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Numerical Investigation of Mixing in Microchannels with Grooved Surfaces

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Abstract. Mixing in microchannels with grooved surfaces were studied numerically by applying the particle tracking technique. Point location, velocity interpolation and a fourth order adaptive Runge-Kutta integration scheme were applied in the particle tracking algorithms. Using these algorithms, streaklines and Poincaré maps were calculated from the 3D velocity field exported from a CFD package for microfluidics (MemCFD™). For small aspect ratio ($\alpha = 0.05$) grooves, the results illustrated there was no significant irregularity in the Poincaré map, and indicated little chaotic effect. In the meantime, the helicity observed from the streaklines and Poincaré maps indicated 3D convection were introduced by the grooved surfaces. Due to the wall boundary condition of viscous flow in microchannels, 3D convection could fold and stretch fluids to increase their interfacial area. As a result, the diffusion path could be reduced. Moreover, the change of flow rate did not affect the helicity very much, so helicity is a function of geometric parameters. For high aspect ratio ($\alpha = 0.30$) grooves, the flow pattern in the microchannel was complex and the jumbled dots in the Poincaré map indicated chaotic effects. In summary, although the microfluidic mixers with grooved surfaces could not always create chaotic effects, the helical flow patterns were always generated. It is a robust mixing strategy to apply grooved surfaces in microchannels and does not require high Reynolds number.

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1. Introduction

In a typical microfluidic device, viscosity dominates flow, and as a result, the Reynolds number is low and the flow is laminar. Therefore, the mixing of two or more fluid streams in microfluidic devices relies on diffusion, which is a slow process. On the other hand, in many microfluidic devices, such as lab-on-a-chip, it is very important to mix two or more reagents and testing samples together. And the mixing needs to be done in a confined area. So, microfluidic mixing is challenging and attracts the attention of many researchers. Based on the mixing mechanisms, micro-mixers have pure molecular diffusion at one end (Kamholz & Yager 2001) and chaotic mixing on the other (Liu et al. 2000, Stroock et al. 2002a). Based on structures, micro-mixers can be categorized in active mixing schemes and passive mixing methods. Most of active micromixers enhance mixing by stirring flow. The stirring can be done mechanically (Lu et al. 2002) or by the means of magneto-hydrodynamic (MHD) (Lemoff & Lee 2000), electro-hydrodynamic (EHD) (Choi & Ahn 2000) or by acoustic streaming (Zhu & Kim 1998, Yang et al. 2000) to create secondary flows. The secondary flows can stretch and fold material lines to reduce the diffusion distance between fluid streams and hence enhance mixing. Active micromixers are particularly suitable for chamber mixing. However, most of the active micromixers are very complex for fabrication and need external power sources to drive. It makes the active mixers expensive to make and difficult for flow control.

Some passive mixers reduce diffusion distance between fluid streams by splitting and recombining (Schwesinger et al. 1996, Koch et al. 1998, Ehrfeld et al. 1999). Recently, passive chaotic micromixers were reported. Chaotic mixing has been studied extensively in the macro-scale since the early 80s (Aref 1984, Jones et al. 1989, Ottino 1989). The knowledge can be borrowed for the design of microfluidic mixers. For instance, using a twisted pipe, secondary flow happens at the bends of the pipe (Jones et al. 1989). Chaotic advection can be a result of these secondary flows. Inspired by the twisted pipe, 3D serpentine channels (Beebe et al. 2001, Liu et al. 2000) were fabricated. The flow in 3D serpentine channels demonstrated chaotic advection at high flow rates ($Re \sim 70$) and good mixing performance. However, the challenges of serpentine mixers are the micro-fabrication of complex 3D structures and the needs of high Reynolds number to stir the fluids to generate chaotic advection. The chaotic microfluidic mixers by patterning grooves in microchannels were compatible with microfabrication processes and could be realized in general micro-machining centers (Johnson et al. 2002, Stroock et al. 2002a, Stroock et al. 2002b). The anisotropic patterned grooves in the micro-channel could create spiral circulation around the flow axis, and can stretch and fold streams of liquids to a complete mixing in a shorter channel length. The mixing effects were investigated over a range of Reynolds numbers. Both chaotic mixing strategies pointed out the design of chaos is one of the effective solutions to enhance mixing in a micro-scaled device.

Patterning grooves in microchannels has the drawback of creating dead volumes, but
it is compatible with microfabrication processes and works at low Reynolds number. So it can be applied in many microfluidic applications, especially the disposable microfluidic devices and those applications needing low flow rate. Under the same conditions, lower flow rate normally means lower pressure drop, and it makes it easier to drive the flow through a microfluidic device.

