

A NOVEL MICROFLUIDIC MIXER USING APERIODIC CIRCULATION PERTURBATIONS

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ABSTRACT

This paper investigates the mixing enhancement of electrokinetically driven flow in a microchannel with aperiodically spatiotemporal variation in heterogeneous zeta potential. Numerical simulations are performed to analyze the effects of the heterogeneous zeta potential on the fluid flow characteristics in the microchannel and the corresponding mixing performance. In this simulation, aperiodic oscillating sources are derived using the Sprott system. By variation of the scaling factor in the Sprott system, an aperiodic oscillating source of adjustable frequency can obtain to modulate the heterogeneous zeta potential over time. The results indicate that the alternate flow circulations induced by the heterogeneous zeta potential are generated over time within the microchannel to stir the species. This mixing scheme proposed in the study provides an effective mixing performance.

Keywords: Micromixer, Active mixing, Electroosmotic flow

INTRODUCTION

Rapid and efficient species mixing is a crucial key in microfluidic applications, such as biological and chemical analysis, drug delivery, DNA hybridization and so on. However, due to the small characteristic scale of microfluidic devices, fluid flow is constrained to the low Reynolds number region. As a result, the flow is laminar and species mixing occurs primarily by the diffusive effect. In the absence of turbulence, species mixing by the laminar flow is very difficult and requires very long mixing length and mixing time. The mixing result cannot be practically applied to microfluidic systems. Hence, a highly efficient mixing device must be developed to support fast analytical processes in microfluidic systems.

In the literature, various mixing approaches used to ensure efficient species mixing have been proposed. These proposed mixing schemes can be categorized roughly as either passive or active. Passive mixing techniques improve species mixing

utilizing geometrical advantages. Typical passive micromixers include the staggered herringbone mixer [1], the three-dimensional serpentine mixer [2], the split-and-recombine mixer [3], the wave configuration mixer [4] and others.

NOMENCLATURE

C	[molm ⁻³]	Species concentration
C_0, C_∞	[molm ⁻³]	Species concentration in completely unmixed and perfectly mixed statuses, respectively
D	[m ² s ⁻¹]	Diffusion coefficient
e	[C]	Charge of an electron
E	[Vm ⁻¹]	Electric field
k	[-]	Scaling factor
k_b	[JK ⁻¹]	Boltzmann constant
F_E	[Nm ⁻³]	Electrokinetic driving body force
n	[-]	Normal direction
n_0	[m ⁻³]	Bulk ionic concentration
P	[Pa]	Pressure
P_i	[-]	Parameters of the Sprott system
t	[s]	Time
T	[K]	Absolute temperature
u, v	[ms ⁻¹]	Velocity components
V	[ms ⁻¹]	Velocity
V_{slip}	[ms ⁻¹]	Helmholtz-Smoluchowski velocity
W	[m]	Width of channel
x_i	[-]	Oscillatory sources
z	[-]	Ionic valence
Special characters		
ϵ	[-]	Dielectric constant
ϵ_0	[Fm ⁻¹]	Permittivity of vacuum
ϕ	[V]	Applied electrical potential
η_m	[%]	Mixing efficiency
μ	[Nsm ⁻²]	Viscosity
ρ	[kgm ⁻³]	Density
ψ	[V]	Potential due to the charge at the wall
ζ, ζ_h	[V]	Homogeneous and heterogeneous zeta potential
ζ_w	[V]	Zeta potential
Subscripts		
in		Inlet of channel
out		Outlet of channel

2 Topics

Compared to passive mixing schemes, active mixing strategies utilize external driving forces or external mechanical components to perturb the species and thus to achieve the enhancement of mixing effect. Many active mixing techniques have been proposed to mixing the species utilizing time-dependent pressure fields [5] or time-varying externally-applied electric fields [6, 7]. Under appropriate operation conditions, these proposed actively mixing schemes can effectively improve the mixing performance in microfluidic systems.

In electroosmotic flow (EOF), applying the heterogeneous zeta potential to the local wall surfaces to alter the surface properties is also an effective method for enhancing the mixing effect. Many studies have demonstrated that utilizing constant heterogeneous zeta potential [8, 9] or using time-varying heterogeneous zeta potential [10, 11] to local wall surfaces can perturb the flow fields to improve the mixing performance.

The vast majority of the active mixing schemes in the literature mix the species using a periodic perturbation source of some kind. By contrast, the utilization of the aperiodic or random perturbation source has seldom considered. Accordingly, in an attempt to improve the mixing performance in microfluidic systems, the aperiodic oscillations are utilized to perturb the species. In the study, the nonlinear Sprott system [12] is used to generate the aperiodic oscillating sources. In the proposed mixing scheme, the zeta potential on the heterogeneous charge surfaces is varied over time according to the oscillatory behaviors of Sprott system. A series of aperiodically alternate circulation structures induced by the heterogeneous zeta potential are generated over time to stir the species to improve the mixing performance. The validity of the proposed approach is verified numerically. The effects of heterogeneous zeta potential on the fluid flow characteristics and the corresponding mixing performance are examined to prove the effectiveness of the proposed mixing approach.

