

ALTERNATE FLOWS IN A MICROFLUIDIC DEVICE

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Abstract — *The mixing properties of systems combining alternate flows with obstacles are studied by numerical methods. Preliminary results show that the layers of high and low solute concentration, created by the alternate flow, are split into smaller chunks of fluid, due to the obstacles inserted in the mixing channel increasing the contact area between high and low concentration regions and decreasing the critical mixing length. The improvement in the mixing process shows that this method is very useful for designing mixers in lab-on-a-chip devices.*

Key Words: *oscillatory flow, alternate flow, fluidic mixer*

I INTRODUCTION

An essential requirement for any practical fully integrated lab-on-a-chip device is the ability to mix two or more fluids thoroughly and efficiently, i.e., in a reasonable amount of time. The microscale conditions have distinctive properties due to its small dimensions and typically low volume flow rate [1]. Rapid mixing becomes a challenging task, as due to strictly laminar flow conditions (it is generally operated at Reynolds numbers of less than 1), turbulent diffusion is absent and the mixing must be achieved by molecular diffusion (which is a rather slow process, even over short distances [2]) or chaotic advection [3,4]. Therefore, while small molecules can diffuse significant distances during the average residence time in the device, large molecules or particles that do not diffuse significantly during the same interval, will not move appreciably from their original stream unless the critical mixing length is small.

It is possible to improve mixing by using periodic flows [5,6], which will create a flow with layers of low and high solute concentration along the mixing channel. However, the thickness of these layers should be smaller than the half channel width.

Pressure driving flows have parabolic velocity profiles. The parabolic profile contributes to mixing since different layers will interpenetrate each other allowing mixing by diffusion in the

transversal direction. However, the fluid in the center of the channel has a small residence time and a high local Peclet Number.

In continuous flow, good mixing can be obtained by the split and join technique. However, this technique is only efficient if it is possible to turn the fluid in a tridimensional way. Splitting without rotation is inefficient.

This work combines alternate flow with the bi-dimensional split and join technique enhanced by obstacles. The function of the alternate flow is to create alternate layers of low and high concentrations. The function of the obstacles is to delay the fluid in the center of the mixing channel and to split the layers into smaller chunks that are easily mixable.

II MIXER DESCRIPTION

The mixer (Figure 1) has two entries, one for the reactant (R) and the other for the sample (S). The purpose is to mix a stream R with a stream S. Stream R is rich in a reactant R and stream S is rich in a sample S.

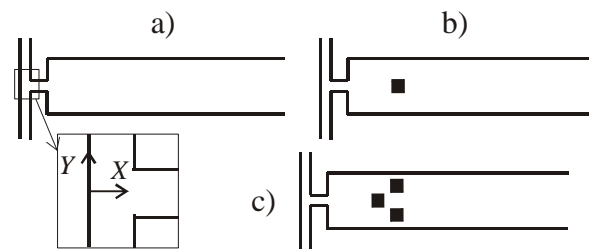


Figure 1. Schematic representation of the mixers studied.

Three versions of the mixer were studied, a version without an obstacle (Figure 1a), a version with a central obstacle (Figure 1b) and a version with three obstacles (Figure 1c). All versions have two

feed channels (of width W and length L_f), an ejector (of width W_e and length L_e), which connects to the mixing channel (of width W_m and length L_m). The width of the squared obstacle is W_{obs} . This geometry was selected so that symmetrical layers could be obtained, even for small frequencies and small Reynolds numbers. The width of the feed channel was taken as the characteristic dimension. The following non-dimensional geometrical variables were defined:

$$l_f = L_f/W; l_e = L_e/W; l_m = L_m/W \quad (1)$$

$$w_e = W_e/W; w_m = W_m/W; w_{obs} = W_{obs}/W \quad (2)$$

II.1 NUMERICAL METHOD

Numerical methods are used to simulate the alternate flow, the mixing, and the reaction in a T mixer. Alternate flow (Figure 2) is described by the following equation:

$$\begin{cases} V_R = 0.5V_0 \{1 + \beta \operatorname{sgn}[\sin(2\pi St \times t + \phi_R)]\} \\ V_S = 0.5V_0 \{1 + \beta \operatorname{sgn}[\sin(2\pi St \times t + \phi_S)]\} \end{cases} \quad (3)$$

where V_0 is the maximum velocity (for $\beta=1.0$), St is the Strouhal number based on the width of the channel (W), ϕ_R is the initial phase of the reactant stream and ϕ_S the initial phase of the sample stream and β is a constant. If this constant is highest than 1 the feed velocities is negative during half of the cycle.

The non-dimensional time, t , is given by:

$$t = V_0 T / W \quad (4)$$

where T is the dimensional time. The Strouhal number is given by:

$$St = fW / V_0 \quad (5)$$

where f is the frequency of the alternate flow.

