Design and simulation of the micromixer with chaotic advection in twisted microchannels

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Chaotic mixers with twisted microchannels were designed and simulated numerically in the present study. The phenomenon whereby a simple Eulerian velocity field may generate a chaotic response in the distribution of a Lagrangian marker is termed chaotic advection. Dynamic system theory indicates that chaotic particle motion can occur when a velocity field is either two-dimensional and time-dependent, or three-dimensional. In the present study, micromixers with three-dimensional structures of the twisted microchannel were designed in order to induce chaotic mixing. In addition to the basic T-mixer, three types of micromixers with inclined, oblique and wavelike microchannels were investigated. In the design of each twisted microchannel, the angle of the channels' bottoms alternates in each subsection. When the fluids enter the twisted microchannels, the flow sways around the varying structures within the microchannels. The designs of the twisted microchannels provide a third degree of freedom to the flow field in the microchannel. Therefore, chaotic regimes that lead to chaotic mixing may arise. The numerical results indicate that mixing occurs in the main channel and progressively larger mixing lengths are required as the Peclet number increased. The swaying of the flow in the twisted microchannel causes chaotic advection. Among the four micromixer designs, the micromixer with the inclined channel most improved mixing. Furthermore, using the inclined mixer with six subsections yielded optimum performance, decreasing the mixing length by up to 31% from that of the basic T-mixer.

1 Introduction

Micro Total Analysis Systems (μTAS) have been developed to undergo a number of analytical processes involving chemical reactions, separation and sensing all performed on a single chip (the so-called "Lab on a chip"). The μTAS research, which is aimed at biochemical analysis miniaturization and integration, has recently made dramatic progress.[1,2] Some unit procedures, such as capillary electrophoresis (CE),[3,4] polymerase chain reaction (PCR),[5–7] sample preconcentration,[8] genomic DNA extraction, DNA hybridization[9] and chromatography,[10] have been successfully miniaturized and can now operate on a single-step chip. However, there is still a considerable technical challenge in integrating these procedures into a multiple-step system.[11]

An important issue for this integration is microfluid management technique, *i.e.* microfluidic transportation, metering, and mixing. The microfluid management devices, such as micropumps, microvalves, microsensors and micromixers, have been rapidly developing over the past few years.[12] Effective mixing is essential to many of the microfluidic systems. Rapid mixing can reduce the analyzing time and improve procedure control in μTAS. Mixing generally involves two steps: first, a heterogeneous mixture of substantially homogeneous domains of the two fluids is created by convection; secondly, diffusion between adjacent domains causes a homogeneous mixture at the molecular level.[13] However, the mixing procedures on the macroscopic scale, such as stirring or creation of turbulent flow cannot be shrunk to fit into the miniaturized systems (whose dimensions are so small that obtaining Reynolds numbers over 2000, the critical value for turbulent flow, are not feasible). The rapid mixing process produced by turbulence is usually not available at the microscale due to the extreme weakness of inertial forces. Thus, some other mechanisms must be employed to enhance mixing.

In the last several years, numerous devices designed to improve mixing on the microscale were reported in the literature. These devices are classified into two categories: active and passive mixers. Active mixers employ some external forces or forms of active control on the flow field by moving parts or varying gradients.[14–17] Conversely, passive mixers[13,18–21] exert no energy input except that of the mechanism used to drive the microfluid flow at a constant rate. Although active mixers may effectively provide rapid mixing, the actuators used in these mixers need extra energy and could be difficult to fabricate. Additionally, the electrical field and heat generated by the active control of these mixers may cause damage to the biological samples during the biochemical processes. The operation and integration of active mixers onto a biochemical system are problems that need to be overcome. Passive mixers have the potential to be an attractive solution due to their simplicity and easy operation.

