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NUMERICAL SIMULATION OF AN ELECTROOSMOTIC MICROMIXER

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ABSTRACT

We present a micromixer fabricated using MEMS technology which takes advantage of electroosmosis to mix fluids. A time dependent electric field is applied and the resulting electroosmosis perturbs the low Reynolds number flow. It is shown that the electric field can be deemed quasi-steady and the electroosmotic slip boundary condition can be applied when the incompressible Navier Stokes equation is solved. Both the electric field and the electroosmotic flow are simulated numerically. Study of the particle traces shows folding and stretching of material lines, and a positive Lyapunov exponent is found which indicates chaotic-like mixing.

INTRODUCTION

The ability to mix two or more fluids thoroughly and in a reasonable amount of time is critical to the creation of fully integrated "on-chip" micro-electromechanical fluid processing systems. But mixing in micron sized channels is difficult due to the low Reynolds numbers that characterize these flows. The flow is restricted to the laminar flow region and there is no turbulence which could assist the mixing. If we rely only on molecular diffusion to mix the fluids, the mixing channel must be extended to be extremely long.

To achieve fast mixing, several passive micromixers have been developed and studied, such as the T-type [1], L-shaped [2],

serpentine pipe [3], flow splitting [4], ridged-floor mixer [5] and so on. They do not improve mixing significantly, and need to be fabricated delicately. A few active micromixers have also been demonstrated. A mixing chamber mimicking a source/sink system [6] is designed to stir fluids effectively using microfabricated valves and phase-change liquid micropumps. Pressure disturbances from side channels have also been added to microchannel flows to enhance mixing [7, 8]. Encouraging progress in enhancing mixing has been reported.

In the past two decades it has been demonstrated that chaos can be used to mix fluids in laminar flows [9], and the chaotic regimes are associated with stretching and folding of material lines [10]. Chaos may arise in a nonlinear dynamical system provided that the system has at least three dimensions. Adding a time dependent external perturbation to a two dimensional flow provides the third dimension, and chaotic mixing may arise.

Here we present a silicon microfabricated mixer with no moving parts, which makes use of time dependent electroosmotic flow to mix two fluids. Numerical simulation is carried out to help understand the mixing of fluids in this micromixer.

DESCRIPTION OF THE MIXER

The geometry of our electroosmotic micromixer is shown in Figure 1. It takes two fluids from different inlets and combines them into a single channel which is $10\mu m$ wide. The fluids then enter the central loop with the inner and outer radii being

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5 μm and 15 μm respectively. Four microelectrodes are positioned on the outer wall of the central loop at angular positions 45°, 135°, -45°, and -135°. These microelectrodes impose a spatially varying electric field, and the fluids are manipulated via the electroosmotic slip boundary condition before they enter the outlet channel. Electric potentials on the microelectrodes are also time dependent, which adds the third dimension necessary for chaotic mixing. The aspect ratio (channel depth over channel width) is 5 : 1, which validates our 2-D assumption in the numerical simulation.

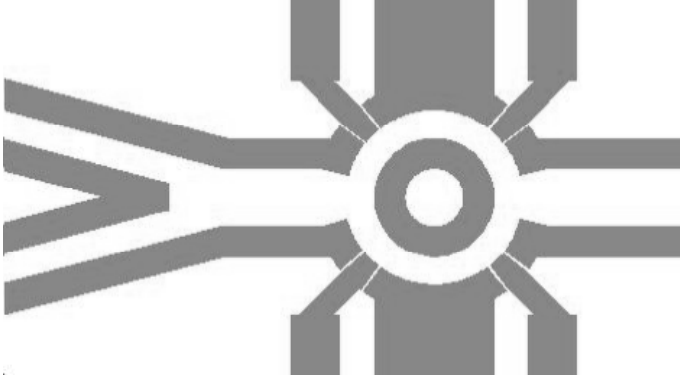


Figure 1. Geometry of the micromixer

FABRICATION

The micromixer is built on a silicon wafer using lithographic and deep etching technique. A Scanning Electron Microscope (SEM) picture of the micromixer is shown in Figure 2. To obtain a sufficiently high aspect ratio of the microelectrodes, heavily Boron doped silicon is used as the fabrication material. SOI (Silicon On Insulator) wafer is used to isolate the device from the substrate bulk material. The surfaces are thermally grown silicon dioxide (quartz), and exhibit a zeta potential when brought into contact with the fluid. The gap between the electrode and the wall is also filled by the thermally grown silicon dioxide.

