Published in final edited form as:

J Micromech Microeng. 2008 March 6; 18: 045015–. doi:10.1088/0960-1317/18/4/045015.

An unsteady microfluidic T-form mixer perturbed by hydrodynamic pressure

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Abstract

An unsteady microfluidic T-form mixer driven by pressure disturbances was designed and investigated. The performance of the mixer was examined both through numerical simulation and experimentation. Linear Stokes equations were used for these low Reynolds number flows. Unsteady mixing in a micro-channel of two aqueous solutions differing in concentrations of chemical species was described using a convection-dominated diffusion equation. The task was greatly simplified by employing linear superimposition of a velocity field for solving a scalar species concentration equation. Low-order-based numerical codes were found not to be suitable for simulation of a convection-dominated mixing process due to erroneous computational dissipation. The convection-dominated diffusion problem was addressed by designing a numerical algorithm with high numerical accuracy and computational-cost effectiveness. This numerical scheme was validated by examining a test case prior to being applied to the mixing simulation. Parametric analysis was performed using this newly developed numerical algorithm to determine the best mixing conditions. Numerical simulation identified the best mixing condition to have a Strouhal number (St) of 0.42. For a T-junction mixer (with channel width = 196 μm), about 75% mixing can be finished within a mixing distance of less than 3 mm (i.e. 15 channel width) at $St = 0.42$ for flow with a Reynolds number less than 0.24. Numerical results were validated experimentally by mixing two aqueous solutions containing yellow and blue dyes. Visualization of the flow field under the microscope revealed a high level of agreement between numerical simulation and experimental results.

Introduction

Rapid developments in micro/nano fabrication technology have enabled versatile lab-on-a-chip applications for fundamental biological research, biomedical diagnostics and therapeutics [1,2]. Significant research has been performed in the area of microfluidic mixing that is a critical step for most biomedical technologies [3,4]. In microfluidic systems, low Reynolds number conditions typically result in laminar flow [1]. As a result, molecular diffusion, rather than turbulence, dominates the mixing process and consumes a majority of the time in lab-on-a-chip processes [5]. Various micro-mixer design strategies have been utilized to enhance mixing [3–5]. Micro-mixers can be classified as either passive or active mixers. For passive mixers,

no unsteady perturbations are applied to enhance mixing. Passive mixers typically rely on three-dimensional complex geometries [3,6–9], multi-lamination or hydrodynamic focusing [10–12] to increase contact interface and decrease diffusion distance. On the other hand, active mixers employ pressure disturbance [13–16], electro-hydrodynamic disturbance [17–23], dielectrophoretic disturbance [24], ultrasonic vibration [25], magnetohydrodynamic (MHD) convection [26], magnetic stirring [27,28], multi-phase convection [29,30] and collision of liquid segments [31] to generate external forces for active mixing of fluids in micro-channels.

Micro-mixer performance has been examined using various experimental methods, including fluorescence and ultraviolet resonance Raman spectroscopy [32], thermal lens spectrometry [33], micro laser-induced fluorescence (μ -LIF), and micro Particle image velocimetry (μ -PIV) [34]. Recently, computational fluid dynamics (CFD) simulations has been developed for micro-mixer design because detailed information regarding flow field, magnetic field, electric field, thermal field and species concentration can be obtained directly from simulation results [9, 11,12,14–16,19,21–23,29,35–37]. In a typical mixing problem, micro-channel mixing of two aqueous solutions with different concentrations of a chemical species is described using a convection-dominated diffusion equation. However, numerical results from algorithms with either first- or second-order special accuracy may result in erroneous conclusions regarding convection-dominated flow due to numerical mixing (also termed false diffusion) caused by truncation.

We have developed high-order transformation-free numerical schemes [38] on non-uniform grids for unsteady convection-dominated diffusion problems. These methods were applied to examine unsteady mixing in a T-form micro-mixer. Due to their simple confluence geometry, the mixing efficiency of T-form micro-mixers has been studied by several groups [11–13,34, 40–43]. In this paper, we applied high-order numerical schemes to study the performance of a two-dimensional T-mixer and identified the best mixing condition. A T-mixer was fabricated using standard micro-fabrication processes and tested with two aqueous solutions to compare experimental results with numerical simulation. An important focus of our paper was on the high-order numerical simulation of mixing to avoid spurious mixing from numerical diffusion. The Taylor dispersion in the axial direction of mixing [37] is outside the scope of our two-dimensional model system but will be considered in future three-dimensional studies.

Physical model

The coordinates and dimensions of the T-mixer model are shown in figure 1. The mixing channel is 3 mm long and 196 μm wide, while the inlet channel before confluence is 1.5 mm long and 117 μm wide. After the fabrication of the mixer by photolithography, the depth of the micro-channel (H) was 82 μm and the measured width of the mixing and inlet channels were 196 μm and 117 μm , respectively. Two aqueous solutions with different concentrations of a chemical species represented by the colors blue and yellow are introduced through inlets **a** and **b**. For inlet **a**, the concentration is 0.0 M and for inlet **b** the concentration is 0.01 M. In an ideal mixer, the concentration of chemical species will become uniform and equal to 0.005 M at the mixing channel exit.

For all micro-mixer designs, the general approach to mixing enhancement is to increase interface area between the two solutions to facilitate molecular diffusion. At room temperature and in aqueous solutions with a typical kinetic viscosity (ν) around $10^{-6} \text{ m}^2 \text{ s}^{-1}$, the typical value for diffusion (D) for most biomolecules, such as RNA, DNA and proteins, is in the order of $10^{-10} \text{ m}^2 \text{ s}^{-1}$.

