Numerical visualization and quantification of chaotic mixing for micromixers

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ABSTRACT

We present a systematic way of visualization and quantification of mixing in chaotic micromixers with a periodic mixing protocol. We name it colored particle tracking method, which consists of three steps. One is flow analysis step to obtain periodic velocity field of a periodic mixing protocol. The other is particle tracking step. At the inlet, depending on the species of the fluids, particles are labeled with a specific color. Then, using the initial distribution of colored particles, we repeat integration procedure up to the end period. Finally, from thus obtained particle distribution, we can evaluate mixing performance. In the present study, we propose a new measure of mixing by adopting the concept of the information entropy. We applied the developed method to three micromixers with patterned grooves and were able to evaluate mixing performance both qualitatively and quantitatively.

Keywords: microfluidics, micromixer, chaotic mixing, Galerkin/Least-squares (GLS) method, particle tracking

1 INTRODUCTION

Micromixer has a variety of applications in many biological processes [1]. It is well known that mixing in microchannel is difficult to achieve because most flows in micro scale belong to the regime of creeping flow, in which mixing is dominated by molecular diffusion.

Since early micromixer relies on only molecular diffusion, it takes very long mixing time to mix two different fluids [2]. But one can achieve enhanced mixing by incorporating chaotic advection [3,4]. In chaotic advection, fluid particles exhibit very complex trajectories even in creeping flow regime. Chaotic advection refers to kinematical phenomena in which motion of fluid particles is chaotic in Lagrangian sense even though the velocity field in Eulerian sense is simple. Since chaotic advection is possible to occur in micro scale, it must be a practically attractive mixing mechanism for micromixers. Many researchers have proposed various micromixers incorporating chaotic advection [5-8].

As far as mixing analysis of micromixers is concerned, most of numerical studies regarding micromixers are focused on solving mass transport equation in order to visualize and evaluate mixing performance of micromixers. But there are several drawbacks in this approach. If the deformation of interface is too complicated or the length of channel is too long compared with the dimension of the height or width, the approach mentioned above may not catch the precise interface due to the numerical diffusion and insufficient resolution of discretization for computational domain. For three-dimensional numerical analysis of flow and mass transport, moreover, it needs enormous computational resources and CPU time to carry out mixing analysis for the entire micromixer. Therefore most of mixing analysis did not cover the entire micromixer but is limited to analyze the basic flow characteristics and mixing pattern in a single period or at most two periods.

Micromixers of interest in current work are patterned grooved micromixers. For this kind of micromixers, recently, there have been several theoretical and experimental works [7,8]. More recently, there has been a numerical study for the patterned groove micromixer by Wang *et al* [9]. To investigate the mixing performance of a micromixer clearly, it is required to carry out a numerical analysis for the whole domain. Therefore, it is essential to have an efficient numerical scheme for the entire domain and a quantitative measure of mixing for the evaluation of mixing performance.

The goal of the present work is to develop a systematic way of visualization and quantification of mixing in chaotic micromixers with a periodic mixing protocol. We name it "colored particle tracking method", which consists of three steps: the first is the periodic velocity field analysis; the second is the particle tracking using particles labeled with a specific color depending on the species; and the third is the quantitative measure of mixing from the particle distribution. Finally, we will present the results of the application of the developed numerical method to three patterned groove micromixers.

2 NUMERICAL METHODS

Colored particle tracking will be introduced in this section method as an efficient numerical method for analyzing micromixers with the help of a periodic mixing protocol. It consists of three steps. First, periodic velocity field of repeating mixing protocol is calculated via Galerkin/Least-squares (GLS) method [10]. Second step is the particle tracking. In this step, many particles are tracked using the velocity field obtained from the first step. The essence of this stage is the color labeled to particles according to their species. Since color information of a particle is an intrinsic property, it is possible to measure mixing from the distribution of colored particles at a specific cross section. The final step is the quantification of mixing with a proper measure. A measure of mixing is introduced by using the concept of information entropy. This overall approach is thought to be a general way of analyzing mixing in a micromixer composed of a periodic mixing protocol. The detailed method is described in the following sections.

