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ABSTRACT

To improve mixing, obstacles have been placed in the channel to try to disrupt flow and reduce the diffusion path. The disruption to flow velocity field alters the flow direction from one fluid to another. In this way, convection may occur to enhance the mixing. Ideally, properly designed geometric parameters, such as layout and number of obstacles, improve the mixing performance without increasing the pressure drop. In this work, the commercial computational fluid dynamics (CFD) tool for microfluidics is used to study the mixing of two liquids in a “Y” channel. The results indicate that asymmetric layout of the obstacle has more effect on the mixing than the number of obstacles. Placing obstacles in the microchannels is a novel method for mixing in microfluidic devices, and the results can provide useful information in the design of these devices.

Key words: Microfluidics, mixing, micro-flow, micromixer, microreactor, microchannel, CFD, Simulation, MEMS

1. INTRODUCTION

The lab-on-a-chip technology has stimulated considerable research in recent years, and for many of such systems, they need to mix two or more fluid streams together to fulfill the task. Therefore, the mixing unit is one of the critical elements of such a system. In general, because the Reynolds number is low in typical microfluidic channels, the viscous forces play a dominant role. As a result, the flow is laminar under normal conditions, especially for liquids.

Therefore, diffusion, rather than turbulence affects the mixing of binary or multi-components fluid streams in a microchannel. Diffusion is a slow process for mixing, even in a microscaled device [1]. For a typical microfluidic device, the length scale is too large for a rapid diffusion and too small to include mechanical agitation. Furthermore, the channel length for fully developed mixing is limited on microscaled chips and increasing the length for mixing also means increasing the pressure drop, and this makes the design of microchips more difficult and the micropump may fail to drive the fluids through the channels.

Therefore, it is necessary to enhance the mixing within the microchip without increasing the pressure drop too much. It is possible to achieve this by dynamic mixing with the assistance of externally forced mass transport, i.e., Yang et al. [2] used ultrasonic waves to enhance mixing, and Knight [3] described fast mixing by forming and controlling nanoscale, submerged fluids jets. However, it is much easier to control mixing in a laminar flow using a static micromixer. The principle of a static micromixer can be categorized into four types. (a) T-shape micromixer. The “T” mixer simply combines two or more fluid streams, which flow parallel to each other in the microchannel, and mixing relies purely on molecular diffusion (Jacobson et al. [4]). The “T” mixer normally has small channel width at the order of tens of microns and sufficient channel length. (b) Geometrically splitting and recombining substreams. In this way, large contact surfaces and small diffusion paths are generated (Ehrfeld et al. [5], Schwesinger, et al. [6], Koch et al. [7] [8]). (c) Chaotic Mixer. Stroock et al. [9] presented this mixer to stretch and fold the streams by rotating the streamline inside the microchannel. The circulation of the streamlines was due to the transverse pressure component created by the anisotropic resistance to viscous flow. Johnson et al. [10] reported similar structures machined by Excimer laser to achieve rapid mixing. However, the obvious drawback for these mixers is the dead volume created by these structures. (d) Altering flow direction laterally. This method tries to create stirring (convective) effects by forcing one fluid stream into another (Liu et al. [11], and He et al. [12]). Liu’s serpentine-shaped micromixer was more favorable to high Reynolds numbers (~70), and He’s in-situ micromixer could alter the flow direction, shrink the channel and divide the main stream into substreams. However, He’s mixer is not likely to be used in a pressure-driven environment, due to the large pressure drop in its packed columns.

The purpose of this investigation is to try to enhance mixing by placing obstacles in the channel. This structure is

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totally compatible with the currently micromachining techniques and can be easily realized by Excimer laser or silicon machining. This paper focuses on several general aspects of static micromixer design and the optimisation of layout of obstacles under a fixed Peclet number. Computer simulation was employed for this work and we also endeavoured to understand the phenomena by theoretical analysis

2. MIXING AT LOW REYNOLDS NUMBER

The Reynolds number is used to relate the inertial forces to the viscous forces, and is given by equation 1.

\[
Re = \frac{\rho \bar{u} l}{\mu} = \frac{\bar{u} l}{v}
\]  

(1)

Where \( \rho \) is the density, \( \bar{u} \) is the average velocity, \( \mu \) is the dynamic viscosity, \( l \) is the characteristic length and \( v \) is the kinetic viscosity.