Chaotic mixers with twisted microchannels were designed in the present work. The tee (T) mixer was used as a basis for comparisons. Additionally, three types of micromixers with inclined, oblique and wavelike microchannels were investigated and the mixing characteristics of these micromixers were performed numerically herein. In the design of each twisted microchannel, the angle of the channels' bottoms alternates in each subsection. When the fluids enter the twisted microchannels, the flow sways around the varying structures within the microchannels. The designs of the twisted microchannels provide a third degree of freedom to the flow field in the microchannel. Therefore, chaotic regimes that lead to chaotic mixing may arise. Simulations using CFD-ACE™ (CFD Research Corporation, Alabama, USA) were performed on a personal computer. The finite element method and three-dimensional unstructured grids were employed to calculate the pressure and velocity fields, as well as species distributions in the micromixers.

2 Designs of the microchannel with chaotic mixing

The phenomenon that a simple Eulerian velocity field may generate a chaotic response in the distribution of a Lagrangian marker is termed chaotic advection.[22] Dynamic systems theory indicates that chaotic particle motion can occur when a velocity field is either two-dimensional and time-dependent, or three dimensional.[23] The twisted-pipe structures with chaotic advection have been investigated to provide effective mixing for those Reynolds numbers larger than 60 on the macroscale.[24–26] Chaotic advection may improve the mixing, even at low Reynolds number regions.[27] Recently, several investigations[19,21,28–30] based on the concept of chaotic mixing have been reported and examined. Volpert *et al.*[28] developed an active micromixer to improve mixing of two fluids in a microchannel. The flow through the main channel of the micromixer was unsteadily perturbed by three sets of secondary flow channels, thereby enhancing the mixing. Lee *et al.*[29] presented a design of the micromixer, which employs unsteady pressure perturbations superimposed to a mean stream to enhance mixing. The channels of their mixer were etched into silicon wafer using the DRIE technique and anodically bonded to Pyrex plates. Liu *et al.*[19] proposed a three-dimensional serpentine microchannel design with a C-shaped repeating unit as a means of implementing chaotic advection to enhance passive mixing. Their micromixer was fabricated in a silicon wafer using a double-sided KOH wet-etching technique. A plastic 3D L-shaped serpentine micromixer was subsequently developed to enhance the mixing of biological sample preparation.[21] Three-dimensional PDMS microfabrication and plastic micromolding technique were employed to fabricate the L-shaped micromixers. Hong *et al.*[20] designed an in-plane passive micromixer (fabricated using PDMS), which employed the "Coanda effect" to improve mixing.

Three-dimensional structures of the twisted microchannel, which induce chaotic mixing in the micromixers, are designed in the present study. The twisted microchannels can be fabricated from the polymer materials, such as poly-methylmethacrylate (PMMA) or PDMS, and are adapted for biochemical analysis. Fig. 1 illustrates the geometries and dimensions of the chaotic micromixers investigated herein. The dimensions of the basic T-mixer are identical to those used in the previous report[31] for the sake of comparison. In addition to the basic T-mixer shown in Fig. 1a, three types of twisted microchannels are illustrated in Fig. 1b–c, the inclined, oblique and wavelike microchannels. The width of the microchannel is 500 μm and the depth is 300 μm for all types of the micromixers herein. The angle of the inclined or oblique planes alternates in each subsection of the microchannel. When the fluids enter the twisted microchannels, the flow sways around the varying structures within the microchannel. The designs of the twisted microchannels provide a third degree of freedom to the flow field of the microfluid in the channel. Therefore, chaotic regimes that lead to chaotic mixing may arise.

3 Numerical simulations

The three designs of the mixers are based on the T mixer whereby two gases enter the two top branches of the mixer and mix by diffusion at the T-junction and lower portion. Simulations were performed using CFD-ACE™ software running on a personal computer. The finite element method and three-dimensional unstructured grids were employed to solve the governing equations. The governing equations in these mixers are the continuity equation, momentum conservation (Navier-Stokes) equations as well as species convection–diffusion equation.[32] The dimensionless forms can be expressed as the following:[31]