The problem was solved numerically by a code developed in house based on the public available library Overture [7]. The study is being complemented by simulation using commercial computational fluid dynamics software, FluentTM.

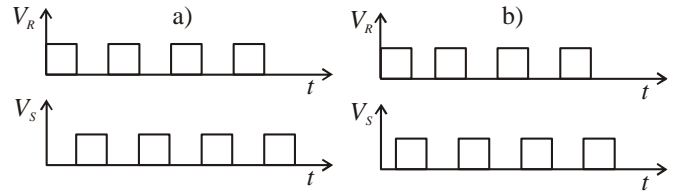


Figure 2. Inflow boundary conditions: (a) $\phi_R - \phi_S = \pi$; (b) $\phi_R - \phi_S = \pi/2$;

The developed code solves the Navier-Stokes equations and the mass transport equations for each component by a finite difference technique. The Navier-Stokes equations, in their velocity-pressure formulation, are:

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = -Eu_0 \nabla p + \frac{1}{Re} \nabla^2 \vec{v} \quad (6)$$

$$Eu_0 \Delta p = -\nabla_{v_x} \frac{\partial \vec{v}}{\partial x} - \nabla_{v_y} \frac{\partial \vec{v}}{\partial y} - \nabla_{v_z} \frac{\partial \vec{v}}{\partial z} \quad (7)$$

where x , y and z are the coordinates normalized by W and Eu_0 is the Euler number:

$$Eu_0 = P_0 / \rho V_0 \quad (8)$$

and Re the Reynolds number based on the channel width:

$$Re = \rho V_0 W / \mu \quad (9)$$

The mass transport equation for each component is:

$$\frac{\partial c_i}{\partial t} + \vec{v} \cdot \nabla c_i = \frac{1}{Pe} \Delta c_i - \alpha Da_i c_i \quad (10)$$

where α indicates if the component i is a reactant or a product ($\alpha=-1$ is a reactant, $\alpha=1$ is a product), Pe is the Peclet number:

$$Pe = V_0 W / D \quad (11)$$

and Da_i is the Damkohler number given by:

$$Da_i = K_i W / V_0 \quad (12)$$

where K_i is the kinetic constant of reaction i .

II.2 MIXING QUANTIFICATION

Mixing of the fluid was measured in vertical lines along the mixing channel. Mixing was quantified by (see [6]):

$$M = 1 - \sqrt{\frac{\sum_{i=1}^N \left(\frac{C_i}{\bar{C}} - 1 \right)^2}{N} \left| \frac{Vx_i}{\bar{V}} \right|} \quad (13)$$

where C_i is the concentration of each point in the vertical line sampled several times during a complete cycle, Vx_i is the tangential component of the local velocity, \bar{C} is the concentration of a perfectly mixed solution and \bar{V} is the average velocity.

III DIMENSIONAL ANALYSIS

The local velocity V in a given position of the mixer is a function of the coordinates of the point, X and Y , the time T , the width of the channel W , the feed velocity V_0 , the frequency of the alternate flow f , the constant β , the initial phase of each stream, the fluid transport properties (viscosity, μ , and density, ρ) and the geometry of the mixer (G):

$$V = f_1(X, Y, T, W, V_0, f, \beta, \phi_R, \phi_S, \mu, \rho, G) \quad (14)$$

The number of parameters of this relation can be significantly reduced by dimensional analysis:

$$v = f_2(x, y, t, \beta, \phi_S - \phi_R, Re, St, G) \quad (15)$$

The local concentration, C , is influenced by the flow field and will depend of the same variables as the local velocity. Additionally, the local concentration is a function of the feed concentration, C_0 , and the Damkohler number.

$$c = g(x, y, t, \beta, \phi_S - \phi_R, Re, Sc, St, G, Da_i) \quad (16)$$

Since mixing is independent of Y , then

$$M = h(x, t, \beta, \phi_S - \phi_R, Re, Re, Sc, St, G, Da_i) \quad (17)$$

For small Reynolds numbers, as the ones in microfluidic systems, the flow pattern is independent of the Reynolds number. In this case, the Schmidt and the Reynolds numbers can be grouped. The functional dependence of the mixing parameter becomes:

$$M = h_2(x, t, \beta, \phi_S - \phi_R, Pe, St, G, Da_i) \quad (18)$$

For non-reacting flow, mixing is independent of t and a function of the position along the mixing channel, the phase difference, the Peclet and Strouhal numbers and the constant β .

$$M = h_2(t, x, \beta, \phi_S - \phi_R, Pe, St, G) \quad (19)$$

IV RESULTS

IV.1 FLOW AND CONCENTRATION FIELDS

Flow and concentration fields were determined for the three versions of the mixers (see Figure 1) and for three operating conditions:

- Continuous flow;
- Alternate flow with $\phi_S - \phi_R = \pi$;
- Alternate flow with $\phi_S - \phi_R = \pi/2$;

Mass transport results are presented in Figure 3. Mixing for continuous flow (Figure 3a) is very small when compared with mixing for alternate flow (Figures 3b to 3f).