MATHEMATICAL MODEL

The fluid motion is governed by the incompressible Navier Stokes equation

$$\rho \left[\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right] = -\nabla p + \mu \nabla^2 \mathbf{V} + \rho_e \mathbf{E}, \quad (1)$$

where ρ_e is the electric charge density, and $\mathbf{E}$ is the electric field intensity. $\mathbf{E}$ is related to the electric potential Φ by

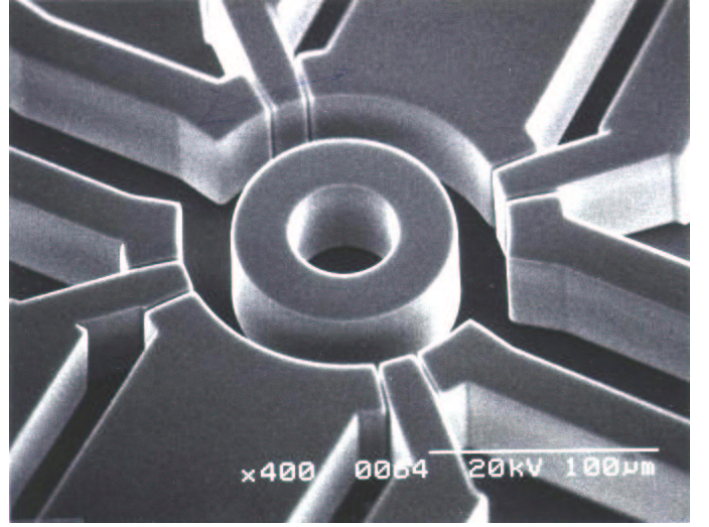


Figure 2. SEM picture of the micromixer

$$\mathbf{E} = -\nabla \Phi, \quad (2)$$

and Φ is governed by the Poisson equation

$$\nabla^2 \Phi = -(\rho_e / \epsilon), \quad (3)$$

where the permittivity ϵ of the medium is equal to the permittivity ϵ_0 of a vacuum multiplied by the dielectric constant (also known as the relative permittivity) ϵ_r . Substituting Equation 2 and Equation 3 into Equation 1, we obtain

$$\rho \left[\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right] = -\nabla p + \mu \nabla^2 \mathbf{V} + \epsilon [\nabla^2 \Phi \cdot \nabla \Phi]. \quad (4)$$

Equation 2 and Equation 3 can be simplified further to obtain a more solvable form. The charge density ρ_e is given by

$$\rho_e = F \sum_i z_i c_i, \quad (5)$$

and the ionic concentration of species i , c_i , is given by the Boltzmann distribution

$$c_i = c_{i\infty} \exp \left(-\frac{z_i F \Phi}{RT} \right), \quad (6)$$

where F is Faraday's constant, R is the gas constant, T is the temperature, z_i is the charge number of species i , and $c_{i\infty}$ is the average concentration of species i . Substituting Equation 6 and Equation 5 into Equation 3, we obtain

$$\nabla^2 \Phi = -\frac{F \sum_i z_i c_i}{\epsilon} = -\frac{F}{\epsilon} \sum_i z_i c_{i\infty} \exp\left(-\frac{z_i F \Phi}{RT}\right). \quad (7)$$

Under the Debye-Hückel approximation [11], $z_i F \Phi \ll RT$, we can expand the exponential term as

$$\exp\left(-\frac{z_i F \Phi}{RT}\right) \approx 1 - \frac{z_i F \Phi}{RT}. \quad (8)$$