In this paper, the authors intended to use CFD models to reveal more information of the performance of chaotic microfluidic mixers with patterned grooves. Extended numerical investigation of the mixing mechanism for micromixers with complex geometric structures was carried out by using particle tracing algorithms. The limitation of chaotic microfluidic mixers and the limitation of CFD simulation are also discussed.

2. Methodology

To evaluate the performance of chaotic microfluidic mixers, numerical approaches were applied in this research. A CFD package for Microfluidic applications was applied to simulate the 3D velocity field, and algorithms to compute rate of shear and particle trajectories were also developed to study the stretching and folding of fluids.

2.1. Numerical Setup

While theory can suggest or predict the occurrence of chaotic advection, which can be explained in Ottino’s book (Ottino 1989), the degree of chaotic effects presented can only be determined for specific examples (Beebe et al. 2001). The existing analytical predictions for chaotic advection in microchannels with grooved surfaces are not accurate for high aspect ratio ($\forall \alpha > 0.1$), which was defined as half of the groove depth to the depth of channel plus half of the groove depth(Figure 1(a)). Therefore, it is necessary to use numerical simulations to evaluate the flow patterns in such channels.

In this paper, T-type microchannels were modelled numerically using the CFD software package MemCFD$^\text{TM}$ v2001.3d from Coventor. MemCFD$^\text{TM}$ uses a finite volume method to solve the Navier-Stokes equations. The grid can be seen in Figure 1(b). The simulation was run as steady, laminar, Newtonian, with 1 or 2 fluids (to evaluate mass fraction). The inlets were assigned flow rate boundary conditions, and all the channel walls were assigned wall boundary condition ($v_i = 0, i = 1, 3$). As the commercial packages rarely publish algorithms for visualizing velocity field, a set of particle tracing algorithms was developed and coded in Fortran77 to compute the particle trajectories and Poincaré maps out of the 3D velocity field exported from the CFD simulations.

The length, width and height of the channels were 5mm, 200$\mu$m and 100$\mu$m respectively. Simulations were performed on Win NT4.0 with Pentium $III$ 800MHz CPU and 512MB memory. The number of mesh elements (cells) in the models is in a range from about 250,000 to 300,000, and shown in Figure 1(b).
2.2. Particle Tracing

To evaluate the performance of a chaotic mixer, one can put non-diffusive particles in the velocity fields. To observe the advection of these particles, the convection of mass transport can be evaluated. In experimental measurement, this can be carried out by inject very fine colored ink streams in the flow fields or by particle image velocimetry (PIV). The numerical approach places virtual particles, which have no physical properties, in the velocity fields. The trajectories of these particles can be computed by the Lagrangian method, which records the spatial positions of the particles at each time step. In a steady flow, particle trajectories can be integrated with the system of Equations (1):

\[
\frac{dp(t)}{dt} = v(p(t), t)
\]

where \( p(t) \) is the particle position at time \( t \), \( v \) is the velocity field. Integrating equation (1) yields:

\[
p(t + \delta t) = p + \int_t^{t+\delta t} v(p(t), t) \, dt
\]

where \( \delta t \) is the time step.

The integral term on the right hand side can be evaluated numerically using a multi-stage method or a multi-step method. Regardless of how it is solved, the end result is a displacement which when added to the current position, \( p(t) \), gives the new particle location at time \( t + \delta t \).

In a discrete velocity field, the velocity of a particle at certain position is interpolated by the element containing this position. So this element need to be located first. After the element is located, the particle velocity can be interpolated. Then, a time step is assigned to integrate its new position. The procedure is repeated until the particle leave the flow domain. The algorithm is described in words below:
find cell containing initial position \( \text{(point location)} \)

\( \text{while } \) (particle in grid) \( \text{determine velocity at current position} \) \( \text{(interpolation)} \)

\( \text{calculate new position} \) \( \text{(integration)} \)

find cell containing new position \( \text{(point location)} \)

endwhile

2.2.1. Point location Point location is required to find the cell that contains a specified point. For the complex mesh of microchannels with grooved surface, it is difficult to locate particle position in the 8-nodes hexahedral elements. So it is necessary to split hexahedral elements into 5 or 6 tetrahedral elements, and 5 tetrahedral elements are used commonly (in Figure 2). For each tetrahedron, assume that we have a point \( p \) with coordinate \( p(x, y, z) \). The simplest way to find the element into which point \( p \) falls is to perform a loop over all the tetrahedrons, evaluating their shape-functions, \( N_i \), with respect to \( p(x, y, z) \) (Equation 3).

\[
\begin{align*}
    x &= \sum_i N_i x_i; \quad y = \sum_i N_i; \quad y_i z = \sum_i N_i z_i; \quad 1 = \sum_i N_i \\
    \text{(3)}
\end{align*}
\]