$$\nabla^* V^* = 0 \tag{1}$$

$$\frac{dV^*}{dt^*} = -\nabla^* P^* + \frac{1}{Re}\nabla^{*2} V^* \tag{2}$$

$$\frac{dC_A^*}{dt^*} = \frac{1}{ReSc}\nabla^{*2} C_A^* \tag{3}$$

where

$$Re = \frac{\rho U D_h}{\mu},\ Sc \frac{\mu}{\rho D_{AB}}$$

C_A is the species concentration. D_h and U are the hydraulic diameter of the microchannel and the inlet velocity of the fluid, respectively. The numerical simulations obtain the pressure, velocity fields and species distributions in the micromixers. The Schmidt number (*Sc*) is defined as the kinematic viscosity

$$\left(\nu = \frac{\mu}{\rho}\right)$$

divided by the diffusivity (D_{AB}). The value of *Sc* is about 0.8 for gases and the diffusivity for the binary gas mixture (methanol and oxygen) is 2.78×10^{-5} m^{2}s^{-1}. Laminar flow and adiabatic boundary conditions are set in this simulation. Compressibility

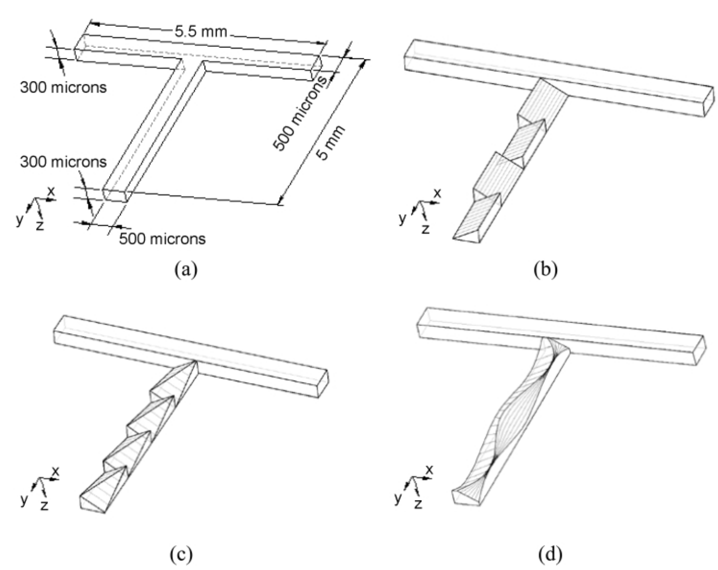

Fig. 1 Schematic diagrams (upside down) of (a) T-mixer, (b) inclined mixer, (c) oblique mixer, and (d) wavelike mixer.

and slip effects of the gaseous flow in the microchannel are negligible.[31] The SIMPLEC method was adopted for pressure–velocity coupling and all spatial discretizations were performed using the first-order upwind scheme. The simulation was implemented in steady state. A fixed-velocity condition was set to the boundary condition at the inlet of *the* micromixer. The boundary condition at the outlet was set at a fixed pressure. The total number of elements was approximately 9,000 in the case of the T-type mixer and 10,000 to 16,000 in the cases of the twisted microchannels with different structures.

4 Results and discussions

Fig. 2 shows the mass fraction contours of oxygen in the T-mixer with different inlet velocities (0.5, 1.0, 2.0 and 2.5 m s^{-1}). As shown in this figure, the mixing lengths increase as the inlet velocities increase. The Peclet number ($Pe = UD_h/D_{AB}$), which represents the product of the Schmidt number (Sc) and the Reynolds number (Re), characterizes the ratio of mass transport by convection to that by diffusion. When the Peclet number is larger than two, the convection dominates the mass transfer process.[33] The mixing occurring in the main channel requires progressively larger mixing lengths as the Peclet number increases. The Peclet number is 6.75 at an inlet velocity of 0.5 m s^{-1}. This demonstrates that the process of mass transfer is controlled by convection for the cases in the present study.