Mathematical model

Governing equations

Constitutive governing equations are the incompressible Navier–Stokes equations for mass and momentum conservation and the unsteady convection–diffusion equation for the evolution of species molar concentration, namely, continuity

$$\nabla \cdot \vec{V} = 0, \quad (1)$$

momentum

$$\frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} = -\frac{1}{\rho} \nabla p + \frac{1}{Re} \nabla^2 \vec{V}, \quad (2)$$

species

$$\frac{\partial c}{\partial t} + \vec{V} \cdot \nabla c = \frac{1}{Pe} \nabla^2 c, \quad (3)$$

where $\vec{V}$ is the velocity vector field, p is the pressure and c is the species molar concentration. Re is the flow Reynolds number that is representing the ratio of inertial force to viscous force and is defined as

$$Re = VL/\nu \quad (4)$$

in which V is the mean base flow velocity at the mixing channel outlet, ν is the kinetic viscosity and the characteristic length scale L is given by the hydraulic diameter,

$$L = 4 \frac{\text{cross section area}}{\text{wetted perimeter}} = 2 \frac{W \times H}{W + H}, \quad (5)$$

where W ($=196 \mu\text{m}$) and H ($=82 \mu\text{m}$) are width and depth of the main channel, respectively. Based on the channel geometries in figure 1, L $115.6 \mu\text{m}$. In the species equation, the Peclet number, Pe , indicating the ratio of characteristic time of diffusion to characteristic time of convection, is defined as

$$Pe = VL/D, \quad (6)$$

where D is the constant mass diffusion coefficient. The Schmidt number, $Sc = \nu/D$, representing the ratio of kinetic viscosity ($\nu = 10^{-6} \text{ m}^2 \text{ s}^{-1}$) to the mass diffusion coefficient ($D = 10^{-10} \text{ m}^2 \text{ s}^{-1}$) typically has a value of 10^4 . The Peclet number is equal to the product of the Schmidt number and the Reynolds number

$$Pe = Sc \times Re \quad (7)$$

indicating that the Peclet number is 10^4 times larger than Reynolds number.

Characteristics of governing equations

From equations (1)–(3), the species concentration does not appear in either the continuity or momentum equation. In other words, the velocity field solution is not dependent on the species concentration. Therefore, the velocity field and species concentration equation can be solved sequentially.

In most microfluidic flow conditions, the Reynolds number is low due to micro-scale geometries and slow flow rates. For instance, at a typical flow rate of $Q = 1.0 \mu\text{l min}^{-1}$ in a micro-channel, mean base flow velocity equals 0.00103 m s^{-1} and the flow Reynolds number is 0.12 as calculated from equation (4). Therefore, the viscosity term in the momentum equation (equation (2)) dominates. After removing the relatively small nonlinear inertial term from equation (2), the momentum equations become

$$\frac{\partial \vec{V}}{\partial t} = -\frac{1}{\rho} \nabla p + \frac{1}{Re} \nabla^2 \vec{V}, \quad (8)$$

which are linear Stokes equations. On the other hand, at a typical flow rate of $Q = 1.0 \mu\text{l min}^{-1}$, the species equation (equation (3)) is convection dominated because the Peclet number is 1200 (from equation (7)).

Boundary conditions

To enhance mixing, the in-line pressure disturbances are introduced from both inlets in figure 1. The inflow condition is specified as

$$\begin{aligned} V_{a,b} &= V_0 + \varepsilon V_0 \sin(2.0\pi ft + \varphi_{a,b}) \\ c_a &= 0.0M, \quad c_b = 0.01M, \end{aligned} \quad (9)$$

where V_0 is the base inflow, ε is the non-dimensional disturbance amplitude from pressure perturbations, f is the disturbance frequency in Hz, t is the time in seconds and $\varphi_{a,b}$ is the phase angle. Non-slip and zero species flux boundary conditions are assumed at the channel wall boundary, while a constant pressure boundary condition is applied at the exit. For periodic flow, the time scale is characterized by the Strouhal number, which is defined as the ratio of the characteristic flow time to the disturbance period

$$St = \frac{L/V}{1/f}. \quad (10)$$

Superimposition of velocity fields

Even for the linear Stokes equation, solving an unsteady flow field is computation intensive because numerous iterations are required to find the appropriate pressure distribution to satisfy the continuity equation at each time step. By considering the linear property of Stokes equations, the principle of linear superposition can be applied to velocity vector fields. If we set two different inflow conditions, V_{in1} and V_{in2} , to obtain different velocity vector fields $\vec{V}_1$ and $\vec{V}_2$, respectively, the linear combination of inflow condition $a \times V_{in1} + b \times V_{in2}$, will yield a velocity vector field, where a and b are arbitrarily held constant.

Instead of introducing disturbances with single frequencies in equation (9), superposition of the steady base flow and disturbances with multiple frequencies are specified as inflow conditions for V_a and V_b in figure 1, i.e.,

$$V_{a,b}=V_0\left(1+\varepsilon_N\sum_{n=1}^N\sin(2.0\pi f_n t+\varphi_{a,b})\right)$$

$$f_n=nf_1,$$
(11)

where ε_N is the disturbance amplitude at all frequencies. In the current test cases, a total of 15 ($N = 15$) frequencies with the lowest frequency, $f_1 = 1$ Hz were considered in numerical simulations. The simulation was carried out until the unsteady state solutions reach a periodic state. Temporal Fourier analysis was performed on the unsteady state solutions for a single frequency to decompose mean flow and disturbances with different frequencies. Specifically, the Fourier transform for the velocity fields leads to

$$u_i(x,y,z,t)=\bar{u}_i(x,y,z)+u_{di}(x,y,z)$$

$$\times\sum_{n=1}^N\sin(2.0\pi f_n t+\varphi_i(x,y,z)),$$
(12)

where $u_i(x,y,z,t)$ ($i = 1, 2$) is the velocity component, $\bar{u}_i(x,y,z)$ is the base flow solution, $u_{di}(x,y,z)$ is the local disturbance amplitude of velocity and $\varphi_i(x,y,z)$ is the phase angle of velocity disturbances.