MATHEMATICAL FORMULATION

Figure 1 illustrates the geometric configuration of the microfluidic mixer considered in the present investigations. In the model, W represents width of the channel, L is the total length of the channel, L_{mix} is the length of the mixing region, L_i is the length of the injection channel, and L_{het} and L_{hom} are the length of the heterogeneous and homogeneous charge patterns in the mixing region, respectively.

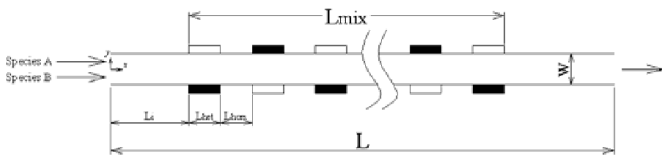


Figure 1 Schematic illustration showing microfluidic mixer configuration. Note that the filled and unfilled blocks are heterogeneous surface patterns. The microchannel includes ten-pair heterogeneous charge patterns within the mixing region.

GOVERNING EQUATIONS

In the current analysis, the governing equations are simplified by making the following assumptions: (i) the flow field is two-dimensional; (ii) the aqueous solutions flowing through the microchannel are incompressible, Newtonian liquids; (iii) the gravitational and buoyancy effects in the fluid flow are ignored; (iv) the two mixing species have the same constant diffusion coefficient; (v) no chemical reactions take place; and (vi) the Joule heating effects are neglected. The various governing equations used to describe the electroosmotic flow are as follows.

POISSON-BOLTZMANN EQUATION

According to electrostatics theory, the electrical double layer (EDL) potential distribution can be described by the Poisson-Boltzmann equation. When symmetric electrolytes are used, the Poisson-Boltzmann equation is given by

$$\nabla^2 \psi = \frac{2n_0 z e}{\epsilon \epsilon_0} \sinh\left(\frac{z e}{k_b T} \psi\right) \quad (1)$$

where ψ is a potential due to the charge at the walls.

LAPLACE EQUATION

The distribution of the externally-applied electric field in a microchannel is described by the following Laplace equation

$$\nabla^2 \phi = 0 \quad (2)$$

where ϕ is the applied electrical potential.

NAVIER-STOKES EQUATIONS WITH ELECTROKINETIC DRIVING BODY FORCE TERM

The modified Navier-Stokes equations incorporating an electrokinetic driving body force term have the form

$$\nabla \cdot \vec{V} = 0 \quad (3)$$

$$\rho \left[\frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \nabla) \vec{V} \right] = -\nabla P + \mu \nabla^2 \vec{V} + \vec{F}_E \quad (4)$$

where \vec{V} is the velocity vector with u - and v -components in the axial and vertical directions, respectively; P is the pressure; \vec{F}_E is the electrokinetic driving body force and is given as

$$\vec{F}_E = 2n_0 z e \sinh\left(\frac{z e}{k_b T} \psi\right) \nabla(\psi + \phi).$$

CONCENTRATION DISTRIBUTION EQUATION

In electroosmotic flow applications, assuming that the electrophoretic effect is sufficiently small to be neglected, the species transport can be described by the following convection-diffusion equation:

$$\frac{\partial C}{\partial t} + (\vec{V} \cdot \nabla) C = D \nabla^2 C \quad (5)$$

where C is the species concentration.

INITIAL AND BOUNDARY CONDITIONS

In this work, in the initial state, the velocity is assumed to be static throughout the microchannel, and species A and B are assumed to have filled the upper and lower microchannels, respectively. In boundary conditions, a constant electric field is applied along the microchannel, and homogeneous and heterogeneous zeta potential are applied to homogeneous and heterogeneous charge patterns on the wall surfaces, respectively. The initial and boundary conditions are specified as

Initial conditions

$$\vec{V}^* = 0, \quad C^* = \begin{cases} 1 & \text{in upper channel} \\ 0 & \text{in lower channel} \end{cases} \quad (6a)$$

Boundary conditions

Inlet

$$\phi = \phi_{in}, \quad \nabla \vec{V} \cdot \vec{n} = 0, \quad P = 0, \quad C = C_{in} \quad (6b)$$

Outlet

$$\phi = \phi_{out}, \quad \nabla \vec{V} \cdot \vec{n} = 0, \quad P = 0, \quad \nabla C \cdot \vec{n} = 0 \quad (6c)$$