Fig. 3 plots the mass fraction distributions of oxygen for the four types of the microchannel (possessing four subsections) with an inlet velocity of 2.0 m s^{-1}. The length of the microchannel is 4.5 mm in Fig. 3. The numerical results illustrated in this figure indicate that the mixing efficiency of fluids in the inclined microchannel is better than that in other structures. The complete mixing of the fluids can be defined as no more than ±1% deviation from the equilibrium composition at all locations in the cross-section. The microchannel is extended one subsection at a time until the mixing length required for complete mixing of the fluids can be obtained. The mixing length for the basic T-mixer required to achieve complete mixing is 7.90 mm. For the inclined mixer, this required mixing length is only 5.64 mm. Therefore, the mixing efficiency in the microchannel of the inclined mixer is better than that of the basic T-mixer by 28.6%. The mixing lengths required for complete mixing in the oblique and wavelike mixers are 6.19 and 7.43 mm, respectively. Thus, the mixing in these micromixers with the twisted microchannels is also enhanced. The tracks of the fluids in microchannels for the four

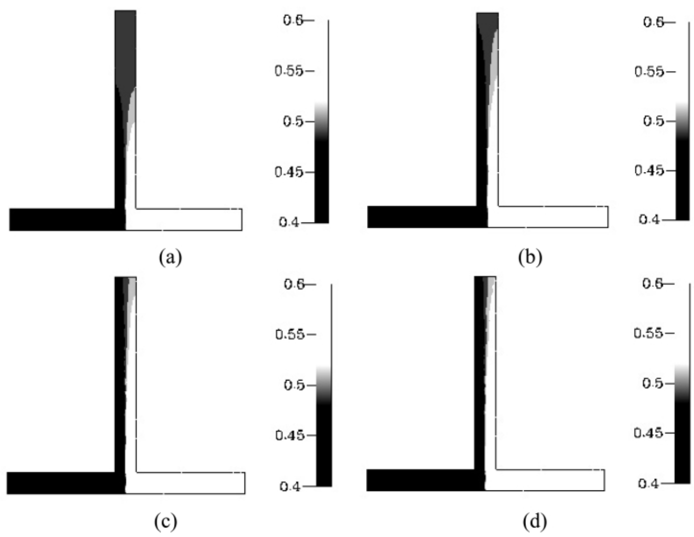

Fig. 2 Mass fraction distributions of oxygen in the T-mixer with different inlet velocities: inlet velocity = (a) 0.5 m s^{-1} (b) 1.0 m s^{-1} (c) 2.0 m s^{-1} (d) 2.5 m s^{-1}.

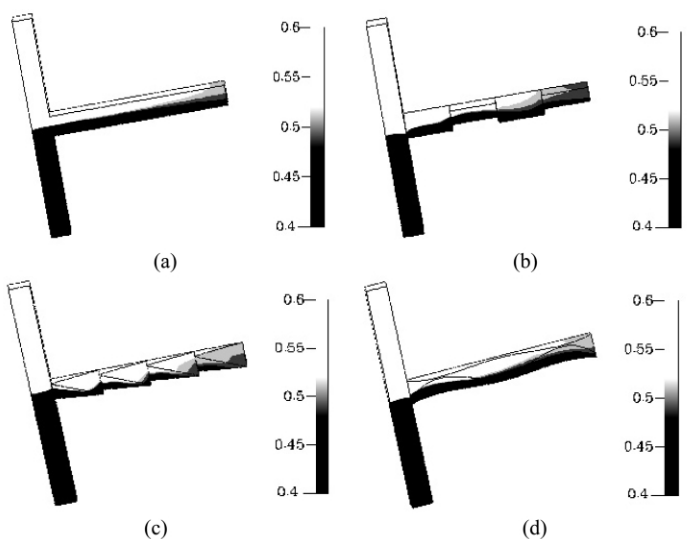

Fig. 3 Mass fraction contours of oxygen for (a) T-mixer (base case), (b) inclined mixer, (c) oblique mixer, and (d) wavelike mixer. (four subsections, inlet velocity = 2.0 m s^{-1})

designs of the microchannel are depicted in Fig. 4. The flow sways around the structures within the twisted microchannel which results in chaotic advection. It is observed that sway of the flow within the inclined micromixer creates the greatest change in amplitude.