Once the velocity fields were obtained at multiple frequencies (equation (12)), the solutions for any combination of different base inflow and disturbances with different amplitudes at any frequency $f = f_n$ for inflow conditions in equation (9) were directly calculated from linear superposition of solutions in equation (12) without the requirement to solve Stokes equation repeatedly. The solutions of velocity fields were plugged into the species equation (equation (3)) to solve distributions of species concentration for each case of interest. This approach has a significantly lower computational cost by avoiding the need to solve Stokes equations for each case.

In our numerical simulations, a commercial software package was used to solve nonlinear Navier–Stokes equations, instead of linear Stokes equations, for velocity fields. In addition, the principle of linear superposition of Stokes equations was employed to calculate velocity fields based on solutions of Navier–Stokes equations and the resulting velocity fields were plugged in to solve the species equation (equation (3)).

Numerical simulations

Numerical grids

The computational domain was divided by rectangular meshes (see figure 2). Only part of the computational domain near the T-junction is shown in figure 2 for clarity. A hyperbolic tangent stretching function was used to cluster denser points near the wall to accommodate boundary-layer effects. In the case of the inlet channel prior to confluence, 41 grid points were used in the x -direction and 301 points in the y -direction. For the mixing channel after confluence, 601 points were used in the x -direction and 81 points in the y -direction. Overall, the inlet channel consisted of 680×40 cells and the mixing channel consisted of 640×80 cells with 40×80 cells in the overlap region. The grid size was chosen based on the estimation of the oscillation wavelength of the species concentration in the mixing channel. For each wavelength, more than 20 points were used to capture the details of the wave structure. The numerical accuracy of this grid assignment was evaluated by numerical grid refinement experiments to ensure that the numerical solutions were grid independent.

Solution procedure

Based on the preceding analysis of characteristics of equations governing unsteady mixing, the momentum equations (equation (2)) are viscosity dominated while the species equation (equation (3)) is convection dominated. Therefore, different numerical methods were applied to solve equations (2) and (3), respectively. In addition, velocity fields and the species concentration equation can be solved in sequence. Velocity fields were solved first and then plugged into equation (3) for solution of the species concentration.

Numerical methods for Navier–Stokes equations

A commercial software package was used to solve the viscosity-dominated momentum equation for velocity fields. Even though the momentum equation has only second-order accuracy in space, the numerical dissipation effect on solutions of velocity fields is relatively small because flow with small Reynolds number is viscosity dominated.

High-order numerical methods for the convection-dominated diffusion equation

We have developed high-order compact finite difference methods to solve the unsteady convection-dominated diffusion equation [38]. Third-order or fifth-order upwind finite difference schemes were derived on compact stencils for discretization of first-order spatial derivatives in convection terms while fourth-order or sixth-order central schemes were used for the second-order spatial derivatives in diffusion terms, namely, spatial discretization

$$\frac{\partial c}{\partial \xi} \quad \text{or} \quad \frac{\partial^2 c}{\partial \xi^2}: \sum_{k=-n_0}^{k=n_0} b_{i+k} c'_{i+k} = \sum_{k=-m_0}^{k=m_0} a_{i+k} c_{i+k} + O(\Delta \xi^m), \quad (13)$$

where $c'(\prime\prime)$ is the first (or second) order derivatives with respect to ξ , ξ is x or y and m is the order of truncation errors. The partial differential equation (PDE) of equation (3) becomes the first-order ordinary differential equation after spatial discretization. Two different numerical methods were employed for time integration, one is the alternating direction implicit (ADI) method and the other is the second-order Runge–Kutta method. For the ADI method, the Crank–Nicolson scheme and ADI factorization were applied for time integration, i.e., ADI methods

$$\begin{aligned} 1 + \frac{\Delta t}{2} \left(u^{n+1} \frac{\partial}{\partial x} - D \frac{\partial^2}{\partial x^2} \right) c^* &= 1 - \frac{\Delta t}{2} \\ &\times \left(u^n \frac{\partial}{\partial x} + v^n \frac{\partial}{\partial y} - D \frac{\partial^2}{\partial x^2} - D \frac{\partial^2}{\partial y^2} \right) c^n \\ 1 + \frac{\Delta t}{2} \left(v^{n+1} \frac{\partial}{\partial y} - D \frac{\partial^2}{\partial y^2} \right) c^{n+1} &= c^*, \end{aligned} \quad (14)$$

where c^* is the intermediate variable for species concentration, superscripts n and $n + 1$ stand for numerical solutions at time step n and $n + 1$, respectively. The multi-dimensional problem becomes a sequence of one-dimensional (1D) problems after ADI factorization. The procedure consists of multiple applications of one-dimensional tri-diagonal matrix solutions which produces a computationally cost effective solution. The combination of hybrid Padé (HPD) schemes and ADI method (HPD–ADI) was developed, which has been demonstrated to be unconditionally stable and able to reach third or fourth order in space for convection-dominated diffusion problems [38].

The second-order Runge–Kutta method involves two steps, prediction and correction, as follows: prediction step

$$c^* = c^n - \Delta t \left(u^n \frac{\partial c^n}{\partial x} + v^n \frac{\partial c^n}{\partial y} + D \frac{\partial^2 c^n}{\partial x^2} + D \frac{\partial^2 c^n}{\partial y^2} \right), \quad (15)$$

correction step

$$c^{n+1} = 0.5 \left(c^n + c^* - \Delta t \left(u^{n+1} \frac{\partial c^*}{\partial x} + v^{n+1} \frac{\partial c^*}{\partial y} + D \frac{\partial^2 c^*}{\partial x^2} + D \frac{\partial^2 c^*}{\partial y^2} \right) \right). \quad (16)$$

The numerical accuracy can reach second order in time for both methods. The performance of both methods, including numerical accuracy and computational efficiency on uniform grids and non-uniform grids without transformation, has been studied and the detailed description on these high-order numerical methods can be found in our previous paper [38].

