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The effect of dilution on the dispersion with respect to microfluidic channel geometries

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ABSTRACT

In most microfluidic devices, single or multiple dilutions of reagents are required to perform reactions or measurements over a range of concentrations using a set of sample solutions to fill the inlets. In this paper, we discuss the results of a study to understand the effects of different dilution schemes on the Taylor dispersion of sample plugs in microchannels. Taylor dispersion arises due to axial spreading of the solute plug due to variations of fluid velocity in the transverse direction. Dilution ratios (*DR*), channel dimensions, and channel layouts are varied. The results show that the one-sided dilution scheme provides a wider plug of 1.9%, 1.2% and 0.7% when $DR = 0.5$, $DR = 0.25$ and $DR = 0.1$, than its two-side dilution counterpart, independent of dilution channel angle and shift. This deviation increases by increasing the Péclet number, where $\sigma^2_{1ch} - \sigma^2_{2ch} \sim Pe^2$. Moreover, we discussed the effects of the compression ratio of the plug, the width ratio between plug and dilution channel, the angle of the dilution channel, the staggered dilution channel, and the 3-dimensional case having different width to height ratios. The compression and width ratios change the final length of the plug dramatically, whereas the channel geometry, i.e. channel angle and shift variation do not. For the 3-dimensional extension, the converged Taylor dispersion values increase with decreasing aspect ratios. These physical understandings and findings for fundamental fluid flow are important for the design of microfluidic devices.

1. Introduction

Microfluidic chips designed for biological and chemical applications have attracted considerable attention in the past decade [1–4]. Many areas of biomedical science, such as biotechnology and chemistry, have benefited from this miniaturization trend [5–9]. The microfluidic chip is capable of performing multiple procedures, such as sample handling, mixing, pretreatment, chemical reaction, and separation, but its primary advantages include having smaller reagent volumes, shorter reaction times, higher selectivity and yield, fewer byproducts, increased process safety, and the possibility of parallel operations, automation, and integrating an entire laboratory onto a single chip [10–14]. In most of the above microfluidic procedures, single or multiple dilutions of reagents are required in order to perform reactions or measurements over a range of concentrations, using only one set of sample solutions to fill the inlets. In Microfluidic High Throughput Screening (mirco-HTS), a device uses a serial strategy to sequentially screen each compound of interest using a common microfluidic channel with a single detection element [15–18]. Mechanically speaking, throughput depends on factors such as flow speed, sample concentration, and the acquisition time of the detector. The most frequently used layout of micro-HTS devices is the cross flow design, which consists of two channels perpendicular to each other. The plug of interest flows towards the microfluidic junction and mixes with reagents. It then travels down the main channel towards the output, where the detection is. As the plug travels down the channel it spreads due to dispersion, and it is thus important to predict the broadening of the plug such that a second plug does not overlap with the first one. It is often a challenge to design the dilution channel or channels for achieving minimal dispersion of the plugs. The design constraints often come from the available pressure or flow control sources. Important parameters in microchip design that affect the plug dispersion include the following: the number of dilution channels, the channel architecture, the dilution ratios, the channel geometry, and the distance between the first and second dilution channels for two-sided channel dilution. To our knowledge, there has been no attempt to systematically study the dispersion of reagents plugs. Furthermore, the optimal

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design parameters required to minimize dispersion within a dilution microchip have not yet been identified.

In microfluidic devices, pressure driven flow results in parabolic velocity profiles in microchannels. Hence, the molecules experience a range of velocities, from zero at the boundary walls to the maximum velocity in the center of the channel. This leads to a broadening of the initial plug known as Taylor dispersion. Taylor dispersion is a result of uneven convective transport and molecular diffusion. Faster flow, occurring in the center of a channel, transports a solute farther within a given time interval, thus creating a concentration gradient in the transverse direction. Molecular diffusion of the solute then acts in the transverse direction to homogenize the solute distribution. The Taylor dispersion regime is reached when the concentration variations across streamlines have fully smoothed out. The velocity variations in the lateral direction $(0 \leqslant y \leqslant w)$ of the fluid flow induce two typical time scales: $O(w^2/D)$ and $O(w/\langle u\rangle)$, where w is the width of channel, D is the molecular diffusivity of solute and $\langle u\rangle$ is the average velocity of the fluid in the channel. The time scale of $O(w^2/D)$ reveals whether the solute plug has had enough time to equilibrate in the lateral direction. Meanwhile, the $O(w/\langle u\rangle)$ time scale reveals whether or not the solute plug has experienced effects of the velocity streams. The ratio between these two time scales is defined as the Péclet number, $Pe = \langle u\rangle w/D$. For a 2-dimensional channel, it has been shown that the effective dispersion is a function of molecular diffusion and the Péclet number, $D^*_{2D} = D(1 + Pe^2/210)$. For a 3-dimensional channel, $D^*_{3D} = D(1 + f(\delta)Pe^2/210)$, where δ is the width to height aspect ratio of the channel [19]. The Taylor dispersion regime is defined when the elapsed time is larger than $O(w^2/D)$ during the convective flow, because at this time point the concentration variations in the lateral direction have smoothed out. Dispersion is an undesired phenomenon in many microfluidics applications since it decreases the efficiency and sensitivity of such devices.