The mass fraction contours of oxygen for the inclined-mixer with different numbers of subsections with a fixed length of 4.5 mm are shown in Fig. 5. However, the simulated results show that a microchannel of 4.5 mm in length could not achieve complete mixing. The mixing lengths required for complete mixing are obtained by extending the microchannel. For the inlet velocity of 2 m s^{-1}, the mixing lengths of the inclined mixer with different designs and their corresponding subsection's lengths are listed in Table 1. The mixing lengths, which are obtained by extending the subsections in the microchannel to varying lengths, are plotted in Fig. 6. The inclined mixer with six subsections yields the optimum mixing length for enhancing mixing. The mixing length of the inclined mixer with six sections is only 5.46 mm, which is about 31% faster than that of the T-mixer. The sway of the fluid in those microchannels, whose number of subsections exceeds six, becomes weaker because the proximity of each subsection is too close. Therefore, the fluid does not have enough time to change direction before entering the next subsection. The inclined microchannels can be fabricated using excimer laser photo-ablation onto polymer materials adapted for biochemical analysis, such as PMMA.

5 Conclusions

Chaotic mixers with twisted microchannels were designed and simulated numerically herein. Micromixers with three-dimensional structures of the twisted microchannel were designed and investigated in the present study. The angle of the channels'

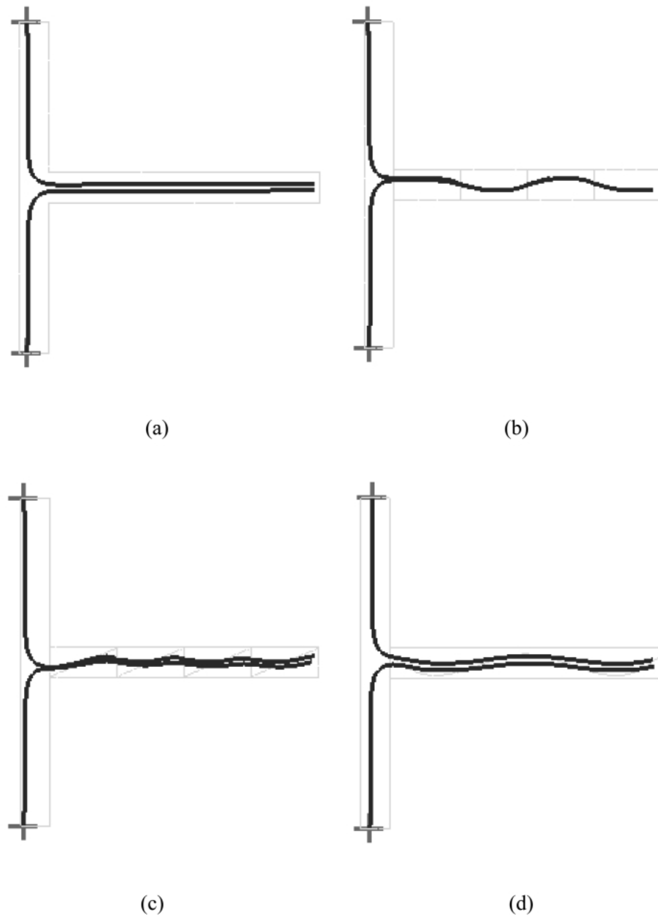

Fig. 4 The tracks of the microfluid flow in the microchannels of (a) T-mixer, (b) inclined mixer, (c) oblique mixer and (d) wavelike mixer.

