Optimization of Mixing in an Active Micromixing Device

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ABSTRACT

Microscale mixers can be divided into two broad classifications - passive and active. Passive mixers rely on geometric properties of the channel shape whereas active mixers rely on time-dependent perturbation of the fluid flow to achieve mixing. In this work, we consider the problem of characterizing the mixing performance of an active micromixer which consists of a main mixing channel within which the flow is perturbed by pressure-driven flow from three pairs of orthogonal secondary channels. Using the newly developed measure of mixing, the so-called "Mix-Norm", we study optimal values for the frequency and amplitude of the oscillating flow in the secondary channels. It is shown that with one side channel operating regions of poor mixing parameter values interlay with good mixing parameter values and that for the second and third channels mixing is good for a large range of parameter values.

Keywords: micromixing, chaotic advection

1 Introduction

Mixing of fluids at the microscale has gained a lot of importance with the rapidly expanding use of microfluidic systems in biology and biotechnology. Flow in microchannels typically have low Reynolds numbers and are therefore laminar. Molecular diffusion across the channels are too slow to cause mixing within reasonable time scales. These limitations make it necessary to design micromixers which efficiently stretch and fold fluid elements so that diffusion needs to act across only smaller length scales to achieve complete mixing. Microscale mixers can be divided into two broad classifications - passive and active. Passive mixers rely on geometric properties of the channel shape to induce complicated fluid particle trajectories and thus cause mixing ([1], [2]). Active mixers rely on time-dependent perturbation of the fluid flow to achieve mixing. In this work, we consider the problem of characterizing the mixing performance of an active micromixer which is based on the concept of chaotic advection. The concept of chaotic advection was introduced by Aref [3] - the basic idea being that even flow fields which have a simple structure from the Eulerian point of view could lead to complex Lagrangian fluid element trajectories, thereby causing efficient stretching and folding of fluid material resulting in the development of finer and finer structures in the advected passive scalar field. Books by Ottino [5] and Wiggins [4] address the problem of mixing using concepts and methods of dynamical systems theory.

To quantify the degree of mixing, we have developed a new measure of mixing called the Mix-Norm [9]. The Mix-Norm is able to capture the efficiency of the "stirring" stage of the mixing process accurately by probing the "mixedness" of the evolving density field at various scales. Previous approaches to this fundamental problem of measurement of mixing include using the entropy of the underlying dynamical system[7] as an objective for mixing and using the scalar variance of the density field which is being transported by a dynamical system[6].

2 Micro-Mixer Geometry and Models

We study an active micro-mixing device proposed in [8] and shown in Figure 1. It consists of a main mixing channel and three pairs of transverse secondary channels. The flow in the main channel is perturbed by a time-dependent pressure-driven flow from the secondary channels, thereby enhancing mixing. Two unmixed fluids, one at the upper half and the other at the lower half, enter the main channel. The two fluids referred to here are not two fluids with different properties, but can rather be thought of as the same fluid with different colored tracer particles in them.

For the purposes of our study, a simple analytical form for the flow field based upon superposition of elementary velocity profiles is assumed. The flow in the main channel follows a parabolic profile in the horizontal direction. The flow from the secondary channels consists of a vertical velocity with a parabolic profile that varies sinusoidally in time at different frequencies. The optimization problem here is to find the amplitude and frequency of oscillation in the secondary channels which give the best mixing. This micro-mixer has been built and studied experimentally [10]. In this analysis, diffusion is neglected and our objective is to optimize the "stirring" phase of the mixing process.

The micro-mixer is divided into three types of re-

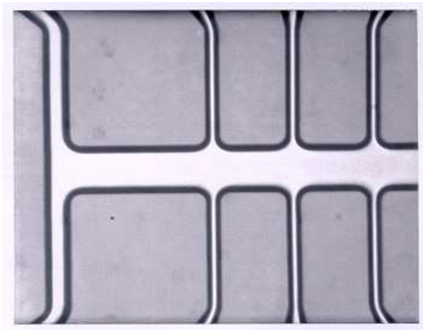


Figure 1: Micrograph of the micro-mixer device (device fabrication courtesy of K.S. Breuer, Brown University and R. Bayt, United Technologies)

gions: the main channel (horizontal), the secondary channels (vertical), and the intersection regions. The dimensions of the mixer are as shown in Figure 2. A characteristic dimension of the mixer device is h, which is the half-width of the main channel, where $h = 100\ \mu m$. In all our discussions, the origin of the $x - y$ plane is assumed to be at the center of the inlet. The ordinary differential equations governing the motion of each particle are as follows:

$$\frac{dx}{dt} = \begin{cases} U_0\left(1 - (\frac{y}{h})^2\right), & |y| \le h \\ 0, & |y| > h \end{cases} \quad (1)$$

$$\frac{dy}{dt} = \begin{cases} 2\pi r_i f_i h \left[1 - \left(\frac{4\bar{x}}{h}\right)^2\right] \sin(2\pi f_i t), & |\bar{x}| \le 0.25h \\ 0, & |\bar{x}| > 0.25h \end{cases}$$

where $\bar{x} = x - (3.5i - 0.25)h$, for $i = 1, 2, 3$. The scaling constant $2\pi r_i f_i h$ is introduced so that in the absence of the main channel flow, a particle along the centerline of the secondary channel oscillates with amplitude $r_i h$. When $r_i = 1$, the amplitude of oscillation is exactly the half-width of the main channel. Therefore we need to optimize the amplitude ratios r_i and the pump frequencies f_i. Introducing a non-dimensional time $\tau = (U_0/h)t$ and using the characteristic dimension h as the unit for distance we get non-dimensional equations of the form:

$$\frac{dx}{d\tau} = \begin{cases} 1 - y^2, & |y| \le 1 \\ 0, & |y| > 1 \end{cases} \quad (2)$$

$$\frac{dy}{d\tau} = \begin{cases} 2\pi r_i F_i \left[1 - (4\bar{x})^2\right] \sin(2\pi F_i \tau), & |\bar{x}| \le 0.25 \\ 0, & |\bar{x}| > 0.25 \end{cases}$$

where $F_i = (h/U_0)f_i$ are the non-dimensional frequencies.

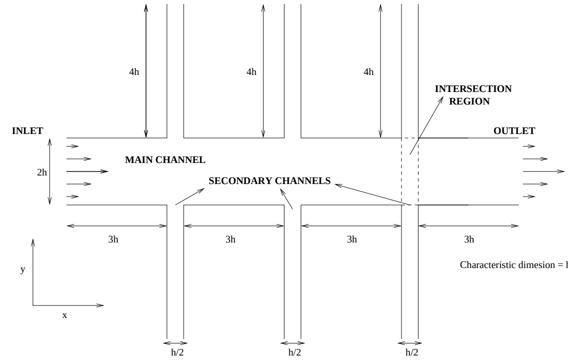


Figure 2: Dimensions of micro-mixer device

3 Simulation

To approximate the evolving density field at the outlet of the mixer a backward particle tracing method is employed here. An intial scalar density field is assumed all over the mixer as follows:

$$c_0(x, y) = \begin{cases} 1, & y > 0 \\ 0, & y < 0 \end{cases} \quad (3)$$

The incoming density field is also of the form (3). One can imagine a density of value 1 to represent a "blue" fluid and a density of value 0 to represent a "red" fluid. This density field is evolving under the dynamics of (2). We are interested only in the "mixedness" of the concentration field at the outlet of the mixer. To make the notation convenient, we define the space $C = \{X_o\} \times [-1, 1] \times [T, T + T_p]$ where X_o is the x-coordinate of the outlet, $[-1, 1]$ is the y-coordinate range at the outlet and $[T, T + T_p]$ is the time period within which we observe the outlet. T_p is chosen to be at least the period of the velocity field in (2) and $T > 0$ is some time beyond which we want to compute mixing. For each tracer particle at the outlet, we simulate the trajectories using (2), but backward in time. To be precise, for each initial condition $(X_o, y, \tau) \in C$, we solve the following ordinary differential equation

$$\frac{dx}{d\tau_b} = -u(x, y, \tau) \quad (4)$$

$$\frac{dy}{d\tau_b} = -v(x, y, \tau)$$

$$\frac{d\tau}{d\tau_b} = -1,$$

where τ_b is a dummy time variable and τ is time. Let $S : C \to \Re^2$ be the solution of (4) which gives the x, y-coordinates of the tracer particles when $\tau = 0$. Then the density field in the space C can be written as

$$c(X_o, y, \tau) = c_0(S(X_o, y, \tau)). \quad (5)$$

4 The Mix-Norm for Quantification of Mixing

In this section we introduce the Mix-Norm. In [9] we study the properties of the Mix-Norm from a theoretical perspective. Here, we de ne the Mix-Norm for a normalized 2-dimensional domain. Let $c : [0,1]^2 \rightarrow \Re$ be a scalar density eld. The function c is assumed to be extended in each direction periodically, oddly or evenly based on the boundary conditions of the problem. All vectors are written in bold font and their respective elements are written in usual font with indices as subscripts and also for a given $\mathbf{s} \in (0,1)^2$ and $\mathbf{p} \in [0,1]^2, A_{[\mathbf{p},\mathbf{s}]} = [p_1 \quad s_1/2, p_1 + s_1/2] \quad [p_1 \quad s_2/2, p_2 + s_2/2]$. To de ne the Mix-Norm let