In this paper, we present a numerical study to investigate the effect of dilution on the spread of a solute plug 50 μm in length, for various channel layouts and parameters. We explored the effects of one and two channel dilution layouts on dispersion for three different dilution ratios. We also studied the effect of the dilution channel angle and the effect of channel aspect ratio for both one and two channel dilution layouts, and the effect of distance between the first and second dilution channels for the case of two-channel dilution. At last, we investigated the extension of 3-dimensional Taylor dispersion for comparison. The data were compared numerically, and the best channel layouts were obtained. These findings provide important insights in optimizing the design of microfluidic devices for dilution applications.

2. Numerical simulations

Fig. 1 shows the dispersion of a solute plug in one-sided and two-sided dilution channels of length L and width w. In these simulations, the value of w was set to 5 μm. The initial plug (50 μm long) of 1 μM concentration was placed right before the channel intersection. The dilution ratio was varied between different runs. The diffusion coefficient of the plug was set to D = 0.25 μm^2/s. The average velocity $\langle u\rangle$ at the mixing channel of Fig. 1 was 2 μm/s and Pe = 40. We chose $\langle u\rangle$ = 2 μm/s, 4 μm/s, 6 μm/s, and 8 μm/s for all the runs, and Pe = 40, 80, 120, 160 for simulations, so that the flow was dispersion dominant.

In all our numerical simulations, we maintained the same flow rate after the mixing junction regardless geometries or dimensions. The dilution ratio was defined as the ratio of the flow rate between the mixing channel and the dilution channel, $DR = Q_{\text{dilution}}/Q_{\text{mixing}}$. Our first set of simulations consisted of one-sided and two-sided dilution channels positioned at a 90° angle with respect to the main channel, and the dilution ratios were varied between DR = 0.5, DR = 0.25, DR = 0.1 and DR = 0. DR = 0 means no-dilution from the side channel, which is used as a control for comparison purposes. The dispersion of the plug was then monitored with respect to time. In our second set of simulations we maintained a dilution ratio of DR = 0.5, and changed the flow rate to study its effect on the Péclet number. In our third set of simulations, the effect of dilution channel geometries such as width of dilution channel, angle of dilution channel of one-sided dilution channels, and the dilution channel shift for two-sided dilution channels was investigated. In our last set of simulations, we extended the study to 3-dimensional geometries to provide applicable context for real microchip design. The results are shown in the following section.

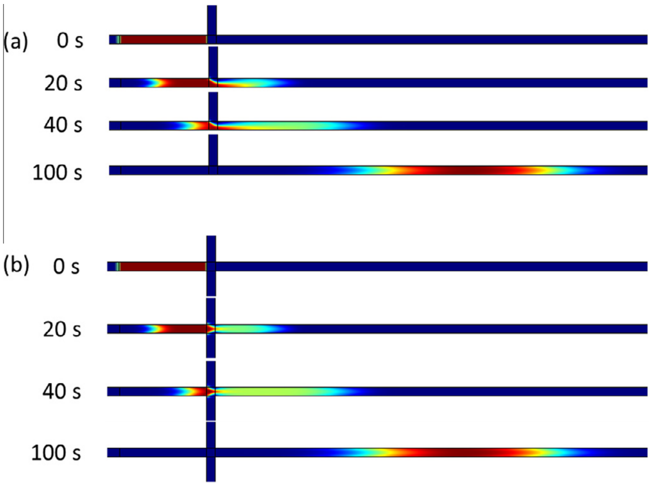

Fig. 1. Broadening of the plug with respect to time for one- and two-channel dilution and their respective concentration profiles. The Péclet number is 40 and dilution ratio DR = 0.5.

3. Results and discussions

3.1. Validation of numerical model

In order to validate our numerical experiments for the different dilution cases, we first numerically solved the Navier–Stokes equation. The velocity profiles of one-sided and two-sided channels were than compared with a known analytical solution. The numerical solution agreed very well with the analytical one, thereby validating the numerical model (details in Supplementary Information). The convection–diffusion equation was then solved numerically for a plug positioned right before the junction. The plug size, position, and concentration were kept constant in all our dilution runs.

The numerically calculated concentration profiles were comparable to the analytical results which is a combination of the error functions of $C(x,t) = \frac{C_0}{2}\left\{erf\left(\frac{l_{plug}/2-x}{\sqrt{4D^*t}}\right) + erf\left(\frac{l_{plug}/2+x}{\sqrt{4D^*t}}\right)\right\}$ when the length l of the plug ranges from $-l_{\text{plug}}/2$ to $l_{\text{plug}}/2$. The numerical solutions at 500 s $(t = 5\,w^2/D)$ are consistent with the analytical solutions, having a small error equal to 0.6% (details in Supplementary Information).

3.2. The effect of one sided and two sided dilution channel systems on dispersion

Fig. 1 shows the results for one-channel and two-channel dilution layouts around the junction of the channel before and after,