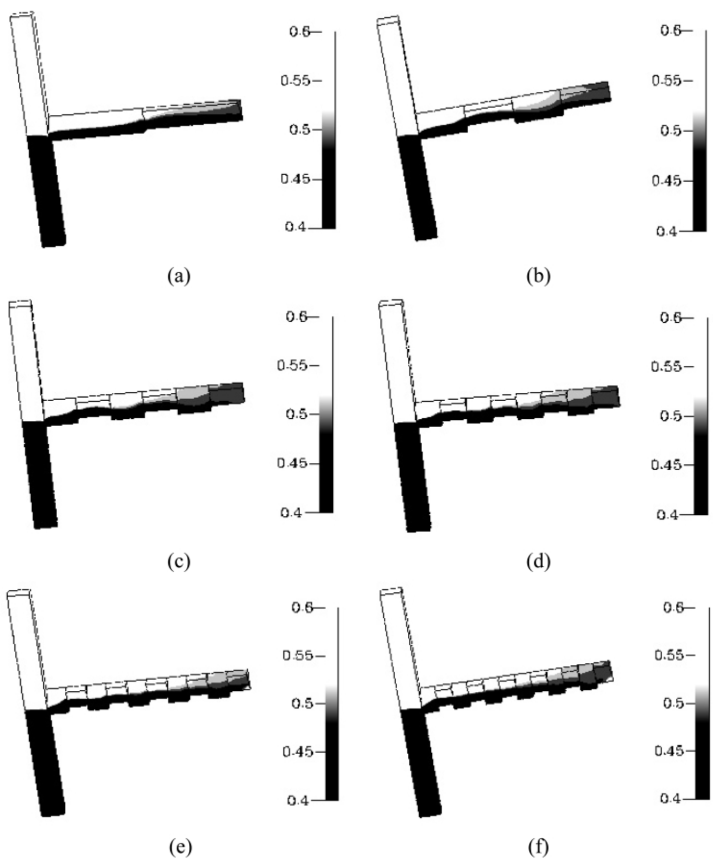

Fig. 5 Mass fraction contours of oxygen for the inclined-mixer with different numbers of sections (inlet velocity = 2.0 m s^{-1}): (a) two, (b) four, (c) six, (d) eight, (e) ten, and (f) twelve subsections.

Table 1 The mixing lengths of the inclined mixer with different designs when the inlet velocity is 2 m s^{-1}.

Numbers of subsections in the fixed length of the microchannel (4.5 mm)	Length per section/mm	Mixing length/mm
2 Subsections	2.2500	6.44
4 Subsections	1.1250	5.62
6 Subsections	0.7500	5.46
8 Subsections	0.5625	5.64
10 Subsections	0.4500	5.71
12 Subsections	0.3750	6.26

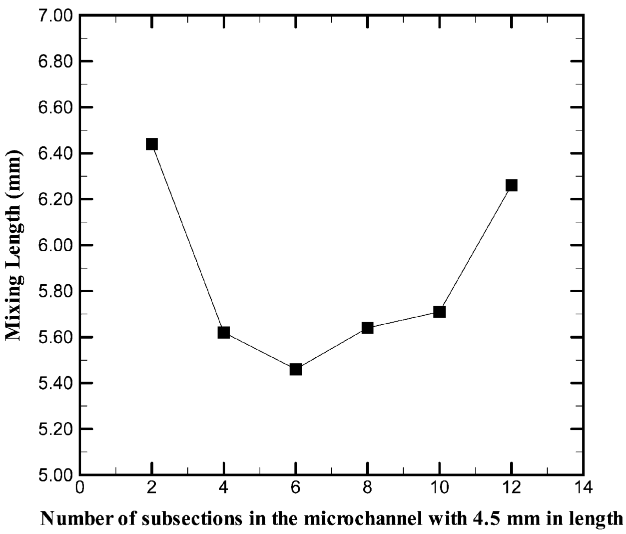

Fig. 6 The mixing length for different numbers of subsections in the inclined microchannel of 4.5 mm length.

bottoms alternates in each subsection. The designs of these microchannels provide a third degree of freedom to the flow field in the microchannel. Therefore, chaotic regimes that lead to chaotic mixing may arise.

If the Peclet number is large enough, the convection in the main channel dominates the mass transfer process and mixing occurs. The numerical simulations indicate that the inclined micromixer most effectively improves mixing. The flow sways around the twisted microchannel due to the alternating inclined structures within the channel, which results in chaotic advection hence improving the efficiency of the microfluid mixing. Furthermore, the inclined mixer with six subsections yields the optimum mixing length for enhancing mixing. The micromixers investigated in this work present an attractive solution for the mixing problem in BioMEMS due to their simple design and easy operation. Furthermore, there is no electrical field or heat generated in the micromixer with chaotic advection so that the mixers proposed herein can avoid damage to the biological samples.

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