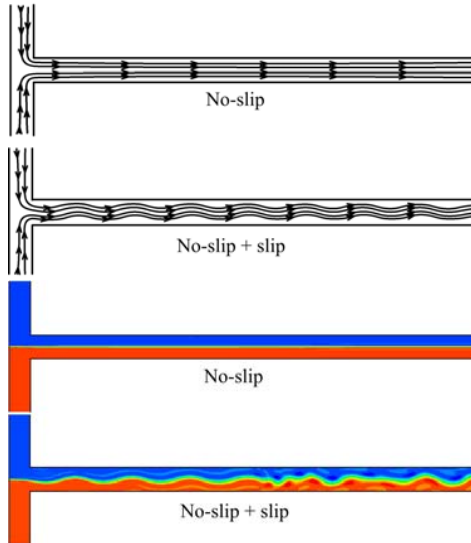

Figure 3. Numerical results of two binary liquids flow in a T-type microchannel with single hydrophilic surface and interval hydrophilic and hydrophobic surfaces, respectively.

The physics of the enhancement of the mixing by surface pattern is to perturb the flow by fluctuating boundary conditions, therefore the length of the surface pattern and the width of the entrance would affect the mixing greatly. To investigate the effect of pattern parameters on the mixing behavior, we define $\beta = h_1/h_2$. Figure 4 shows the visualized species density contours at $\beta = 1.6$ with different ratio of hydrophilic length to entrance width, h_2/h_3. The h_2/h_3 has significant influence on the mixing behavior, when the h_2/h_3 is 0.5, the mixing effect is very weak; with increasing h_2/h_3 to 1.6 and 2.0, the mixing effect becomes significant. The most likely explanation of this phenomenon is that the perturbation from the boundary needs enough space to develop. If the frequency of the perturbation from the boundary is too high, i.e., if the length of the surface pattern is too short, then the mixing would be suppressed; if the frequency of the perturbation from the boundary is too low, the mixing would be certainly weak. This would provide us a hint there should exist an optimum spacing ratio for the micro mixing.
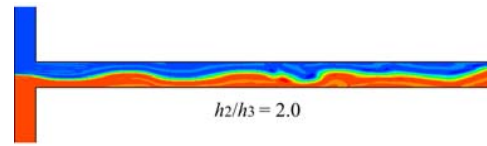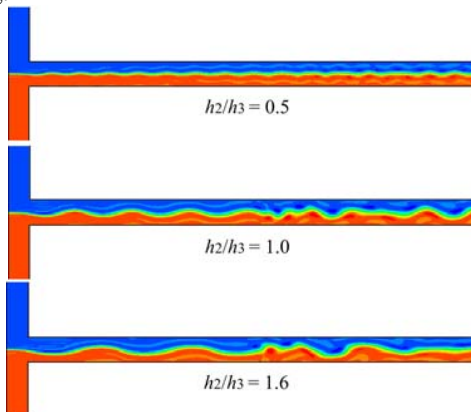

Figure 4. Species concentrations for the mixing microchannel with the different ratio of the no-slip length h_2 to the import length h_3 when the ratio β (h_1/h_2) of 1.6.

To further study the effect of the surface pattern on mixing behavior, Figure 5 shows the visualized species density contour at $h_2/h_3 = 1.0$ with different ratio of hydrophobic to hydrophilic length, β. Similar to Figure 4, when β is lower, the mixing is weaker; with increasing β, the mixing behavior is apparently enhanced.
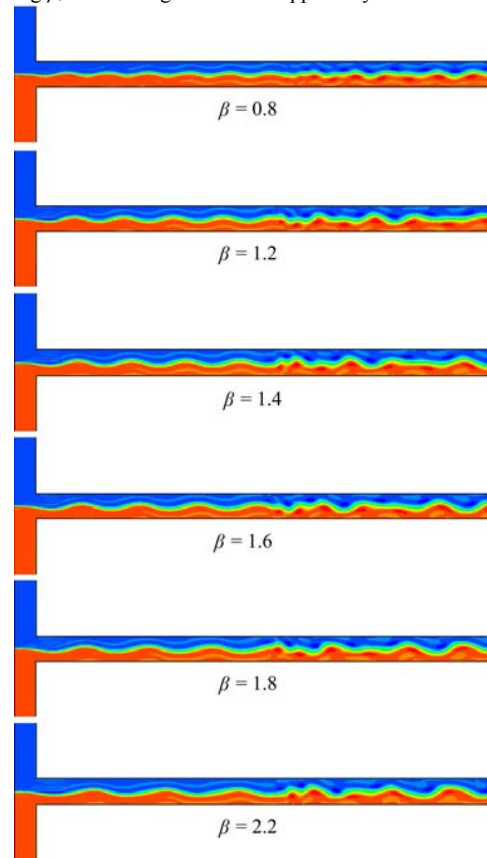

Figure 5. Influence of patterned composite boundary on the species concentration in the mixing microchannel with the different the ratios β (h_1/h_2).