In microfluidic devices, due to the low velocity of the flow and the micron size channels, the Reynolds number is usually low. This means that the viscosity plays a dominant role in microchannels rather than inertia and the vortices cannot exist in such a viscous flow. One classic paper by Purcell [13] describes fluid dynamic differences at the low Reynolds number. When \( Re << 1 \), the inertia dies off from the Navier-Stokes equation, and gives the governing equation at such low Reynolds number as

\[
\rho \nabla ^2 u = \nabla p
\]  

(2)

Where \( p \) is the pressure and \( u \) is the velocity.

Equation 2 indicates that the velocity is determined only by the pressure distribution, therefore, inertial force is irrelevant at low Reynolds number, and all motion is symmetric in time, as described by Brody [1]. At low Reynolds number, diffusion is dominant and mechanical agitation is ineffective at \( Re << 1 \) [13].

Molecular diffusion is a random process, and the diffusion time \( t_D \) to cross a distance \( l \) was given by Einstein in his paper about Brownian motion [14] in equation 3,

\[
t_D = \frac{l^2}{2D}
\]  

(3)

For the typical small molecular liquids with diffusion coefficient \( D \) of \( 10^3 \mu m^2/s \), the diffusion time to cross a 100 \( \mu m \) distance is about 5 seconds, but for 1\( \mu m \), the mixing time is more than 8 minutes, which is unrealistic in a microscaled device. For the mixing to be completed in millisecond, the diffusion path should be of the order of 1\( \mu m \). From equation 3, it is clear that diffusion is quite efficient when dimensions are of the order of microns, however, mixing needs to be enhanced when the length scale increases to hundreds or even tens of microns.

We consider microfluidic devices with microchannels of the order of hundreds of microns. Here, the diffusion is not very efficient due to the large diffusion path. It is helpful if we can introduce convection to enhance the mixing. The Reynolds number is so small that there will not be any turbulence in a microchannel, and convection may be the only means the mass transport in laminar flows compared to molecular diffusion. From Purcell [13], the mixing time by convection, \( t_c \), is

\[
t_c \sim \frac{l}{u_c}
\]  

(4)

where \( u_c \) is the convective velocity or stirring velocity that is consistent to the diffusion direction. The ratio of convection time \( t_c \) to molecular diffusion \( t_D \) is

\[
Pe = \frac{lu_c}{lD}
\]  

(5)
where $Pe$ was called Stirring number by Purcell and referred to as the Peclet number in the literature. Nevertheless, the Peclet number is the ratio of bulk mass transfer (Convection or Stirring) to molecular diffusitivity. The convection works only when the Peclet number is larger than 1, and hence we will try to enlarge the Peclet number to enhance mixing. For consistency with other literature, and also because the stirring velocity is the partial component of the mean velocity in the channel, the mean velocity $\bar{u}$ was used to calculate the Peclet number,

$$Pe = \bar{u} / D$$

Furthermore, the channel length $Lm$ for a complete diffusion mixing is,

$$Lm = \bar{u} \times t_D = Pe \times l$$

For a typical microchannel, when $Pe$ is less than 100, the length for pure molecular diffusion mixing $Lm$ is within one to several centimeters, which is the size of most of the microchips. Therefore, this research will focus on the Peclet number is larger than 100, which converting to Reynolds number, i.e. for water, is $Re > 0.1$. For others fluids, the relation between Reynolds number and Peclet number can be calculated by,

$$Re = \frac{Pe \times D}{\nu}$$

where $\nu$ is the kinetic viscosity.

Furthermore, it is also not necessary to study mixing in a micro-device for the Peclet number that is larger than $10^6$, because the amount of liquids can be easily mixed in a traditional way. For example, for low molecular liquids, the amount is about 1ml for 10 seconds through a 100µm by 100µm channel and can be shaken and mixed in a test tube. From the cost saving aspect of view, higher Peclet number large than $10^6$ is not preferable for the expensive reagent and samples. For the Peclet number ranging $10^2$ to $10^6$, the Reynolds number is still far below the critical transition threshold ($Re = 2300$), so the flow is in the laminar regime.

3. **ASPECT RATIO**

The height to width aspect ratio is one of the critical technical specifications for fabrication of microchannels. For a given flow rate, the mixing performance acts differently for different aspect ratio. For two fluids flowing parallel in a channel, the diffusion occurs at the interface of the two fluids (Figure 1). The fabrication of low aspect ratio microstructures is generally easier, however, for mixing, low aspect ratio microfluidic devices give small contact area between fluids.