2.1 Finite element formulation

A steady state, incompressible Stokes equation and boundary conditions are represented by

$$\nabla \cdot (2\mu \mathbf{D}) - \nabla p = 0 \qquad \text{in } \Omega \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{in } \Omega \tag{2}$$

$$\mathbf{u} = 0 \qquad \text{on } \Gamma_\mathrm{w} \tag{3}$$

$$\mathbf{t} = -\Delta p \mathbf{n} + 2\mu \mathbf{D} \cdot \mathbf{n} \qquad \text{on } \Gamma_\mathrm{i} \tag{4}$$

$$\mathbf{t} = 2\mu \mathbf{D} \cdot \mathbf{n} \qquad \text{on } \Gamma_\mathrm{o} \tag{5}$$

where **u** is the velocity, p is the pressure, μ is the viscosity, **D** is the rate of deformation tensor, Δp is the pressure drop within one period, **n** is the outward normal vector to the boundary surface, and **t** is the traction force. In above equations, Ω, Γ_w, Γ_i, and Γ_o denote bounded domain, wall boundary, inlet boundary, and outlet boundary respectively. In addition to boundary conditions described above equations, periodic boundary condition is applied to the set of two corresponding nods, one for inlet and the other for outlet.

$$\mathbf{u_i} = \mathbf{u_o} \quad \text{on } \Gamma_\mathrm{i} \text{ and } \Gamma_\mathrm{o} \tag{6}$$

Since periodic velocity condition is a kind of constraint to be satisfied by the velocity at the inlet and outlet surface, this condition is implemented via Lagrangian multiplier method as follows.

$$\sum \boldsymbol{\lambda} \cdot (\mathbf{u}_i - \mathbf{u}_o) = 0 \tag{7}$$

The final weak form incorporating periodic boundary condition is obtained by adding additional terms due to the Lagrangian multiplier to the original weak form of Galerkin/Least squares (GLS) method. In equation (8), φ is the weighting function for Lagrange multiplier, $\boldsymbol{\lambda}$. By employing GLS method, we can circumvent the compatibility condition of velocity and pressure interpolation function so that equal order interpolation function may be used [10]. In the present finite element formulation, we use tri-linear interpolation function for all variables, **u**, p, and $\boldsymbol{\lambda}$.

$$\begin{aligned} &\int_\Omega 2\mu \mathbf{D}(\mathbf{u}) : \mathbf{D}(\mathbf{v})\, d\Omega \\ &- \int_\Omega p(\nabla \cdot \mathbf{v})\, d\Omega + \int_\Omega (\nabla \cdot \mathbf{u}) q\, d\Omega \\ &+ \sum_k \int_{\Omega_k} (\nabla p - \nabla \cdot (2\mu \mathbf{D}(\mathbf{u}))) \cdot (\boldsymbol{\tau} \nabla q)\, d\Omega_k \\ &+ \sum [\varphi \cdot (\mathbf{u}_i - \mathbf{u}_o) + \boldsymbol{\lambda} \cdot (\mathbf{v}_i - \mathbf{v}_o)] = \int_{\Gamma_i \cup \Gamma_o} \mathbf{t} \cdot \mathbf{v}\, d\Gamma \end{aligned} \tag{8}$$

2.2 Particle tracking

During the particle tracking procedure, one can identify the species of particles by their intrinsic color assigned initially. The problem of tracing the position of particles can be stated as integrating the following equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{u} \tag{9}$$

where **x** is the particle position vector, **u** is the particle velocity, and t is the time. Instead of dealing with the original equation (9), it turns out to be helpful to modify it to a two-dimensional problem as

$$\begin{aligned} \frac{dx}{dz} &= \frac{u}{w} = \tilde{u} \\ \frac{dy}{dz} &= \frac{v}{w} = \tilde{v} \end{aligned} \tag{10}$$

In equation (10), u, v, and w are the velocity component of x, y, and z coordinate, respectively. The 4th order Runge-Kutta method is used to integrate the set of ordinary differential equations.