$$d(c,\mathbf{p},\mathbf{s}) = \frac{\int_{\mathbf{x}\in A_{[\mathbf{p},\mathbf{s}]}} c(\mathbf{x})d\mathbf{x}}{s_1.s_2} \quad (6)$$

for all $\mathbf{s} \in (0,1)^2$ and $\mathbf{p} \in [0,1]^2$. $d(c,\mathbf{p},\mathbf{s})$ is the mean value of the function c within the subset $A_{[\mathbf{p},\mathbf{s}]}$. Now de ne

$$(c,\mathbf{s}) = \left(\int_{[0,1]^2} [d(c,\mathbf{p},\mathbf{s})]^2 \, d\mathbf{p} \right)^{\frac{1}{2}}. \quad (7)$$

$(c,\mathbf{s})$ is the L^2 norm of the averaged function $d(c,.,\mathbf{s})$ for a xed scale $\mathbf{s} \in (0,1)^2$. Then the Mix-Norm of c is given by

$$\Phi(c) = \left(\int_{\mathbf{s}\in(0,1)^2} {}^2(c,\mathbf{s})d\mathbf{s} \right)^{\frac{1}{2}}. \quad (8)$$

For our purposes, the density distribution $c : C \rightarrow \Re$ is periodically extended in the τ-direction and even-extended in the y-direction and we compute $\Phi(c \quad 0.5)$. For perfect mixing, any set with nonzero area within C should have an equal amout of "red" and "blue" uid. The basic idea behind the Mix-Norm is to parametrize all rectangular sets within C and to measure the variance of the mean values of the function c within all these sets from the mean $c_m = 0.5$. For good mixing, $\Phi(c \quad 0.5)$ will be almost zero whereas for poor mixing, $\Phi(c \quad 0.5)$ will be close to 0.5. Also, if we know the function $c : [0,1]^2 \rightarrow \Re$, in terms of its Fourier expansion as follows

$$\begin{aligned} c(x_1,x_2) &= \sum_{m=\ \infty}^{m=\infty} \sum_{n=0}^{n=\infty} a_{m,n} e^{i2\pi m x_1}.(e^{i\pi n x_2} + e^{\ i\pi n x_2}) \\ &= \sum_{m=\ \infty}^{m=\infty} \sum_{n=0}^{n=\infty} a_{m,n} f_{m,n}(x_1,x_2), \end{aligned} \quad (9)$$

where $a_{m,n} = \langle c, f_{m,n}\rangle / \langle f_{m,n}, f_{m,n}\rangle$, then its Mix-Norm is given by

$$\Phi(c) = \left(\sum_{m=\ \infty}^{m=\infty} \sum_{n=0}^{n=\infty} \lambda_m^p \lambda_n^e a_{m,n}^2 \langle f_{m,n}, f_{m,n}\rangle \right)^{1/2}, \quad (10)$$

where

$$\begin{aligned} \lambda_m^p &= \begin{cases} 1 \text{ if } m = 0 \\ \int_0^1 \frac{sin^2(m\pi s)}{(m\pi s)^2} ds \text{ if } m \neq 0 \end{cases} \\ \lambda_n^e &= \begin{cases} 1 \text{ if } n = 0 \\ \int_0^1 \frac{sin^2(\frac{n}{2}\pi s)}{(\frac{n}{2}\pi s)^2} ds \text{ if } n \neq 0. \end{cases} \end{aligned} \quad (11)$$

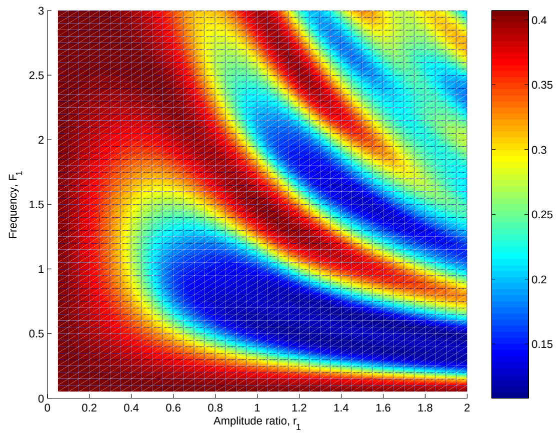
Here, λ_m^p and λ_n^e are the eigenvalues of certain symmetric de nite operators [9] and both of them are of $O(1/k)$ where k is the wavenumber.