The mixer geometry facilitates the creation of layers of fluid of different compositions (Figures 3c, 3d and 3e). Due to the parabolic flow, the layers have a curved interface between each other. Mixing is improved due to the increase of the area between different layers and Taylor dispersion. However, the fluid in the centre of the channel doesn't mix as effectively as the fluid near the wall because the residence time and the thickness of the layer are larger.

The introduction of an obstacle in the axis of the channel (Figure 3d) contributes to delay the fluid, to break the layers into smaller chunks and to increase de interfacial area between fluids with different composition. This effect is further increased by the introduction of two new obstacles

which break the smaller chunks into smaller ones (Figure 3e). Figure 4 shows that, with the introduction of obstacles, the mixing index increases in the region located downstream of the obstacles.

Comparison between Figure 3b and Figure 3c shows that the mixing is more efficient for phase difference equal to π .

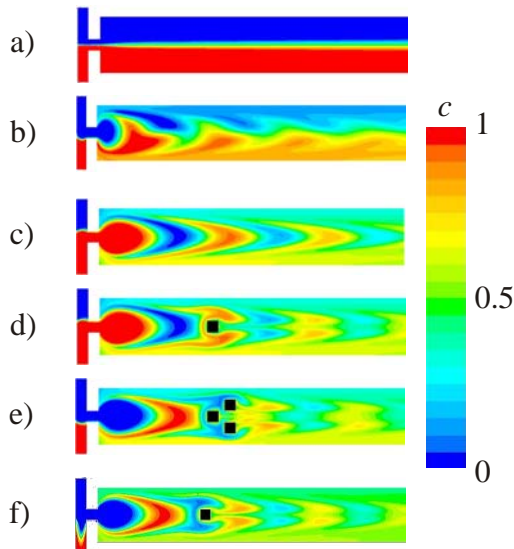


Figure 3. Concentration field for steady state ($Re=0.01$, $Pe=100$, $St=3.33 \times 10^{-3}$, $w_{obs}=1$, $w_e=1$ and $w_m=5$):
 (a) continuous flow; (b) alternate flow with $\phi_R - \phi_S = \pi/2$ and $\beta=1.0$; (c) alternate flow with $\phi_R - \phi_S = \pi$ and $\beta=1.0$;
 (d) alternate flow with an obstacle and $\phi_R - \phi_S = \pi$;
 (e) alternate flow with three obstacles and $\phi_R - \phi_S = \pi$ and $\beta=1.1$; (f) alternate flow with an obstacle and $\phi_R - \phi_S = \pi$ and $\beta=1.2$;

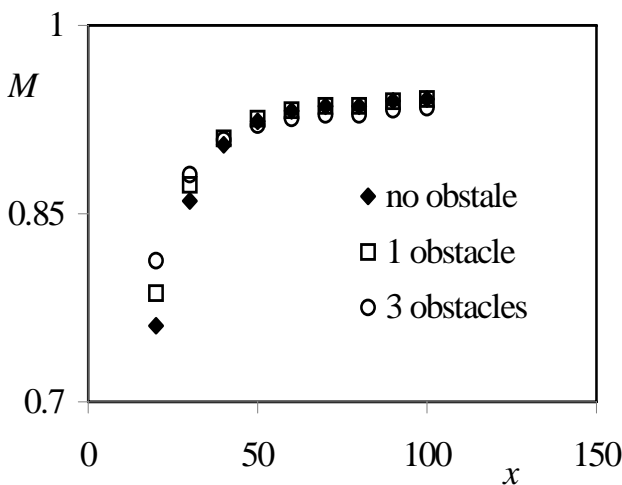


Figure 4. Mixing index along the mixing channel ($Re=0.01$, $Pe=100$, $St=3.33 \times 10^{-3}$, $w_{obs}=1$, $w_e=1$, $\phi_R - \phi_S = \pi$, $\beta=1.2$, and $w_m=5$).

The concentration field in Figures 3c, 3d and 3e is asymmetric because the ejector is not completely cleaned after each cycle. This problem can be partially solved by allowing negative inflow velocities ($\beta > 1.0$). Comparison between Figures 3d and 3f shows that mixing improves for $\beta > 1.0$.

V CONCLUSION

Mixing of two streams in a microfluidic system combining alternate flow with obstacles located along the mixing channel was studied by numerical methods. Preliminary results show that this method can improve mixing in a T mixer. In addition, for biological fluids analysis using lab-on-a-chip devices, this improvement can lead to faster results and to low cost mixers fabricated by planar lithographic technology.

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