What we need in integrating equation (10) is the information of velocity at a certain spatial location. In this particular case, velocity field is obtained from the solution of finite element formulation. Therefore velocity data is available at the nodal points. Thus, after searching the element in which a specific particle is located, spatial interpolation is required to find out the velocity at the desired location. Then a particle can be moved to a new position and at that location particle has the information of coordinates and species.

2.3 Measure of mixing

This section presents a way of characterizing mixing performance quantitatively by employing mixing entropy. First, a cross sectional area of micromixer is divided by finite number of cells. Then, for a certain particle configuration of multiple species, the mixing entropy is defined as a sum of the entropy of individual cells constituting the cross sectional area:

$$S = -\sum_{i=1}^{N_c}\left[w_i \sum_{k=1}^{N_s}\left(n_{i,k}\log n_{i,k}\right)\right] \tag{11}$$

In the definition of mixing entropy, equation (11), i is the index for the cell, k is the index for the species, w_i is the weighting factor for the cell, N_c is the number of cells, Ns is the number of species to be mixed, and $n_{i,k}$ is the particle number fraction of the k^{th} species in the i^{th} cell. Since we are dealing with binary fluids mixing in the current study, N_s is 2. Weighting factor, w_i, is devised such that it is set to zero for the cell with no particle at all or having only single species.

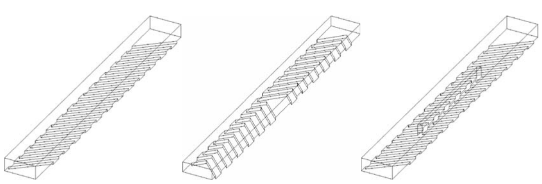
Since the value of mixing entropy itself is not a practically meaningful quantity, degree of mixing (κ) was introduced as a measure of mixing. Degree of mixing (κ) is defined as a normalized entropy difference.

$$\kappa = \frac{S - S_0}{S_{\max} - S_0} \tag{12}$$

In equation (12), S is the mixing entropy of a cross section where κ is evaluated, S_0 is the mixing entropy of inlet particle distribution, and S_{max} is that of uniformly distributed particles. In the case of uniform particle distribution, which is the case of perfect mixing, κ is 1. At inlet, κ is fixed to be 0 by the definition of κ.

3 RESULTS

We applied the developed numerical method to three micromixers. Three micromixers of interest in this study, as depicted in figure 1, are slanted groove micromixer (SGM), staggered herringbone micromixer (SHM), and barrier embedded micromixer (BEM). These micromixers have patterned grooves on their bottom surface in order to induce rotational flow.



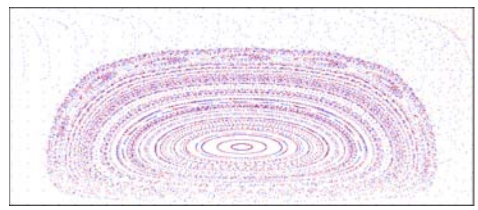
(a) SGM (b) SHM (c) BEM

Figure 1: Geometry of the periodic unit of three micromixers.

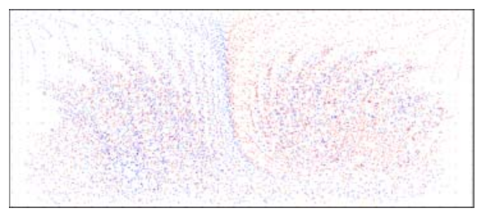
The geometrical parameter of SGM and SHM is from the paper by Stroock *et al* [7]. In the case of BEM [8], the height of barrier is 2/3 of the channel height, thickness of barrier is 20 μm, and the length of barrier is 720 μm, which corresponds to the length of six grooves.

The most important feature of a micromixer is its flow characteristics, which determines final mixing performance. Therefore, accurate velocity field is essential for the mixing analysis by particle tracking. In the particle tracking stage, particles are just the fluid particle; thus there is no interaction between particle and flow so that particles are just convected with the given velocity field of a micromixer.