Code validation

An unsteady problem concerning the convection–diffusion of a Gaussian pulse in the square domain $[0, 2] \times [0, 2]$ is considered here to examine the validity and effectiveness of computational codes based on high-order numerical methods. An analytical solution to this problem is given as

$$\phi(x, y, t) = \frac{1}{4t+1} \times \exp \left(-\frac{(x-ut-0.5)^2}{D^x(4t+1)} - \frac{(y-vt-0.5)^2}{D^y(4t+1)} \right). \quad (17)$$

The initial and Dirichlet boundary conditions are taken directly from the analytical solution. The flow parameters are given in table 1. This is a typical convection-dominated diffusion problem. To compare numerical accuracy and computational cost, the well-known ADI method proposed by Peaceman and Rachford (PR-ADI), based on second-order central schemes, and three other high-order numerical methods [38] developed previously by our group were applied to the uniform grid with mesh size $\Delta x = \Delta y = 0.025$. Very small CFL numbers ($\text{CFL} = 0.08$) are employed case and numerical integrations are advanced in time for 5000 steps to examine time-independent spatial accuracy. Figure 3 compares numerical contour plots (solid lines) with the exact solutions (dotted lines) at $t = 0.0125\text{s}$ for the PR-ADI and third-order explicit methods. The results show that there is significant distortion on contour plots in figure 3(a) resulted from the second-order central scheme using the PR-ADI method, while numerical results from third-order explicit methods are almost indistinguishable from exact solutions (see figure 3(b)). Excellent agreement between numerical results and exact solutions were also obtained for the HPD–ADI and fifth-order explicit methods (not plotted here to avoid redundancy). The L^2 -norm of errors, maximum error and CPU time used by four different schemes are compared in table 1. The comparison shows that numerical errors produced by high-order numerical schemes [38] are one order of magnitude smaller than those produced by the second-order PR-ADI method. Additionally, the CPU time required for high-order numerical methods are higher than those required for the PRADI method. This test case demonstrated that numerical schemes with high-order (at least third order) accuracy are required to simulate a convection-dominated diffusion problem. In terms of high-order numerical accuracy, the HPD–ADI method was computationally most cost effective. For this reason, we calculated most of the numerical mixing results using the HPD–ADI method unless otherwise specified. Explicit third-order and fifth-order methods were applied in numerical experiments to cross check and ensure the accuracy of the HPD–ADI results.

Experimental validation

In this paper, numerical simulations with high-order accuracy were applied for development of a prototype unsteady T-form mixer. The numerical results were validated by experimental tests. The micro-channel device was fabricated at the Nanoelectronics Research Facility (NRF) at UCLA. Negative photo resist SU8–2050 from MicroChem (Newton, USA) was used to fabricate a mold using photolithography. SU-8 is a negative epoxy-based photoresist capable of producing high-aspect ratio features. The height of the SU-8 mold was measured using a Dektak-8 profilometer (Veeco Instruments Inc., Woodbury, New York, USA). Polydimethylsiloxane (PDMS, Sylgard™ 184, Dow Corning) was poured into the SU-8 mold and then carefully peeled off after curing at 65 °C for 4 h. The mixer was formed by sandwiching the PDMS channel between two microscope slides. Three holes were drilled in one of the microscope slides to form flow inlets and outlet. A twin-channel syringe pump (Harvard Apparatus, Holliston, USA) drove DI water containing two different dyes through two inlets into the micro channel. Two pinch valves (Bio-Chem Valve, Boonton, USA) were used between the syringe pumps and flow inlets to generate in-line pressure disturbances. The pinch valves were controlled by the circuit shown in figure 4. A wave generator (Agilent 33120A, Agilent Technologies, Inc., Palo Alto, USA) was used to generate the sinusoidal or square wave for the control signal. For the positive control signal from the wave generator, the NPN bipolar junction transistor (BJT) is on and pinch valve 1 is energized, while the PNP BJT and pinch valve 2 are turned off. Alternatively, the NPN BJT and pinch valve 1 are turned off for negative control signal, while the PNP BJT and pinch valve 2 are turned on. In-line pressure disturbances are generated by two pinch valves with 180° phase difference. The frequency of disturbance generated by this setup can reach up to 160 Hz. The function of the pinch valves here is to generate pressure disturbances rather than pinching off the flow. Therefore, the voltage to drive pinch valves can be lower than their standard working voltage. The pressure disturbance amplitudes were adjusted by two potentiometers (see figure 4). The flow fields were visualized by two different dyes and recorded using a microscope (Nikon Eclipse TE2000-U) and CCD camera (Sony SSC-DC 50A). Flow pattern images were compared with the numerical results on a species concentration contour.

Results and discussion

Numerical simulations: linearity of flow fields

In this paper, the principle of linear superimposition was employed for velocity fields with different combinations of mean input flow and pressure disturbances. Two different flow rates, $Q = 0.8 \mu\text{l min}^{-1}$ and $Q = 2.0 \mu\text{l min}^{-1}$, were considered. The corresponding flow Reynolds numbers are 0.096 and 0.24, respectively. First, the linearity of the flow field was examined by comparing the steady flow solutions of stream lines with two different flow rates, shown in figure 5. Again, only partial flow fields at the vicinity of the T-junction was plotted for clarity. The stream function at $Re = 0.096$ (solid lines) was multiplied by a factor of 2.5 to compare with that at $Re = 0.24$ (dash lines). Overall, streamlines at $Re = 0.096$ after linear amplification were indistinguishable from that at $Re = 0.24$, which means that the steady flow fields were linear at such low Reynolds number conditions ($Re \leq 0.24$).