To quantify the mixing behavior, we use the oscillating velocity ratio between y-direction velocity root-mean-square value and inlet velocity ($U_{y\text{-RMS}}/U_{\text{in-mean}}$) to express the fluid mixing intensity. The velocity root-mean-square is defined

$$U_{y-RMS} = \sqrt{\frac{\sum\left(U_y - \bar{U}_y\right)^2}{n}} \quad (11)$$

Figure 6 shows the variation of the oscillating velocity ratio ($U_{y\text{-RMS}}/U_{\text{in-mean}}$) along the centerline of the micro channel with different surface pattern parameters. Generally, when $h_2/h_3 < 1.0$, the oscillating velocity ratio is quite low, indicating a weak mixing behavior. With $h_2/h_3 = 1.0 \sim 1.6$, the oscillating velocity ratio reaches its maximum; when further increasing h_2/h_3 to 2.0, the oscillating velocity ratio decreases apparently. This indicates that $h_2/h_3 = 1.0 \sim 1.6$ is the optimum ratio.
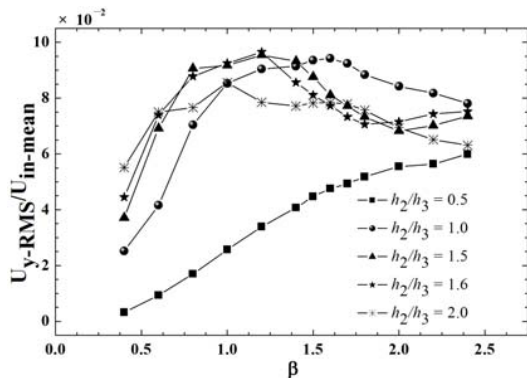
Figure 6. Variation of oscillating velocity with the ratio of hydrophobic to hydrophilic length, $\beta = h_1/h_2$, at different ratio of no-slip length to entrance width, h_2/h_3.

The ratio between hydrophobic and hydrophilic length, β, is also crucial to the micro mixing behavior. When $h_2/h_3 = 1.0$, i.e., the hydrophilic length is the same as the entrance width, the oscillating velocity ratio reaches the maximum at $\beta = 1.6$. It is interesting to note, with increasing h_2/h_3, the maximum oscillating velocity ratio occurs at lower surface pattern ratio β. For example, when $h_2/h_3 = 1.5$ and 1.6, the optimum β is around 1.2.
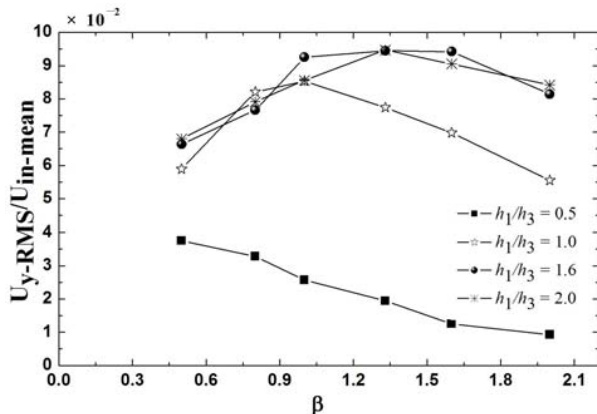

Figure 7. Variation of oscillating velocity with the ratio of hydrophobic to hydrophilic length, $\beta = h_1/h_2$, at different ratio of slip length to entrance width, h_2/h_3.

From the discussion of Figure 6, it seems that the golden mean (1.618) plays some role in micro mixing enhancement. To further evaluate the effect of this optimum number, the effect of hydrophobic length is also studied. Figure 7 shows the variation of the oscillating velocity ratio ($U_{y-RMS}/U_{in-mean}$) along the centerline of the micro channel with β at different ratio of hydrophobic length to entrance width. It is surprising to note, when the ratio of hydrophobic length to entrance width is 1.6, $h_1/h_3 = 1.6$, the velocity oscillation reaches its maximum within a quite wide range of β (= 1.0 ~ 1.6). At other h_1/h_3 ratio, the oscillating velocity is either lower or reaches the maximum within a very narrow band of β. For example, at $h_1/h_3 = 2.0$, the oscillating velocity reaches its maximum at only $\beta = 1.3$; at $h_1/h_3 \leq 1.0$, the oscillating velocity becomes apprantly lower. This indicates that the golden mean number 1.618 is the optimum surface pattern parameter in micro mixing. The most likely explanation of this amazing phenomenon is that the slip perturbation on the wall can be delivered to the middle within just $1.6h_3$, if the slip section is shorter, the perturbation can not be developed fully; if the slip section is longer,

then the perturbation from both sides would interact and suppress each other.

5 Conclusion

The binary fluid mixing in a microchannel is numerically studied using lattice Boltzmann method. To enhance the micro mixing, the surface pattern is designed as alternatively hydrophobic and hydrophilic conditions. The simulation results lead to following conclusions:
(1) The composite boundary conditions can enhance the micro mixing effectively. The entrance width, the hydrophobic and hydrophilic length together with their ratios has significant influence on the micro mixing.
(2) There exist the optimum ratios between the hydrophilic length and the entrance width, i.e., when this ratio, $h_2/h_3 = 1.0 \sim 1.6$, the oscillation velocity ratio can reach its maximum value.
(3) The golden mean number is the optimum ratio between hydrophobic length and entrance width, in which the micro mixing can be enhanced significantly.
(4) The ratio between hydrophobic and hydrophilic length, β, is also crucial, the optimum ratio β may vary with different h_2/h_3.

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