Tetrahedrization is only performed in the cells along the path of the line and the results do not have to be stored. For each tetrahedral element, it has 4 shape-functions \( (i = 4) \). So, the above equations can be written into a linear system (Equation (4)), and shape functions can be evaluated by standard Gaussian elimination.

\[
\begin{align*}
    \mathbf{x} &= \mathbf{X} \cdot \mathbf{N}, \quad \mathbf{N} = \mathbf{X}^{-1} \cdot \mathbf{x}_p \\
    \text{(4)}
\end{align*}
\]

\[
\begin{align*}
    \text{min}(N_i, 1 - N_i) > 0, \forall i \\
    \text{(5)}
\end{align*}
\]

The criterion set forth in Equation (5) is used to determine whether a point lies within the confines of an element. Geometrically, the shape functions are the ratios of four volumes divided by point \( p(x, y, z) \) to the volume of the tetrahedron (in Figure 3) (Li et al. 1999). For any negative value of \( N_i \), it means that the point \( p(x, y, z) \) is outside this tetrahedral element. Then, the point location proceeds by advancing to, and crossing the respective face into the adjoining tetrahedron. The worst violator of the four conditions is used to predict which tetrahedron to try next. Even if the bounding tetrahedron is not found in the immediate neighbor, by always moving in the direction of the worst violator it will converge upon the correct cell.

2.2.2. Interpolate velocity One of three techniques may be used for the spatial interpolation of velocity: physical space linear interpolation, volume weighted interpolation, and linear shape function interpolation. All three are mathematically equivalent and produce identical interpolation functions (Kenwright & Lane 1996). The linear shape function was the most efficient technique for this application because
it reused the shape function $N_i$, $i = 1, 4$ computed during point location. The linear shape function for spatial velocity interpolation is:

$$u = \sum_{i=1}^{4} N_i \times u_i$$  \hspace{1cm} (6)

where, $u_i$ are the velocity vectors at the 4 vertices of the tetrahedron.

2.2.3. Integration  Many integration methods are shown in the literature, ranging from the simple first-order Euler scheme to the fourth-order Runge-Kutta scheme or even higher-order methods, applied with fixed or variable time steps. The fourth order Runge-Kutta scheme, becomes:

$$p(t + \delta t) = p(t) + (k_1 + 2k_2 + 2k_3 + k_4)/6$$

$$k_1 = \delta t \cdot v(p(t), t)$$

$$k_2 = \delta t \cdot v(p(t) + k_1/2, t + \delta t/2)$$

$$k_3 = \delta t \cdot v(p(t) + k_2/2, t + \delta t/2)$$

$$k_4 = \delta t \cdot v(p(t) + k_3/2, t + \delta t/2)$$  \hspace{1cm} (7)
where \( k_i, i = 1 \sim 4 \) are the parameter decided by particle position \( p \), velocity \( v \), time \( t \) and time step \( \delta t \). Thus, using equation (7), a particle can be numerically integrated and traced through the flow field. In this paper, an adaptive variable time steps 4th-order Runge-Kutta scheme was used.

3. Results and discussion

With the algorithms described in the above section (2.2), one arbitrary periodical flow section (Figure II(a)) of the exported velocity field for a single fluid flow was extracted to be used to compute the streaklines and Poincaré map. Mixing of two fluid streams was also presented in Figure 7 to demonstrate the twisting of the interfacial line between them.

3.1. Flow patterns

One periodical flow was illustrated for vector planes in Figure 4, which corresponded to cut planes \( (\frac{\pi}{2}, i = 0 \sim 4) \) in Figure 1(a)). The void areas in the vector planes indicated the cross section of the solid parts of the grooves. The flow patterns for high aspect ratio (\( \alpha = 0.30 \)) grooves were more complex than that of low aspect ratio (\( \alpha = 0.05 \)). The rotating like flow patterns can be called secondary flow. So, a higher aspect ratio created stronger secondary flow.

3.2. Streaklines

A streakline is defined as a line formed by the fluid elements which pass through a given location in the flow field. A streakline can be made visible by injecting a dye into the fluid at the given location. In a steady flow, the streaklines coincide with the particle traces and the streamlines, which are lines to which the velocity vectors are tangent at all points.

To visualize the effects of the mixing numerically, it can be intuitive to trace a particle along the streakline. In Figure 5 the set of streaklines are twisting like a helical shape. This indicates folding and stretching of fluids, which favors mixing. For the grooved surfaces with the periodic configuration, the velocity field can be used repeatedly. CFD simulations were limited by computer resources and could not simulate the whole channel length. But streaklines could be computed by reusing the periodic velocity field and did not limit the length of channel in principle.