To examine the linearity of unsteady flow fields, two different types of inflow conditions, described in equations (9) and (11), were enforced at two inlets (figure 1). Again, two different flow rates, $Q = 0.8 \mu\text{l min}^{-1}$ and $Q = 2.0 \mu\text{l min}^{-1}$ were considered. For single frequency disturbances, the Strouhal number (equation (10)) was fixed at $St = 0.56$ and the disturbance amplitude ε equals 20 for both flow rates. The corresponding frequency is $F = 4 \text{ Hz}$ for $Q = 0.8 \mu\text{l min}^{-1}$ and $F = 10 \text{ Hz}$ for $Q = 2 \mu\text{l min}^{-1}$, respectively. For disturbances with multiple frequencies in equation (11), a small disturbance amplitude $\varepsilon_N = 0.25$ was chosen for all different component with different frequencies. As described in the mathematical model

section, unsteady simulations were carried out until flow fields reached a periodical state in time, followed by a Fourier transformation to analyze mean flow and disturbances with different frequencies. The nonlinear effects from inertial terms in equation (2) would lead to the distortion of mean flow and the generation of a new disturbance component with double frequency. The distortion of mean flow, superposition of velocity disturbances and generation of disturbances with double frequency are discussed as follows.

Figure 6 compares the mean flow (solid lines) with distortion from unsteady disturbances ($St = 0.56$, $\varepsilon = 20$) with steady flow solutions (dash lines) at $Re = 0.096$. There was little difference in velocity fields in the side channels before confluence and in the mixing channel after confluence, while there was an obvious difference located mainly near the T-junction due to unsteady distortion. For flow with higher Reynolds number at $Re = 0.24$, there was a more significant distortion of the mean flow (figure 7) compared with the lower flow rate case (figure 6). This increased distortion is not surprising because there was more nonlinear effect from inertial terms in equation (2) for flows with higher Reynolds numbers. In this paper, the unsteady distortion on mean flow is not considered when the principle of linear superposition is employed to calculate velocity fields. The nonlinear effect including unsteady distortion of mean flow on mixing results will be discussed later in this section.

Figures 8 and 9 compare the amplitude of velocity disturbances from solutions of Navier—Stokes equations with solutions from superimposition for two different flow rates. The disturbance amplitude is adjusted by a factor of 80 ($\varepsilon_N \times 80 = 20$) after Fourier transformation to match the results from unsteady simulation with single frequency. For $Re = 0.096$, there is a close agreement in contour plots of velocity disturbance amplitudes (figure 8), while there is visible distortion for flow at $Re = 0.24$ (figure 9) due to increasing nonlinear convective effect at the higher Reynolds number.

Figure 10 shows the amplitude of velocity disturbances at double frequency ($F = 20$ Hz) resulting from unsteady inflow at $Re = 0.24$ with disturbance frequency $F = 10$ Hz and amplitude $\varepsilon = 20$. Compared with the amplitude of disturbances in figure 9, the amplitude of disturbance generated at double frequency is approximately one order of magnitude smaller. The amplitude of disturbances at double frequency for $Re = 0.096$ and $St = 0.56$ is even smaller with relatively less nonlinear effects at lower Reynolds number (data not shown). Therefore, the nonlinear effect on mixing from the disturbances at double frequency is negligible for $Re \leq 0.24$, $\varepsilon \leq 20$.

Numerical simulations: motion of unsteady flow

Transient streamlines are plotted in figure 11 to show the motion of unsteady flow with $Re = 0.096$, $St = 0.56$ and $\varepsilon = 20$. Unsteady velocity fields were calculated from linear superposition. Figure 11(a) represents streamlines at positive peak disturbances while figure 11(b) shows streamlines at negative peak disturbances. It is obvious that there is separation of streamlines at the lower confluence corner in figure 11(a), which leads to some of the blue reagent from lower inlet a entering the mixing channel and traveling into upper inlet b while displacing the yellow solution (see figure 12). After half of the period of perturbation, the pulse reaches the negative peak value (figure 11(b)), and the blue solution is pushed back by the yellow solution. Driven by the yellow solution, the blue solution that had previously flowed into the upper inlet was expelled into the mixing channel and partially retreated back to inlet a. The flow was periodical and symmetric in time. As a result, both the and yellow solutions were separated into small layers and entered the mixing channel alternately, significantly increasing interface area and inducing the diffusion effect to achieve mixing.

Numerical simulations: species concentration

Species concentration was solved from the species equation (equation (3)) using high-order accurate numerical methods the velocity fields were given.

Figure 12 displays species concentration contours at flow conditions $Re = 0.096$, $St = 0.56$, $\varepsilon = 20$ derived from two different numerical methods, i.e., the software package and fifth-order explicit method. Two different solutions with different concentrations, 0.01 M and 0.0 M represented yellow and blue respectively, mixed in the confluence channel. Without disturbances, there was a distinct interface between yellow and blue solutions after confluence, as shown in figure 1. With pressure disturbances, the two solutions were separated into small layers in the confluence channel (see figure 12). Each layer stretched forward from the two corners of the T-junction and propagated downstream with the flow. Due to viscous friction from the channel wall, the flow moved much more quickly near the center of the channel than the inside of the boundary layer. The leading head of each layer traveled with maximum velocity in the channel while the trailing edge of each layer stretched back to the two corners of the T-junction. As a result, each piece was stretched into a crescent shape, and continued to be elongated during downstream propagation. Near the wall boundary, each elongated layer alternated between the yellow and blue solution. The folding of multiple alternate layers of blue and yellow solutions in the vicinity of thin boundary layer yielded efficient mixing and rendered the color green for the mixture in this region.

It should be noted that due to the boundary-layer flow effect, there was a sharp pulse-shaped mixture pattern, rather than a regular rectangular segment, as the blue solution traveled into the upper inlet channel. The thickness of the multiple alternating layers near the wall boundary can be significantly reduced or totally eliminated if the amplitude of disturbance was not high enough for the blue solution to reach the top right corner of the T-junction or for the yellow solution to reach the bottom right corner of the T-junction. The effect of disturbance amplitude on mixing will be discussed in more detail later in this section.

