



Analyzing mixing quality in a curved centrifugal micromixer through numerical simulation



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ABSTRACT

The Lab On a CD (LOCD), also known as Centrifugal Microfluidics, has evolved into a sophisticated platform for performing biomedical assays due to its marvelous miniaturization and accurate simulation of biological reactions. Among the numerous applications of the LOCD is fluid mixing. In this paper a centrifugal, serpentine micromixer is simulated and reformed toward better mixing performance. The micromixer was chosen to be curved as a curved design was found to be thrice as functional and compact as a rectilinear design, mixing-wise. The two angular velocity and opening radius parameters were originally hypothesized to affect mixing performance. Effect of angular velocity was studied over a broad range starting from quite low values. It was gathered that with increasing angular velocity, mixing performance initially drops and upon reaching a minimum at a threshold angular velocity, begins to continuously increase. The threshold angular velocity was found to be the spot at which the mixing regime changes from diffusion to secondary flow. It was also realized that increasing the opening radius enhances mixing performance only insignificantly, such that it would not be a practical means of making micromixers more efficient.

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1. Introduction

The Lab-On-A-Chip (LOC) is a microfluidic miniaturization platform used in many chemical, biological and biomedical assays; e.g. the Point Of Care Testing (POCT) (Figeys and Pinto [1], Haeberle et al. [2], Lee and Choi [3], Chin et al. [4], Ryu et al. [5]). Because of its small dimensions, the amount of the consumed sample and reagent is significantly less than other known experimental platforms; i.e. nanoliters vs. milliliters, making the LOC extremely efficient concerning material expenses (Srinivasan et al. [6], Fair [7]). Several modules or operational units could be erected on the LOC for various applications in biological assays such as mixing, valving and separation (Strohmeier et al. [8]). The problem with the LOC is that each operational unit requires a separate micropump, mostly syringe pumps, as its driving force to operate. For this reason, multifunctional LOCs are rather scarce since employing several micropumps in an LOC complexes its design, making it harder to fabricate. To overcome the limitation on multifunctionality, the Lab-On-A-CD (LOCD) was introduced. The LOCD is also a microfluidic miniaturization platform which is a

rotating disk in the shape of a CD [9]. Through use of the centrifugal force induced due to the rotation of the platform around its central axis, the LOCD does not require a micropump for the propelling movement of the fluid. All operational units within an LOCD such as mixing, separation, valving, droplet generating, and etc. could operate using a single rotational motor [10–13]. The disk is mounted on a shaft through the CD hole and the shaft's rotation generates centrifugal force within the fluid, propelling it from the input through the operational units and toward the output [14].

Due to the simplicity of its design, the LOCD is a convenient platform when it comes to biomedical assays such as biochemical and enzymatic studies (Lee et al. [15], Kim et al. [16], Lai et al. [17]), DNA studies (Jia et al. [18]) and POCT (Gorkin et al. [19]). For such analyses to occur, operational units such as valving (Madou et al. [20]) and mixing (Noroozi et al. [21]) units are developed for the LOCD (Chakraborty [22]).

If any chemical reaction is to be effective, first the reagents of that reaction need be thoroughly mixed. In large scales, fluid mixing is achieved rather simply through available solutions. However, it still remains a challenge to achieve a proper mixing of two fluids in microfluidic scales. In microfluidic systems the fluid flow is greatly laminar and the Reynolds number is rather small, hence, there can be no turbulent mixing occurring due to the natural stirring of the fluid caused by turbulence vortices.

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There are two general types of micromixers: active and passive. Active micromixers utilize an external energy source or force field such as magnetic (Wang et al. [23]) or electrical (Wu and Liu [24]) to operate. Passive micromixers, however, simply rely on the geometry of the LOCD design (Tofteberg et al. [25], Hessel et al. [26]).

A pressure-driven, passive micromixer for mixing fluids at rather small Reynolds numbers was developed by Stroock et al. [27]. Special obstacles were embodied on the microchannel floor such that the fluids would be mixed upon flowing over them. Multiple micromixers were devised for the LOCD [28–33]. Current micromixers mostly do not show appropriate mixing performance in spite of their rather complex design. A centrifugal micromixer was introduced by Haerberle et al. [2] which was implemented on a straight, radial microchannel. This micromixer functioned based on the transverse flow created due to the Coriolis force which is one of the main volume forces exerted on the fluid within an LOCD. Despite having a quite simple design, their micromixer had limited mixing performance since it was extremely dependent on the LOCD's angular velocity and its resulting Coriolis force. Batch-mode mixing in an LOCD was achieved by Grumman et al. [10] through distributing magnetic particles within the two to-be-mixed fluids. A reciprocating micromixer consisting of two reservoirs connected via U-shaped microchannels was devised by Noroozi et al. [21] which had a high mixing performance. However, due to its geometric limitations, implementing this micromixer in an integrated LOCD setting faces complications. Serpentine microchannel arrangements within an LOCD were introduced by Duffy et al. [34], Puckett et al. [35] and Zoval and Madou [36] for enzymatic, bacterial and protein-ligand analyses, respectively. Their serpentine design was employed only to lengthen the flow path such that the fluid had enough time to freely diffuse. By securing the necessary diffusion time, sufficient mixing was ensured. Yet a thorough observation of the mixing process was not given.