Since $\sum_i z_i c_{i\infty} = 0$ (to preserve electroneutrality in the bulk electrolyte), Equation 7 becomes

$$\nabla^2 \Phi = \frac{\Phi}{\lambda_D^2}, \quad (9)$$

where the Debye length λ_D is given by

$$\lambda_D = \left(\frac{\epsilon RT}{F^2 \sum_i c_{i\infty} z_i^2}\right)^{1/2}. \quad (10)$$

Combining Equation 3 and Equation 9, we obtain the following expression for the charge density

$$\rho_e = -\epsilon \frac{\Phi}{\lambda_D^2}. \quad (11)$$

When the Debye length is small (typically 10nm) and the ζ potential is not large (typically 0.1V), the distribution of charged species near the wall is governed mainly by the ζ potential, and is affected very little by the external electric field [12]. The charge, and hence the potential, distribution near the wall can be determined independent of the external electric field. The effect of the fluid motion on the charge distribution can also be neglected when the fluid velocity is small, i.e., when the inertial terms in the momentum equation are not dominant or when the Debye length is small. Under these assumptions, the electric field and the fluid field can be decoupled, and the potential Φ can be decomposed into a potential due to the external electric field ϕ , and a potential due to the ζ potential ψ

$$\Phi = \phi + \psi, \quad (12)$$

where ψ is determined by Equation 9, and ϕ is determined by

$$\nabla \cdot (\epsilon \nabla \phi) = 0, \quad (13)$$

when the spatial charge density is zero in the bulk of the fluid.

Thus, the fluid velocity inside the electric double layer is governed by

$$\rho \left[\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right] = -\nabla p + \mu \nabla^2 \mathbf{V} + \epsilon \nabla^2 \psi E, \quad (14)$$

where the electric field intensity E is given by

$$E = -\nabla \phi. \quad (15)$$

If the Debye length is small compared with the channel width, then the curvature terms can be neglected and Equation 14 reduces to the one-dimensional form appropriate to the electroosmotic flow past a long plane channel

$$\mu \frac{\partial^2 u}{\partial y^2} = \epsilon \frac{\partial^2 \psi}{\partial y^2} E_x, \quad (16)$$

where x and y are the coordinates along and normal to the channel wall.

Integrating Equation 16 twice with boundary conditions $\psi = \zeta$ at $u = 0$ and $\partial u / \partial y = \partial \psi / \partial y = 0$ at $y \rightarrow \infty$, we obtain the slip velocity at the edge of the electric double layer

$$U_{slip} = -\frac{\epsilon \zeta E_x}{\mu}. \quad (17)$$

This is known as the Helmholtz-Smoluchowski equation [11]. The velocity “slips” at the wall, and the fluid moves as in plug flow, assuming the double layer thickness is very small compared with the characteristic length, say $d/\lambda_D \gg 100$.

In the bulk of the fluid (outside the electric double layer), ψ vanishes, and the fluid motion is governed by the Navier Stokes equation

$$\rho \left[\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right] = -\nabla p + \mu \nabla^2 \mathbf{V}, \quad (18)$$

with the slip boundary condition given in Equation 17.

MODEL VALIDATION

Cummings et al. [13] showed that to apply the Helmholtz-Smoluchowski Equation 17 at the fluid-solid boundaries, the electric field must be at least quasi-steady in order to neglect the transient effects. In other words, the time scale of the unsteady electric field must be much larger than that of the transient flow.

In Stokes' first problem, i.e., the flow due to the impulsive motion of a flat plate parallel to itself, the fluid velocity satisfies

$$\frac{u}{U} = 1 - \operatorname{erf} \left[\frac{y}{2\sqrt{\nu t}} \right]. \quad (19)$$

The similarity solution is shown in Figure 3, where y is the distance from the plate, ν is the kinematic viscosity of the fluid and U is the velocity of the plate.