Wall surfaces

$$\nabla \phi \cdot \vec{n} = 0, \quad \vec{V} = \vec{V}_{slip}, \quad \nabla C \cdot \vec{n} = 0 \quad (6d)$$

where ϕ_{in} and ϕ_{out} are the electric potential applied at the inlet and outlet, respectively; \vec{V}_{slip} is the Helmholtz-Smoluchowski slip velocity and is defined as $\vec{V}_{slip} = -\frac{\epsilon\epsilon_0\zeta_w}{\mu}E$ [13]; ζ_w is zeta potential on the wall surface; E is the electric field; C_{in} is the species concentration in the inlet and is given as $C_{in} = 1$ and 0 for species A and B, respectively; and n denotes the normal direction to the surface. Note that ζ_w is given as $\zeta_w = -|\zeta|$ and $\zeta_w = \pm|\zeta_h|$ to homogeneous and heterogeneous charge patterns, respectively. The ζ_h is a time-varying zeta potential and it is introduced as described next section.

OSCILLATORY SOURCES

In this study, to stir effectively the species, aperiodic circulation perturbations induced by the heterogeneous zeta potential are utilized to enhance the mixing performance. The aperiodic oscillating sources can be generated by using the nonlinear Sprott system. The system can be expressed as [12]

$$\dot{x}_1 = kx_2 \quad (7a)$$

$$\dot{x}_2 = kx_3 \quad (7b)$$

$$\dot{x}_3 = k[-p_1x_1 - p_2x_2 - p_3x_3 + p_4\text{Sign}(x_1)] \quad (7c)$$

where x_1 , x_2 , and x_3 are the oscillatory sources, $p_1 = 1.2$, $p_2 = 1.0$, $p_3 = 0.6$, and $p_4 = 2.0$ are the parameters of the system, and k is the scaling factor. Note that the Sprott system can be solved by using the Runge-Kutta algorithm. When the initial values are given as $(x_1, x_2, x_3) = (0.1, 0.1, 0.1)$, the oscillatory orbit of x_1 is shown in Figure 2. It can be seen that

the oscillatory frequency of x_1 can be controllable via the variation of the scaling factor.

Utilizing the oscillatory orbit of x_1 above, the variation of the zeta potential on heterogeneous charge surfaces over time is set as (see Fig. 1)

Figure 2 Oscillatory orbits

2 Topics

On filled blocks

$$\zeta_w = \begin{cases} -|\zeta_h| & \text{if } x_1 > 0 \\ +|\zeta_h| & \text{if } x_1 < 0 \end{cases} \quad (8a)$$

On unfilled blocks

$$\zeta_w = \begin{cases} +|\zeta_h| & \text{if } x_1 > 0 \\ -|\zeta_h| & \text{if } x_1 < 0 \end{cases} \quad (8b)$$

Accordingly, an aperiodically time-varying zeta potential of an adjustable frequency can be produced and applied to the heterogeneous charge surfaces.

NUMERICAL METHOD

With the corresponding initial and boundary conditions, this study adopts a numerical approach to solve the governing equations in Eqs. (2)-(5) by using the finite-volume method [14]. Notably, in this study, it is assumed that the thickness of the EDL is very thin than the characteristic length of the microchannel. The Helmholtz-Smoluchowski slip velocity is valid to character the electroosmotic velocity near the wall surfaces [13]. In other words, the flow characteristic within the EDL is neglected and the Helmholtz-Smoluchowski slip velocity is applied to replace the flow characteristic within the EDL. As an assumption, the electrokinetic body force term in Eq. (4) is omitted, and it is unnecessary to solve the Poisson-Boltzmann equation in Eq. (1). In the discrete process, the transient time term is treated using one-order Euler method, and the nonlinear convection terms in Eqs. (4) and (5) are discretized using a second-order scheme. The SIMPLE C algorithm [15] is utilized to couple the velocity and pressure fields. The discretized algebraic equations are then solved numerically using the TDMA (tridiagonal matrix algorithm) iteration scheme. Note that prior to the simulations, a grid-sensitivity analysis was performed to establish a suitable mesh size and time step to yield a satisfactory numerical accuracy.

MIXING EFFICIENCY

To quantify the mixing performance, the mixing efficiency (η_m) in any cross-section of the microchannel was computed as follows. [8]

$$\eta_m = \left[1 - \frac{\int_{-W/2}^{W/2} |C - C_\infty| dy}{\int_{-W/2}^{W/2} |C_0 - C_\infty| dy} \right] \times 100\% \quad (9)$$

where C is the species concentration across the width of the channel; C_∞ is the species concentration with perfect mixing, and C_0 represents the species concentration under the completely unmixed condition.