For an LOCD to be used in POCT diagnostics it should most of all be disposable; Therefore, its fabrication should be simple and cost-effective. Hence, as long as a sufficient mixing performance is ensured, a simple passive design without any additional components such as electrodes or magnets is preferred to rather complex active designs. Such simple passive design is conveniently fabricated (even in mass-production scales), portable, cost-effective and easy to use. A centrifugal serpentine micromixer (CSM) was developed by La et al. [37] for an LOCD platform. They compared the CSM and its mixing performance with a pressure-driven serpentine micromixer (PSM). The PSM yielded limited mixing performance since the two laminar flows within it could only mix through diffusion and inertial stirring effects occurring within the microchannel's sharp corners. Yet the CSM showed superior mixing performance due to having an additional secondary flow caused by the Coriolis force. To find a direct approach for quantifying mixing performance is greatly appreciated. However, this goal is not simply achieved for there are many micromixers available and yet no standard criterion exists for determining mixing performance in them all. (Falk and Commenge [38]). Because of this, several studies were conducted in the past couple of years in order to define a quantified index resembling mixing performance. Experimental methods were employed in a couple of these aforementioned studies such as particular chemical reactions and fluorescent microscopy (Ehrfeld et al. [39], Falk and Commenge [38]). Although they grant qualitative analyses of mixing in micromixers, they are unable to offer a quantitative assay such as mixing length or mixing time data (Aubin et al. [40]).

Methods previously used to evaluate the mixing performance of macromixers were employed for the same purpose in

micromixers. One of them applied a Lagrangian analysis in following two to-be-mixed fluid streams (Zalc et al. [41]). The concentration distribution was statistically analyzed at each section of the mixer, thus quantifying the mixture's homogeneity. This analysis was derived from Danckwerts' "intensity of segregation" concept which calculates the variance of the concentration (σ^2_c) with respect to its mean (c_{avg}) throughout different locations (Danckwerts [42]). Shamloo et al. adopted the mixing quality term from this concept and implemented it in their study to quantify mixing performance (Shamloo et al. [43]). They investigated the mixing quality of a centrifugal, serpentine micromixer employed on an LOCD through multiple different setups. The effect of several design parameters of the LOCD including inlet angle, angular velocity and cross-sectional profile was studied on the mixing quality. Their designed microchannel was rectilinear and had sharp corners in microchannel turns.

In this paper, a curved microchannel is devised instead and the effect of the new curved geometry on the mixing quality is investigated. Secondly, the mixing behavior is studied over a broad range of angular velocities to acquire a profound understanding of the effect of this critical parameter on mixing quality in LOCDs. Finally, the effect of the opening radius at which the microchannel starts (from the origin of coordinates being the LOCD's center) on the mixing quality is assessed.

2. Numerical formulation and governing equations

Three well-known PDEs govern the physics of the presented micromixer problem. The incompressible, steady-state Navier-Stoke's momentum equations and the incompressible, steady-state continuity equation govern the fluid flow while the fluid is considered to be Newtonian with constant properties. Also the steady-state, constant-diffusivity convection-diffusion equation directs the concentration distribution within the medium. Having applied the aforementioned assumptions, the governing equations are given as Eq. (1) through Eq. (3):

$$\rho(\nabla \cdot \mathbf{u}) = -\nabla P + \mu \nabla^2 \mathbf{u} + \mathbf{f}_b \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

$$\mathbf{u} \cdot \nabla c = D \nabla^2 c \quad (3)$$

all above equations are numerically solved in three dimensions. In these equations, $\mathbf{u}$ is the velocity vector (m/s), c is the concentration (mol/m³) and they both are the unknown variables for which the equations are solved. P and $\mathbf{f}_b$ denote pressure (Pa) and volumetric force vector (N/m³), respectively. Finally, the constants ρ , μ and D are material constants indicating fluid density (kg/m³), dynamic viscosity (Pa s) and diffusivity constant (m²/s). The volumetric force vector here is the vector sum of the centrifugal and Coriolis volumetric forces generated due to the angular motion of the LOCD and is given in Eq. (4).

$$\mathbf{f}_b = -\rho \vec{\omega} \times (\vec{\omega} \times \mathbf{r}) - 2\rho \vec{\omega} \times \mathbf{u} \quad (4)$$

where $\vec{\omega}$ denotes the LOCD's angular velocity vector. As was mentioned earlier, the index appropriate for indication of mixing performance is the Mixing Quality (M.Q.) which is calculated as follows in Eq. (5) through Eq. (6):

$$CoV = \frac{\sqrt{\sum_{i=1}^n (c_i - c_{avg})^2}}{c_{avg}} \quad (5)$$

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