5 Optimization of Mixing

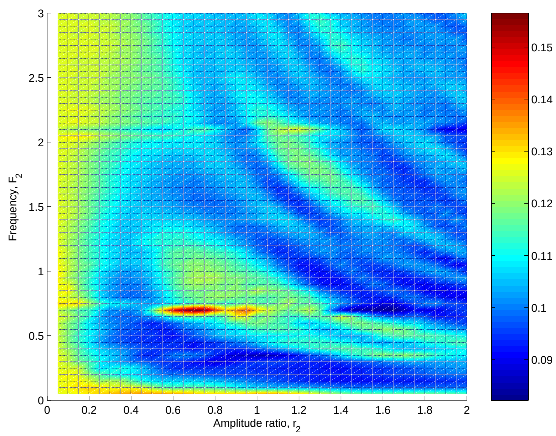
By doing the simulations as in Section 3 and quantifying the mixing as in Section 4, we can study how the optimization parameters (amplitude ratios and frequencies of the pumps) in uence the mixing. The space C de ned in the above section is discretized uniformly in both directions and for each grid point, we solve (4) using a 4^{th} order Runge-Kutta method. In all our computations, we set $T = 30$ and $T_p = 10$. Then the density eld in the space C is approximated using (5).

First we discuss the selection of optimum parameters when only one pump is turned on, i.e, in (2) we set $F_2 = F_3 = 0$ and optimize for F_1 and r_1. Figure 3(a) shows the Mix-Norm as a function of the frequency, F_1 and amplitude ratio, r_1. There is an element of non-robustness as regions of poor mixing parameter values interlay with good mixing parameter values. The optimum parameters with lowest energy input to the mixer are $F_1 = 0.7$ and $r_1 = 1.0$. Note that these optimum parameters are also more robust when compared to other minimas. Even with high energy input to the micromixer, one can achieve very poor mixing as can be seen with parameter values $F_1 = 1.5$ and $r_1 = 1.0$. This shows how crucial the selection of the actuation frequencies are.

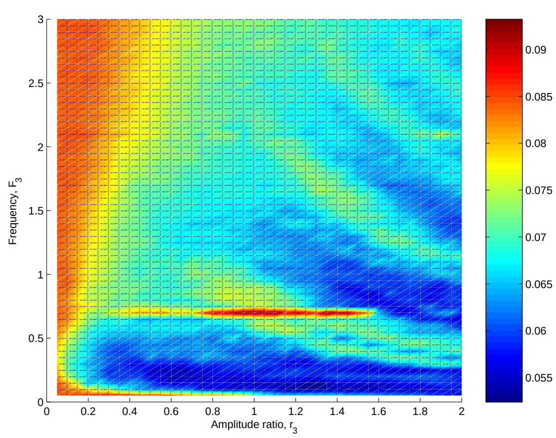
Next we discuss the variation of the Mix-Norm when the rst two pumps are turned on. We set $F_3 = 0$, keep the rst pump xed at its optimum parameters ($F_1 = 0.7$, $r_1 = 1.0$) and vary F_2 and r_2. Figure 3(b) shows the Mix-Norm as a function of F_2 and r_2. It can be seen that reasonable mixing is achieved for a large range of frequency and amplitude values. Note that when $F_2 = 0.7$, for amplitude ratio values ranging from 0.5 to 1.0, there is a sharp decrease in the mixing performance and for amplitude ratio values ranging from 1.4 to 1.7, there is a sharp increase in the mixing performance. This clearly proves that keeping all the



(a)



(b)



(c)

Figure 3: (a)$\Phi(c \quad 0.5)$ as a function of F_1 and r_1 with 2^{nd} and 3^{rd} pumps o . (b))$\Phi(c \quad 0.5)$ as a function of F_2 and r_2 with $F_1 = 0.7, r_1 = 1.0$ and $F_3 = 0$. (c))$\Phi(c \quad 0.5)$ as a function of F_3 and r_3, with $F_1 = 0.7, r_1 = 1.0, F_2 = 0.7$ and $r_2 = 1.5$

pumps at the same parameters gives the worst mixing. Another interesting observation is that for the parameter space of the rst pump which gave reasonable mixing, the second pump gives poor mixing and vice versa. Also, for low amplitude values around $r_2 = 0.5$ we get good mixing, the reason being that the length scales which need to be mixed decreases after the rst pump. Finally, keeping the second pump parameters xed at $F_2 = 0.7$ and $r_2 = 1.5$, we optimize for the third pump. Figure 3(c) shows the Mix-Norm as a function of F_3 and r_3. The same observations as seen for the second pump optimization can be clearly seen for the third pump optimization.

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