RESULTS AND DISCUSSION

The model that is presented in Fig. 1 is applied to perform a series of numerical simulations to study the effects of the heterogeneous zeta potential on fluid flow characteristics and the corresponding mixing performance. In the simulations, the width of the channel is specified as $W = 50 \mu m$, the length of

the injection channel is $L_i = 10W$, and the length of a homogeneous charge surface in the mixing section is $L_{\text{hom}} = 0.5W$. The intensity of externally applied electric field is taken as $E = 200V/cm$. The zeta potential on wall surfaces is assumed to be $\zeta = -75mV$ except the heterogeneous charge patterns.

Figure 3 illustrates the flow streamlines within the microchannel. It can be seen that a series of circulation structures near the heterogeneous surfaces are generated via the application of a heterogeneous zeta potential on the heterogeneous charge patterns. In electroosmotic flow, an electrokinetic driving force is produced by the interaction between the EDL potential and the externally applied electric field. The electrokinetic driving force acts only on the fluid near the wall. The bulk fluid is moved via a momentum coupling effect with the driven flow near the wall surfaces. When externally applied electric potentials are constant across the two ends of the microchannel and the zeta potential on all wall surfaces are homogeneous, the direction of electrokinetic driving force is the same near the wall surfaces to drive the fluid. The results indicate that circulation phenomenon is not occurred within the microchannel. Assuming that the externally applied electric field is constant along the microchannel and the heterogeneous zeta potential is applied to local wall surface, the direction of fluid movement near these heterogeneous charge surfaces is opposite to the homogeneous charge surfaces. As a result, the interaction of these local flow fields with the bulk flow induces local flow circulations in the vicinity of the heterogeneous surface to satisfy the continuity condition. Therefore, when time-varying zeta potential applies to the heterogeneous charge surfaces, the circulation structures near these heterogeneous surfaces are generated repeatedly to stir the species.

(a)

(b)

Figure 3 Flow streamlines. (a) The zeta potential on the filled blocks is given as $\zeta_w = -|\zeta_h|$ and the zeta potential on the unfilled blocks is set as $\zeta_w = +|\zeta_h|$, and (b) the zeta potential on the filled blocks is given as $\zeta_w = +|\zeta_h|$ and the zeta potential on the unfilled blocks is set as $\zeta_w = -|\zeta_h|$. Note that ζ_h is taken as $\zeta_h = 75mV$.

In general, in microfluidic systems, because fluid flow is constrained to the low Reynolds number region, the generation of the circulation phenomenon is very difficult. Utilizing the characteristics of EOF, the circulation phenomenon can be generated by altering local surface properties under an application of a constant electric field. In this study, heterogeneous zeta potential is applied to heterogeneous charge surfaces to generate a series of circulation structures within the mixing region. These flow recirculations capture local species to stir them within the circulation regions. When the recirculations change their directions, a portion of the mixed species is mixed with unmixed species by other circulation structures. Therefore, the species can be stirred repeatedly. Consequently, utilizing the aperiodic oscillating source to generate a series of random-like perturbation behaviors, the species can be effectively stirred to greatly enhance the mixing performance in the proposed mixing scheme.

To further understand the mixing performance in the microchannel, Fig. 4 plots the evolution over time of the mixing efficiency at the position $x = 2000\mu\text{m}$. Because the variation over time of the circulation structures is aperiodic, the species can be stirred irregularly within the mixing region. Therefore, it can be seen that the evolution over time of the mixing efficiency is random. At lower values of the scaling factor, because the oscillatory frequency is slower, the alternative frequency of the circulation structures within the microchannel takes place more slowly. The local unmixed species can be not captured by the circulation structures. Therefore, the local unmixed species can be unperturbed by these circulation structures and pass through directly the microchannel. As a result, the mixing performance can be lower. As increase the scaling factor, a rapider perturbing frequency is generated. As a result, local unmixed and mixed species can be stirred fast by these alternate circulation structures within the mixing region to enhance the mixing performance. Hence, a more effective mixing performance is produced. Consequently, an appropriate perturbing region to the oscillatory source can enhance greatly the species mixing.

CONCLUSION

This paper presents a novel microfluidic mixing scheme in which species are mixed by applying aperiodically spatiotemporal variation in heterogeneous zeta potential within a microchannel. In the proposed mixing scheme, the Sprott system is utilized to generate an aperiodic oscillating source of adjustable frequency and the source is applied to vary the zeta potential on the heterogeneous charge surfaces. Numerical simulations are performed to analyze the influences of the aperiodically heterogeneous zeta potential on the fluid flow characteristics and corresponding mixing performance. The simulation results have shown that alternative circulation structures induced by the variation of the heterogeneous zeta potential are generated near the heterogeneous surfaces over time to stir the species. The results have demonstrated that the proposed mixing scheme herein can effectively enhance the mixing performance within microfluidic systems.

Figure 4 Evolution of mixing efficiency at $x = 2000\mu\text{m}$ as function of time.

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