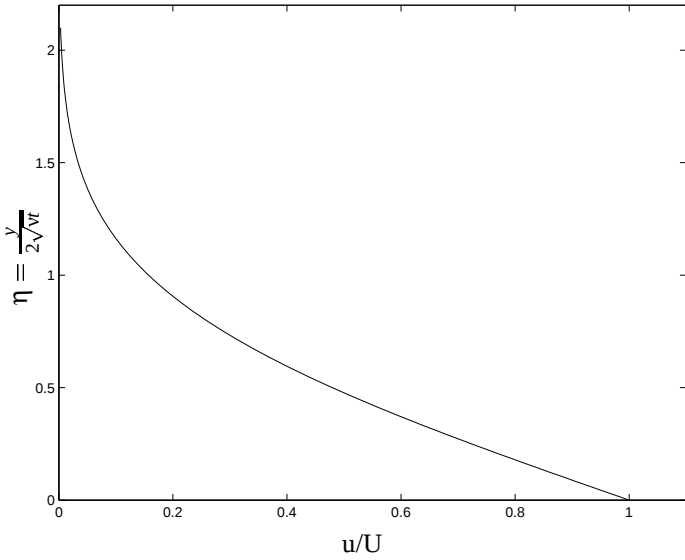


Figure 3. Similarity solution of laminar flow due to an impulsively started flat plate

In this impulsively started flow, the initial vorticity is simply diffused outward, resulting in an increase in the width of flow. We define the characteristic time t_{trans} featuring the transient flow as the time required for u to reach 95% of U across the channel width. From Figure 3, $u/U = 0.95$ corresponds to $\eta = 0.0443$. Therefore

$$\frac{\delta}{2\sqrt{\nu \cdot t_{trans}}} \sim 0.0443, \quad (20)$$

where $\nu = 10 \times 10^{-6} \text{m}^2/\text{s}$ is the kinematic viscosity of the water. $\delta = 10 \mu\text{m}$ is the width of the channel, and of the central loop as

well. Thus we obtain an estimate of the time scale of the transient effect in the micromixer as $t_{trans} = 0.0127 \text{sec}$.

If we apply sinusoidal (in time) electric potentials on the microelectrodes with frequencies between 0.1Hz and 10Hz , the corresponding time scales are between 10sec and 0.1sec . Compared with the time scale of the transient flow, the electric field changes at a much slower rate and can be deemed quasi-steady.

NUMERICAL SIMULATION

Both the electric field and the flow field are solved in FEM-LAB [14]. Equation 13 is solved for the electric potential in a rectangular domain (Figure 4) with insulation boundary conditions on the four sides of the rectangle.

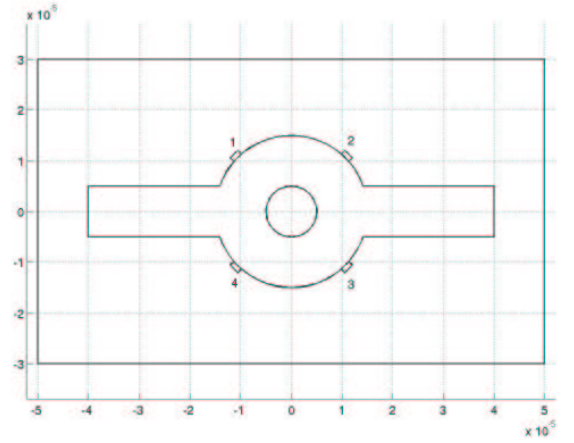


Figure 4. Computational domain

The electric potentials on the four microelectrodes are sinusoidal in time with the same maximum value of 0.1V and the same frequency of 8Hz , but alternate in polarities. Potentials on electrode 1 and electrode 3 are $\phi = \phi_{max} \cos(2\pi ft)$, and potentials on electrode 2 and electrode 4 are $\phi = -\phi_{max} \cos(2\pi ft)$. Water in the channel has a relative permittivity of 78.3. Everywhere else is assumed to be vacuum with the permittivity of $8.854 \times 10^{-12} \text{CV}^{-1}\text{m}^{-1}$.