3.3. Poincaré map

To generate a Poincaré map in a spatially periodic system, one passive particle (or a series of particles) is advected by the periodic velocity field and passes through a series of periodic planes in the system. For the mixer considered here the plane is located at the exit of each mixing segment, and each position of the particle which hits this plane
Figure 4. Cross section velocity vector planes, $0 \sim 2\pi$. 

$\alpha = 0.05$ 

$\alpha = 0.30$
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Figure 5. Streaklines, sample points from two fluids streams

is recorded. The plane is called the Poincaré map. Regular patterns in the Poincaré map indicate integrable (non-chaotic) behavior, while jumbled patterns indicate chaotic behavior. In Figure 6(a), a small aspect ratio ($\alpha = 0.05$) had a regular recirculation pattern. With high aspect ratio, the irregularity of the flow patterns indicated chaotic effects (in Figures 6(b & c)). The small island (in Figure 6(b)) stopped other parts of the flow entering this area. But, as the dimension of this area was only a few tens of microns, diffusion could be effective for the mixing. Under a low Reynolds number, such an island disappeared. So, unlike 3D serpentine chaotic mixers requiring high Reynolds number, microchannels with grooved surfaces provide a robust solution to mixing at low or high Reynolds numbers.

3.4. Rate of shear

In the paper about microfluidic chaotic mixers (Stroock et al. 2002b), by analyzing the rate of shear just below the flat plate, a measure of the helicity of the flow was obtained by comparing the transverse and longitudinal rate of shear. It was complicated to interpret the sinusoidal terms. In this paper, the rate of shear was computed from the 3D velocity field exported from the CFD simulations. The measurement of rate of shear can be provided by the angle $\Omega$ between the channel axis $x$ and interfacial line of two fluid streams, which is shifted by the helical flow pattern(Figure 7).

In Figure 8, the average of numerical and analytical predictions were illustrated. Three experimental measured points (Stroock et al. 2002b) were also added for comparison. Obviously, when $\alpha > 0.1$, the numerical prediction does not agree with the analytical ones. The measured data were in between the numerical and analytical predictions. However, the distortion of the measuring optics, the diffusion of the coloring and other reading errors can be added to the inaccuracy of the measurement. In the meantime, the height to width aspect ratio practically is not infinitely small to satisfy $w >> h$, where $w$ is the width of the channel, and $h$ is the height of the channel.
Moreover, the analytical prediction gives the average measurement of the helicity. The periodic terms are not counted in the calculation. In Figure 9, the helicity was computed numerically along the channel longitudinal direction. The number of peaks in wave form coincide the number of periodic grooves in the channel.

The amplitudes of the waves were proportional to the $Re$ number, though the average of the amplitudes remains the same. The average of helicity only relies on groove aspect ratio $\alpha$, width of the grooves and height of channel. To emphasis here, aspect ratio, $\alpha$, contributes the most to the helicity. This means deeper the grooves, better the mixing performance. The periodic terms of the velocity form the wave shape of the helicity.

Figure 6. Poincaré map, 45° grooved surfaces: a) $\alpha = 0.05$, flow rate = 1000nl/sec, b) $\alpha = 0.30$, flow rate = 1000nl/sec, c) $\alpha = 0.30$, flow rate = 2nl/sec
Figure 7. Two fluids streams flow into a T-type channel with grooved surfaces. The interfacial line is indicated by the bright mixed region. The helicity was measured by the angle \( \Omega \) between this interfacial line and the channel axis.

Figure 8. Rate of shear measured by the angle \( \Omega \)

Figure 9. Rate of shear at different Reynolds number, numerical estimations

4. Conclusions

It will be an ideal goal to generate chaos in the microfluidic mixers (Beebe et al. 2001). However, in a typical microfluidic device, the Reynolds number is low. It makes the transfer of momentum through inertia not practical, and chaos is difficult to create under such low Reynolds number \((Re < 1)\). The passive microfluidic mixers patterned with grooved surfaces were studied numerically. Although these mixers could not always create chaotic effects, the helical flow patterns were always generated. The helicity is a
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function of geometric parameters and increases with these parameters. Helicity in such microchannels can provide sufficient folding and stretching to fluids, and then, diffusion is efficient for mixing when the diffusion path is reduced to a few microns. So, it is a robust mixing strategy to apply grooved surfaces in microchannels.

The obvious drawback for these mixers is the dead volume created by the grooves. Contradictory to reduce dead volume, deeper grooves makes better mixing efficiency of the mixers. As the grooves are critical for generating helicity, it has not yet any direct solution to reduce the dead volume in such mixers. Nevertheless, this mixing strategy still can be used in many applications. For instance, disposable microfluidic devices for medical diagnosis and other applications that do not need to clean the grooves after using them.

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