In figure 12(a) (results from the software package), the interface between yellow and blue solutions was very clear near the T-junction. Due to diffusion, the interface gradually blurred and the color of the mixture turned green further downstream. In contrast, in figure 12(b) the interface between the yellow and blue solutions remained clear near the exit of the channel in figure 12(b) based on the results using the fifth-order explicit methods. Comparing the mixing results shown in figures 12(a) and (b), better mixing was obtained from the software package. The species concentration contours in figures 12(a) and (b) were calculated based on same velocity fields, while different numerical methods were applied to solve the species equation. To determine which numerical solution was correct, distributions of the instantaneous species concentrations along the central line of the mixing channel from different numerical methods for the same flow conditions and numeral grids were compared in figure 13. For different numerical methods, second-order numerical schemes were employed for integration in time, while different numerical schemes were utilized for spatial definition of PDE. Significant oscillations in concentration curves were observed due to the alternate movement of blue and yellow solutions in the mixing channel. The numerical results based on the present HPD—ADI methods, explicit-third and fifth-order methods were indistinguishable, indicating that the numerical accuracy of computational-cost effective HPD—ADI methods was high enough to capture the detailed structure of the species concentration oscillations based on current numerical grids. For results shown in the rest of this paper, HPD—ADI methods are applied without specification. The oscillation amplitude decayed very rapidly during downstream propagation using first-order spatial accuracy numerical method. This oscillation amplitude decay was due to high erroneous numerical diffusion from the low-order numerical scheme in spatial definition of PDE. The quality of numerical results from the software package was better than that of the first-order method, but there was significant damping of oscillation due to high

erroneous numerical diffusion. The high numerical diffusion can explain the spurious mixing shown in figure 12(a).

Numerical simulations: evaluation of mixing degree

To quantitatively evaluate mixing efficiency at each station along the mixing channel, the time average mixing index was defined as

$$I_{ave} = AVE \left(1.0 - \frac{1}{\bar{c}} \sqrt{\frac{\sum_{i=1}^{N_1} (c_i - \bar{c})^2 \left(\frac{V_i}{\bar{V}} \right)}{N_1}} \right), \quad (18)$$

where c_i and V_i are species concentration and time averaged velocity in the i th cell across the channel, respectively, $\bar{c}$ ($=0.05$ M) is the output concentration for an ideal mixer and $\bar{V}$ is the mean velocity. Thirty-two points were evenly chosen in one period to calculate the time averaged mixing index. Figure 14 compares the time average mixing index computed from two different methods. For two different flow rates with flow Reynolds numbers $Re = 0.096$ and $Re = 0.24$, respectively, the software package consistently over predicts the degree of mixing. For a very low Reynolds number, $Re = 0.096$, the maximum difference in the values of the average mixing index between the two different numerical methods was more than 26%, even though the difference at $x = 3$ mm between 76% and 80% from different methods was relatively small. At $Re = 0.24$, mixing index could only achieve 70% at $x = 3$ mm based on current results, though the value using the software package reached 94%. Therefore, there was a serious numerical diffusion problem using low-order-based numerical software to solve the convection-dominated diffusion equation at higher Peclet number. Due to spurious mixing from numerical diffusion, the software package predicted better mixing for high Reynolds number flow when Strouhal number is fixed at $St = 0.56$ and a disturbance amplitude equals 20. From the present simulation, the mixing efficiency at $x = 3$ mm is 6% lower for $Re = 0.24$ to compared the case for $Re = 0.096$. This can be explained by the difference in residence time for mixing. The blue and yellow solutions are separated into small layers and laid out alternately in the mixing channel by pressure perturbations. After separation, mixing occurs mainly through boundary-layer flow with elongation of mixture patterns, which can continuously increase the interface. The last mixing step leading to homogenization is molecular diffusion, which is highly dependent on interface area and the gap between two different solutions. Similar mixture patterns can result from separation of solutions due to the pressure disturbance and subsequent stretching with boundary-layer flow at the same Strouhal number for different flow Reynolds numbers. However, the residence time of mixture in the channel is longer for lower Reynolds number flow compared to high Reynolds number flow. Consequently, there was more molecular diffusion that resulted in better mixing for low Reynolds number flow.

Numerical simulations: the nonlinear effect on the degree of mixing

The linearity of flow fields has been examined at the beginning of this section. The solutions from the Navier—Stokes equations and the superimposition without linear effect are plugged into equation (3) to examine the nonlinear effect on mixing efficiency. Figure 15 compares the mixing index with and without nonlinear effect at fixed $St = 0.56$, $\varepsilon = 20$ for two different flow Reynolds numbers, $Re = 0.096$ and $Re = 0.24$. As expected, there was a much smaller difference in mixing index curves for the lower Reynolds number case described in figure 15. If we neglect the transient effect near the T-junction, the difference in mixing index curves with/without nonlinear effect is less than 3% for $Re = 0.096$. For the higher Reynolds number $Re = 0.24$,

there was about 6.8% difference in mixing index at $x = 3$ mm due to more significant distortion of mean flow as shown in figure 7.

Numerical simulations: the effect on mixing from the disturbance amplitude

To study the effect on mixing from disturbance amplitude, five evenly distributed disturbance amplitudes ranging from 5 to 15 were selected to construct unsteady velocity fields using superimposition. The flow conditions are specified as $Re = 0.096$ and $St = 0.42$. The mixing results at different amplitudes are plotted in figure 16. There is a clear trend for higher mixing degree with increasing disturbance amplitudes. In fact, exactly the same instantaneous species concentrations along the central lines were obtained for different disturbance amplitudes, which are similar to those shown in figure 13. In other words, the increasing disturbance amplitude does not improve mixing near the center of the mixing channel. However, when the disturbance amplitude increases, more blue solution can enter the top boundary layer and more yellow solutions can enter the bottom boundary layer of the mixing channel; this greatly enhances mixing near the wall boundary. This phenomenon explains why the overall mixing index increases for higher disturbance amplitudes. The mixing index at $x = 3$ mm increases from 68.3% to 78% when disturbance amplitude increases from 5 to 15.