Gobby, et al. investigated the aspect ratio with constant width [15], and we extend this investigation to a constrained area. For simplicity, we assume the bi-fluids travel at same velocity $\bar{u}$/flow rate, $Q$, through a channel with cross
section area $A$. Thus,

$$Q = Au$$

(9)

where

$$A = 2lH$$

(10)

and the height to width ratio $\alpha$ is

$$\alpha = \frac{H}{2l}.$$ 

(11)

We have,

$$\bar{u} = \frac{Q}{4\pi d^2}.$$ 

(12)

Using equations 3 and 12, we can obtain the travel distance $L_m$ for mixing in time $t$,

$$L_m = \bar{u}t = \frac{Q}{8\pi d}.$$ 

(13)

Therefore, if the flow rate is constant, the minimum length of the channel for a complete mixing, $L_m$, is identified as the reciprocal of the aspect ratio of the channel.

Equation 13 is a rough estimation of mixing length. Due to the Poiseuille-like velocity distribution, the velocity in the centre of the channel is higher, and the layers of liquid close to the walls have zero velocity. Therefore the fluid close to the centre of the channel has less time to diffuse than the fluid close to the wall. The fluid close to the wall will have more time to mix [16-19]. Clearly, the large height to width aspect ratio is not welcomed due to uneven distribution of the diffusion along detection section [20]. Conversely, the increased contact surface of fluids benefits process chemistry productivity, which is the main goal of mixing.

When the mixing due to pure molecular diffusion, equation 13 can be true. The diffusion works efficiently when the flow rate is small and the height to width ratio is high (Figure 2). On the other hand, the pressure drop, $\Delta p$, for fully developed laminar flow in a microchannel with an arbitrary cross section configuration is approximately,

$$\Delta p = \frac{128\mu Q}{\pi d_h^4}.$$ 

(14)

Where hydraulic diameter $d_h$ is given by the equation 15

$$d_h = \frac{4 \times \text{Area}}{\text{wetted \ perimeter}}.$$ 

(15)

Figure 3 shows examples of how the design of channel could affect the pressure drop. When designing a microchannel for mixing applications, the aspect ratio should be optimised to favor the mixing, but in addition, the pressure drop needs to be considered as well.
Figure 2. Aspect Ratio and flow rate affect the total length to achieve complete mixing

Figure 3 Pressure drop in a microchannel with same cross section area, different height to width aspect ratio, and different flow rate

4. MIXING BY THE ASSISTANCE OF OBSTACLES

From the analysis in section 3, we can see that mixing in a microchannel only by diffusion is difficult if the diffusion path is hundreds of microns. Our approach to improving mixing is to place obstacles inside the microchannel. Obstacles in the channel do not generate turbulence in the low Reynolds number flow, but can stir the fluid to create lateral mass transport to improve the mixing. Simulations were conducted of two fluid streams mixing in a Y-Channel.

4.1. Simulation of mixing in Y-Channel with obstacles

The Y-channel has two inlet and one outlet ports, and the angle between the inlets is 60 degrees. The width of the inlets is 200µm, the width of the outlet channel is 300, and the height of the channel is 100 µm. The length of the channel is 1.2mm for reducing computing time, except for the two obstacle arrays (configuration no.8) with a length of 2 mm. The diameter of the obstacle is 60µm. Table 1 gives the number of the obstacles in eight different designs. Figure 5 illustrates the layout of design no.6, no.7 and no.8, and the spacing for other designs are the same.

Figure 4 3D model of a Y-channel with 2 obstacles
Table 1  Configuration of microchannel with obstacles

<table>
<thead>
<tr>
<th>Configuration number</th>
<th>No.1</th>
<th>No. 2</th>
<th>No. 3</th>
<th>No. 4</th>
<th>No.5</th>
<th>No.6</th>
<th>No.7</th>
<th>No.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of obstacles</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>9</td>
<td>9</td>
<td>18</td>
</tr>
</tbody>
</table>

Figure 5  Layout of square and triangular configuration of obstacle array. (a). configuration No.6. (b). configuration No.7  (c). configuration No.8