The incompressible Navier Stokes equation (Equation 18) is solved for the fluid velocity in the mixer, with the slip boundary condition (Equation 17) on the inner and outer wall of the central loop. A ζ potential of 0.1V is used in Equation 17. Water is flowing in from the left and the inlet velocity is parabolic with a mean value of 10^{-4}m/s . Since the microelectrodes must be in contact with the fluid to facilitate ion exchange, silicon dioxide

is removed on the surface of the electrode that is also part of the mixing chamber wall. A no-slip boundary condition is applied on these electrode surfaces. Because the electric field decays exponentially away from the microelectrodes and the slip velocity is proportional to the electric field intensity, we can neglect the slip velocity along the wall of the horizontal inlet and outlet, where a no-slip boundary condition is used.

Figure 5 shows the equal potential contour lines in the central loop region at $t = 0.25\text{sec}$. Fluid streamlines at $t = 0.25\text{sec}$

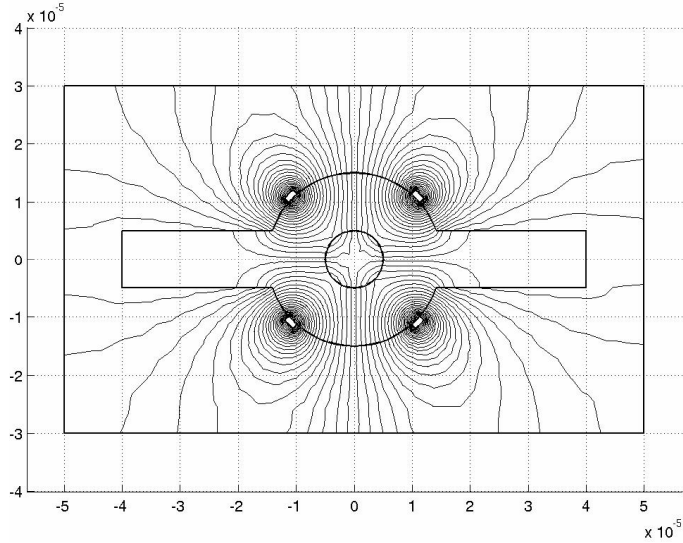


Figure 5. Equal potential contour lines at $t = 0.25\text{sec}$

are shown in Figure 6. We can see that in the central loop the flow splits into domains with eddy rotations separated by separating streamlines near the microelectrodes. A properly chosen time-varying protocol of the actuation will cause the separatrix to break up.

Simulation of the fluid particle trajectories shows that fluid particles stay in the central loop, and experience stretching and folding, for a sufficiently long time before they enter the horizontal outlet. This fact not only indicates chaotic advection, but also facilitates the final stage of mixing: molecular diffusion. Figure 7 depicts this kind of stretching and folding by tracking a small volume of fluid released in a small rectangular box near the channel symmetry axis in the upstream region. We see that this rectangular volume turns into a complicated pattern very quickly. There does exist a set of stretching and folding of material lines in the central loop that is needed for the chaotic mixing.

Lyapunov exponent (LE), as the average exponential rate of divergence of nearby trajectories, can be used to describe chaotic mixing in a quantitative manner. A positive Lyapunov exponent