Numerical simulations: the optimal Strouhal number for efficient mixing

Better mixing can be obtained from higher disturbance amplitudes, but higher amplitude requires higher external energy. Another parameter that can significantly affect mixing efficiency is disturbance frequency, which is represented by the Strouhal number for the fixed base flow rate. Parametric study was conducted to determine the best mixing condition in terms of the Strouhal number. Two flow rates with flow Reynolds numbers $Re = 0.096$ and $Re = 0.24$ were considered. For each flow rate, a total of 15 frequencies ($f_n = nf_1, f_1 = 1$ Hz) with the lowest frequency of $f_1 = 1$ Hz were used. The corresponding Strouhal numbers range from 0.14 to 2.1 for $Re = 0.096$, and from 0.056 to 0.84 for $Re = 2.4$. A disturbance amplitude of $\varepsilon = 20$ was chosen for $St = 0.56$. For other cases, the disturbance amplitudes were chosen to be proportional to the Strouhal number ($\varepsilon = 35.7 \times St$) to keep the pulse volume independent from pressure disturbances [12].

Figure 17 shows contours of species concentrations at $Re = 0.096$ with different disturbance frequencies, (a) $F = 1$ Hz, $St = 0.14$, (b) $F = 2$ Hz, $St = 0.28$, (c) $F = 4$ Hz, $St = 0.56$, (d) $F = 8$ Hz, $St = 1.12$, respectively. It was obvious that coarse mixture patterns with crescent shape were obtained for lower frequencies ($F = 1-2$ Hz), while the mixture pattern were refined for higher frequencies ($F = 4, 8$ Hz). The blue and yellow solutions were separated into much smaller layers in the mixing channel at higher frequencies, thus significantly increasing the interface area between the two solutions and thereby improving mixing. Intuitively, higher disturbance frequency would be expected to improve mixing efficiency. This effect was observed for mixing near the center area of mixing channel. However, judging by the color of mixture near the wall boundary shown in figure 17(d) for high frequency ($F = 8$ Hz, $St = 1.12$), higher disturbance frequency worsened the mixing efficiency. Specifically, yellow solution occupies the top boundary and blue solution occupies the bottom boundary in figure 17(d). The profiles of species concentrations at $x = 3$ mm were compared in figure 18 for $Re = 0.096$ with different Strouhal numbers. For the lowest frequency case ($f = 1$ Hz, $St = 0.14$), the strongest oscillation in species concentration occurred near the center of the channel. The oscillation in concentration profiles near the center decreased as disturbance frequency increased. In contrast, the species concentration near the wall was closer to the results of an ideal mixer (0.005 M) for the lower frequencies, while the concentration near the wall was closer to the initial condition for higher frequencies. In other words, better mixing near the wall was obtained at lower frequencies. Mixing was considered optimal when the overall concentration dispersion across the channel was minimized.

Figure 17(d) shows a case in which the space nearest the mixing channel wall was occupied either by yellow solution (near upper wall) or by blue solution (near lower wall). Mixing would be greatly enhanced if more blue and yellow solutions could be moved into the top and bottom layers, respectively. From the above discussion, there was sharp pulse-shaped mixture pattern when the blue and yellow solutions traveled to the wall opposite the vertical inlet channel due to the boundary-layer flow effect. At higher disturbance frequencies, the disturbance amplitude is proportionally higher to maintain the same pulse volume. The flow inside the boundary layer lags further behind for higher central flow velocities. At higher frequencies, the pulse shape of each solution becomes sharper in the vertical inlet channels. As a result, higher frequencies reduce the volume of blue (or yellow) solution entering the top (or bottom) layer of the mixing channel, leading to less efficient mixing near the channel wall (figures 17(d) and 18).

Figure 19 compares the overall mixing index for four different Strouhal numbers at a fixed Reynold's number, $Re = 0.096$. There was a dramatic increase in mixing index curves at different disturbance frequencies due to splitting and folding of solutions by pressure perturbation. At the lowest frequency ($St = 0.14$), there is strong oscillation in species concentration due to the coarse mixture pattern near the center of the channel (see figure 17) that leads to a low global mixing index. When frequency increases to 0.28, the mixing index also increases due to better mixing in the center of the channel. However, the overall mixing degree at $St = 0.56$ is lower than that at $St = 0.28$ due to less efficient mixing near the boundary layer. At very high frequency ($St = 1.12$), the overall mixing degree is further reduced, and the slope of the mixing index curve becomes almost flat due to slow molecular diffusion in unmixed solutions near the channel wall.

The mixing index as a function of the Strouhal number (non-dimensional disturbance frequency) is plotted in figure 20 for two different flow Reynolds numbers $Re = 0.096$ and $Re = 0.24$. The mixing index became much higher at lower flow rates due to longer diffusion time. It is obvious that the mixing index peaks around $St = 0.42$, which is the optimal mixing condition for disturbance frequency at different flow rates. At optimal disturbance frequency $St = 0.42$, the maximum mixing degree is 78% and 74% for $Re = 0.096$ and $Re = 0.24$, respectively. The corresponding disturbance amplitude is $\varepsilon = 15$. Based on the above discussion regarding the effect of disturbance amplitude on mixing, an even better degree of mixing can be achieved with higher disturbance amplitude.

Experimental validation

Based on the results of numerical simulation, we designed, fabricated and tested the T-mixer. The performance of the mixer was tested using aqueous solutions containing yellow and blue dyes. The image of the flow was compared with the numerical results in terms of the species concentration contour. Figure 21 compares the species concentration distribution between the numerical results (on the top) and the experimental results (on the bottom) with fixed $Re = 0.096$ for (a) $St = 0.28$, (b) $St = 0.56$ and (c) $St = 1.12$, respectively. There was good agreement in mixture patterns between numerical and experimental results, which qualitatively validated our simulation of the T-form mixer. Better mixing was observed from experimental results based on the flow patterns shown in figure 21 due to integrated effect (3D effect) from the z -direction when picture was taken. Quantitative measurement and study of 3D effects on mixing will be conducted in our future work.