The Y-channel is one of the T-type microchannels, and to improve mixing performance of the Y-channel, we placed obstacles in a microchannel. Simulations were performed using MemCFD by CoventorWare™ on Win NT4.0 with Pentium III 800MHz CPU and 128MB memory. Due to the limitation of the computer resource, the model was built in a 2D domain. The accuracy of the simulation will depends on the height to width aspect ratio. At low aspect ratio, the simulation is more accurate than that of at a high one. The aspect ratio we applied was 1:3 for demonstrating the concept. The sample fluids used in the simulation were water and ethanol (Table 2) . Steady flow with a Peclet number of 200 was assumed in the simulation. The results demonstrated the evolution of the design layouts using cylindrical obstacles in the microchannels (Figure 5 and 6). In Figure 6, the dark shading area was the fluid not mixed and bright area was the mixed area. The wider the bright area at the outlet, the better mixing.

Table 2  Properties of water and ethanol at 20 °C

<table>
<thead>
<tr>
<th>Fluids</th>
<th>Viscosity (kg/µm/s)</th>
<th>Diffusivity (µm²/s)</th>
<th>Density (kg/µm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>9.0e-10</td>
<td>1.2e3</td>
<td>9.998e-16</td>
</tr>
<tr>
<td>Ethanol</td>
<td>1.2e-9</td>
<td>1.2e3</td>
<td>7.89e-16</td>
</tr>
</tbody>
</table>
To evaluate the performance of mixing, mixing efficiency can be calculated by equation 16 [21],

\[
\text{mixing efficiency} = \left( \frac{\int_{0}^{2L} |c - c_{\infty}| \, dx}{\int_{0}^{2L} |c_{0} - c_{\infty}| \, dx} \right) \times 100\% \quad \text{(16)}
\]

where \( c \) is the mass concentration distribution across the transverse direction at the outlet, \( c_{0} \) is the initial distribution of the concentration before any mixing, and \( c_{\infty} \) is the concentration of a complete mixing. The simulation results of mixing efficiency and pressure drop in the Y-channel were calculated and plotted in Figure 7.
4.2. Discussion

The simulation results (Figure 6 and 7) illustrate that mixing increases as the number of obstacles increases. The increased mixing can be interpreted as the obstacles causing the parabolic velocity distribution to be evened out and give more time for the diffusion at the interface of the two liquids. However, the improvement of mixing performance is not proportional to the increasing of pressure drop or the number of obstacles. Configuration no.2&3 have approximately the same pressure drop, but configuration no.3 has much more mixing. Configuration no.6&7 have the same amount of obstacles, but no.7 has lower pressure drop and higher mixing efficiency. These results show that the asymmetric arrangements are favoring mixing better than symmetric ones.

For a given flow rate, the total time for the flow through the channel remains the same, because the average velocity at inlets and outlet remains the same for incompressible fluids (mass conservation). The local velocity, where the obstacles are, is increased to keep the constant flow rate. The asymmetric layout of obstacles gives different resistance to the flow in the lateral direction, so the fluids find their path through the lower resistance area, similar to the electric circuit. This means that part of the fluid flow is distorted and the redirection of the flow from one component to another and this illustrates the convective effect (Figure 8) and mixing relies largely on the velocity in the lateral direction.

5. CONCLUSION

With viscosity dominating flow in microchannels, mixing of two fluid streams mainly depends on diffusion. The mixing performance of the Y-channel mixer was examined by theoretical analysis and CFD simulation. The mixing for
a constrained flow rate and channel transversal area is affected by aspect ratio, and the increased height to width aspect ratio benefits the mixing. On the other hand, visualisation analysis in Y-channel (T-sensor) needs flat distribution of flow pattern, and a low aspect ratio is preferred. However, the theoretical foundation is the same for the industrial production and analysis in the laboratory. For industrial processing chemistry, the design requires shorter diffusion width, so that mixing can be completed in less time. When Y-channels are used for chemical analysis, they mostly require a very small height to width aspect ratio to reduce the distortion of flow pattern. A small height to width aspect ratio increased the width for the fluids to travel, and thus it has a poor mixing performance. To improve the performance of Y-channels, the use of obstacles was investigated. Obstacles in a microchannel with a low Reynolds number can not generate eddies or turbulence. However, the results demonstrated that obstacles can improve mixing performance by affecting the flow pattern, and the asymmetric arrangement of obstacles alter the flow directions and force one fluid to flow into another to create lateral mass transport. In this paper, this phenomenon was called convective effect to differ from the pure molecular diffusion.

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