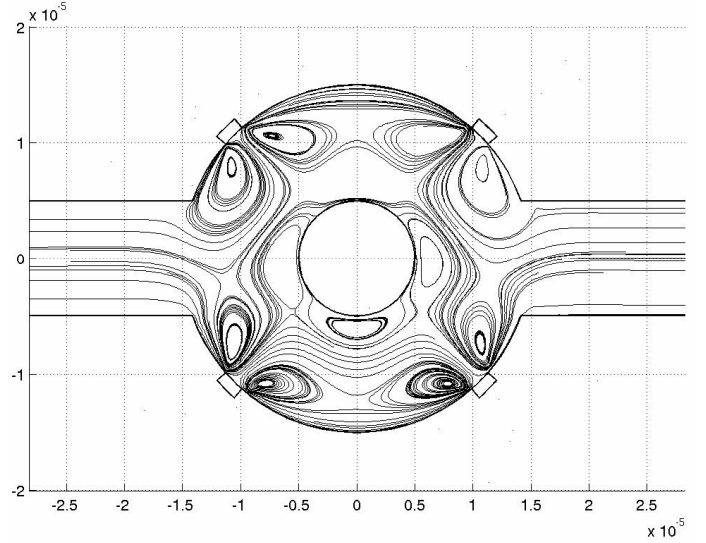


Figure 6. Streamlines at $t = 0.25\text{sec}$

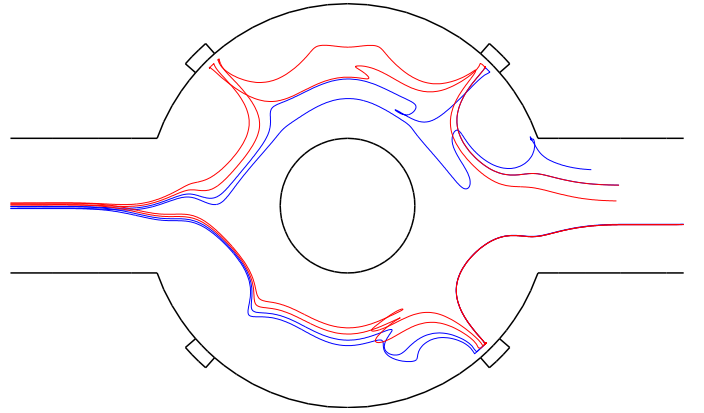


Figure 7. Stretching and folding of a small volume of fluid. Red and blue curves are particle trajectories starting from the upper and lower half of the inlet respectively.

is indicative of chaotic mixing. In Figure 8 we plot $\ln(\delta(t))$ versus t , where $\delta(t)$ is the distance between two nearby particles released near the symmetry axis of the inlet channel. We see that the two particles travel close to each other in the horizontal inlet channel, until they enter the central loop. Then the $\ln(\delta) \sim t$ curve goes up linearly with a positive slope. This positive slope is the Lyapunov exponent. We note that the curve is never exactly straight, having wiggles because the strength of the exponential divergence varies somewhat along the strange attractor. Because of the bounded geometry, the divergence also stops when particles get close to the wall. This explains the leveling off or saturation of the curve in Figure 8.

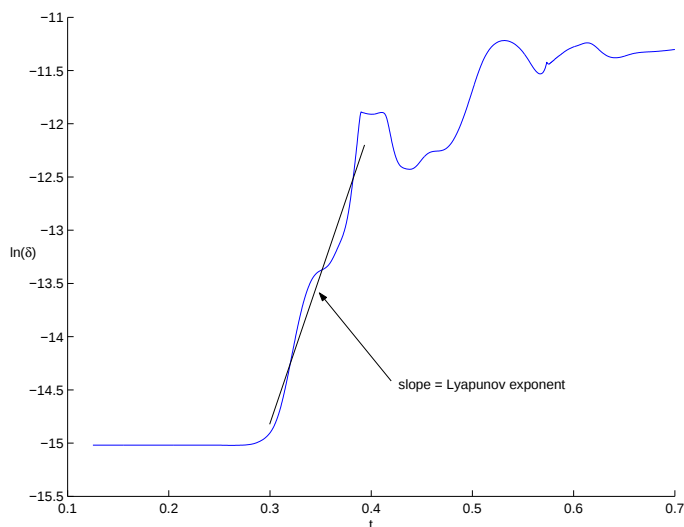


Figure 8. Evolution of the distance between two nearby particles. A positive slope implies an exponential divergence.

CONCLUSIONS

An active electroosmotically actuated micromixer is designed and investigated numerically. The existence of chaotic behavior is demonstrated by the observation of stretching and folding of the material lines. A positive Lyapunov exponent, indicative of chaotic mixing, is found by simulation of particle trajectories and evaluation of the separation rate of neighboring fluid particles. Further investigation is under way to optimize fluid mixing in this micromixer by identifying the proper time-varying electric field. As a part of the future work, numerical results will also be compared with experimental data.

ACKNOWLEDGMENT

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