Conclusions

An unsteady T-form mixer with simple confluence geometry was designed and improved utilizing hydrodynamic pressure disturbances. Computational fluid dynamic (CFD) simulations were applied to improve mixing index.

It was found through numerical experiments that low-order-based commercial software packages are not suitable to simulate a convection-dominated mixing process due to erroneous computational dissipation. New numerical algorithms with high numerical accuracy and computational-cost effectiveness were proposed to solve the convection-dominated diffusion problem, which were validated by numerical tests.

The principle of linear superposition was employed to calculate velocity fields, which were then plugged in to solve the scalar equation for species concentration. This approach resulted in significant computational time savings and made it feasible to conduct parametric studies to find the best mixing condition.

Based on our numerical simulation results, the best mixing condition in terms of the Strouhal number was found to be $St = 0.42$ for flow Reynolds numbers less than 0.24. The mixing index reaches the range of 75% at $x = 0.3$ mm, disturbance frequency of $St = 0.42$ and disturbance amplitude of $\varepsilon = 15$ for flows with Reynolds number less than 0.24.

The numerical results were validated by the experimental observation of mixing of two aqueous solutions containing visualizing dyes under the microscope. The flow patterns from the numerical results qualitatively matched those from the experimental results.

Acknowledgments

The research work was supported by Bioengineering Research Partnership grant EB00127 from the National Institute of Biomedical Imaging and Bioengineering, NIH, Metabolomics Project (1R33DK070328) from NIH, and by the Pacific-Southwest Center for Biodefense and Emerging Infections Diseases Research UC Irvine/NIH NIAID Award (1 U54 AI 065359) 2005-1609.

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Figure 1.
Dimensions and coordinates of the T-form mixer model.

Figure 2.
Computational grids for the T-form mixer.

Figure 3.

Contour plots of the Gaussian pulse at $t = 0.0125$ s. (a) PR-ADI [44]; (b) third-order explicit methods. $\Delta t = 2.5 \times 10^{-5}$, $\Delta x = \Delta y = 0.025$, $u = v = 80$, $D = 0.01$. Solid lines: numerical solutions; dotted lines: exact solutions.

Figure 4.
Control circuit for pinch valves to generate pressure disturbances.

Figure 5. Comparison of streamlines (stream function) between $Re = 0.096$ and $Re = 0.24$. Solid lines: $Re = 0.096$; dash lines: $Re = 0.24$.

Figure 6. Comparison of mean flow with steady flow solutions. (a) $\bar{u}$; (b) $\bar{v}$. Solid lines: mean flow, dash lines: steady flow solutions, $Re = 0.096$, $St = 0.56$.

Figure 7. Comparison of mean flow with steady flow solutions. (a) $\bar{u}$; (b) $\bar{v}$. Solid lines: mean flow; dash lines: steady flow solutions, $Re = 0.096$, $St = 0.56$.

Figure 8.

Comparison of amplitude of velocity disturbances. (a) u' ; (b) v' . Solid lines: solutions of Navier—Stokes flow; dash lines: solutions from superimposition. $Re = 0.096$, $St = 0.56$.

Figure 9.

Comparison of amplitude of velocity disturbances. Solid lines: solutions of Navier—Stokes flow; dash lines: solutions from superimposition. (a) u' ; (b) v' . $Re = 0.24$, $St = 0.56$.

Figure 10.

Amplitude of velocity disturbances at double frequency resulting from the nonlinear effect.

(a) u' ; (b) v' . $Re = 0.24$, $St = 0.56$.

Figure 11. Numerical results of streamlines at positive peak disturbances (a) and negative peak disturbances (b). $Re = 0.096$, $St = 0.56$, $\varepsilon = 20$.

Figure 12. Contour plots of species concentration from different numerical methods. (a) Software package; (b) present method (Explit fifth). $Re = 0.096$, $St = 0.56$, $\varepsilon = 20$.

Figure 13. Comparison of species concentration along the central line of the mixing channel. $Re = 0.096$, $St = 0.56$, $\varepsilon = 20$.

Figure 14.

Comparison of the mixing index from two different methods. $St = 0.56$, $\varepsilon = 20$.

Figure 15.
Comparison of the mixing index with/without nonlinear effects at fixed $St = 0.56$, $\varepsilon = 20$.

Figure 16.

Comparison of the mixing degree at fixed $Re = 0.096$, $St = 0.42$ with different disturbance amplitudes. (a) Mixing degree along the mixing channel; (b) mixing degree at the exit of the channel ($x = 3$ mm).

Figure 17. Contour plots of species concentration at the same flow rate with different Strouhal numbers. (a) $St = 0.14$, $\varepsilon = 5$; (b) $St = 0.28$, $\varepsilon = 10$; (c) $St = 0.56$, $\varepsilon = 20$; (d) $St = 1.12$, $\varepsilon = 40$.

Figure 18.
Comparison of profiles of species concentration at $x = 3$ mm for $Re = 0.096$ with different Strouhal numbers.

Figure 19.
Comparison of the mixing index at $Re = 0.096$ with different Strouhal numbers.

Figure 20.
Degree of mixing as a function of Strouhal number at two different Reynolds numbers.

Figure 21.

Comparison of species concentration distribution between numerical results (top) and experimental results (bottom) with fixed $Re = 0.096$. (a) $St = 0.28$; (b) $St = 0.56$; (c) $St = 1.12$.

Table 1

Numerical errors and CPU times used by four different schemes for a Gaussian pulse problem.

Method	L^2 -norm error	Maximum error	CPU time (s)
PR-ADI	2.18	3.74×10^{-1}	1.88
HPD—ADI	5.15×10^{-2}	1.24×10^{-2}	2.98
Explicit third	3.61×10^{-2}	5.99×10^{-3}	4.57
Explicit fifth	2.57×10^{-3}	5.53×10^{-4}	5.54

$\Delta t = 2.5 \times 10^{-5}$, $t = 0.0125$, $\Delta x = \Delta y = 0.025$, $u = v = 80$, $D^x = D^y = 0.01$.