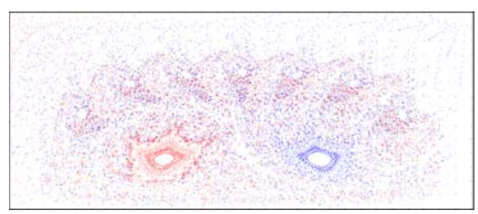
Before mixing analysis via colored particle tracking, Poincaré sections are plotted to examine the dynamical system of three micromixers. As shown in figure 2, chaotic mixing takes place over the most cross section in SHM. In the case of BEM, mixing is also chaotic except two unmixed islands surrounded by KAM. However, in the case of SGM, one can expect that poor mixing will result in.



(a) SGM



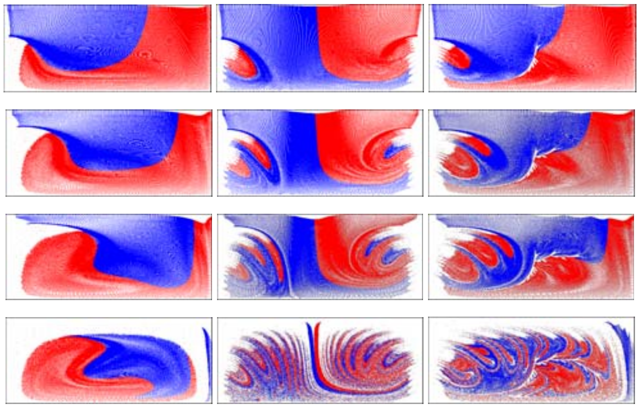
(b) SHM



(c) BEM

Figure 2: Poincaré sections

We carried out colored particle tracking for three micromixers with the velocity solution obtained from finite element method mentioned in previous section. Particles, depending on their species, are labeled with a specific color and the color is inherent to each particle. Therefore, at a certain cross section of micromixer, the configuration of colored particles can reflect the status of mixing both qualitatively and quantitatively. From the distribution of colored particle in figure 3, one can easily figure out the progress of mixing through a micromixer.



(a) SGM (b) SHM (c) BEM

Figure 3: Visualization of mixing; Distribution of colored particles at 1st, 2nd, 3rd, and 10th period. The number of initial particle is 80000 for three micromixers

Now we have the distribution of colored particles at all periods. Accordingly, we can calculate degree of mixing (κ) from equation (12). The change of κ along the down channel direction is plotted in figure 4. As expected from Poincaré sections and colored particle distribution, mixing performance of the SGM is the worst as expected and that of the SHM seems better than BEM of the current design. In the case of SHM and BEM, one can observe a rapid increase of κ and then convergence to an asymptotic value.

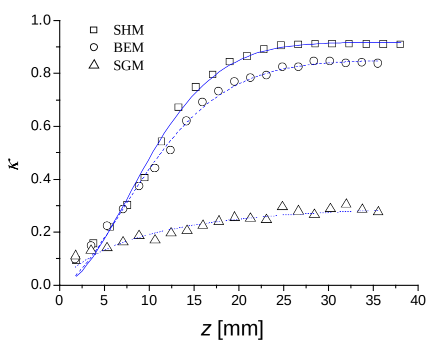


Figure 4: Degree of mixing (κ). κ was plotted to the 20th period for all micromixers.

4 CONCLUSIONS

A systematic way of mixing analysis was proposed to carry out direct numerical simulation of the chaotic mixing in micromixers with a periodic mixing protocol. Instead of solving mass transport equation, colored particle tracking was employed to visualize and quantify the mixing of two different fluids. This colored particle tracking method was applied to three micromixers. From the results of numerical simulation, we were able to obtain the flow characteristics of micromixers and the configuration of colored particles. From thus obtained particle distributions, we could evaluate the mixing performance quantitatively with the new measure of mixing. This method is not limited to a specific geometry but can be applied to general micromixers with a periodic mixing protocol.

Even though two fluids were involved in current study, colored particle tracking method could be extended to the mixing of three or more fluids without loss of generality. Furthermore, this numerical scheme is thought to be a useful tool in optimization of micromixers through design of experiment.

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