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Design of micromixers using CFD modelling

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Abstract

The effect of various geometrical parameters of a grooved staggered herringbone micromixer on the mixing performance has been investigated using computational fluid dynamics. Mixing quality has been quantified with spatial data statistics, maximum striation thickness and residence time analyses. The results show that the number of grooves per mixing cycle does not affect the mixing quality in an important way. On the other hand, a larger groove depth and width allow the maximum striation thickness to be rapidly reduced, without increasing the pressure drop across the mixer. Wide grooves, however, create significant dead zones in the microchannel, whereas deep grooves improve the spatial mixing quality.

Keywords: Mixing; Micromixer; Laminar flow; Computational fluid dynamics (CFD); Striation thickness; Spatial analysis

1. Introduction

Micromixers play a significant role in micro chemical processing and are employed in a multitude of tasks, including blending, emulsification and suspension, as well as for chemical reaction and also in combination with integrated heat exchangers. Due to the small dimensions of the micro channels, the flow is predominantly laminar and mixing is therefore limited by molecular diffusion. In order to effectively mix in a reasonable time, fluids must be manipulated so that the interfacial surface area between the fluids is increased massively and the diffusional path is decreased, enhancing the molecular diffusion to complete the mixing process (Ehrfeld et al., 2000). A number of mechanisms exist for fluid contacting and mixing, including multilamination, splitting and recombination, hydrodynamic focussing, T- and Y-junctions (Ehrfeld et al., 2000), as well as chaotic advection (Beebe et al., 2001; Lui et al., 2000; Stroock et al., 2002a,b).

Due to the relatively young age of microreactor engineering, common design rules for micromixers have not yet been developed. However, one can see that apart from their minute size, microreactors are merely continuous laminar flow reactors, which suggests that design approaches for mixing in micro channels could be dealt with in a similar manner to that of laminar mixing in macro scale pipe flow. In undisturbed laminar flow, the streamlines run parallel to one another and there is no convective mixing in the radial or tangential directions, which results in a high degree of *spatial* inhomogeniety. In addition, the parabolic velocity profile of the laminar flow gives rise to *temporal* inhomogeneities, which translates into wide residence time distributions. Thus in order to disturb the flow and facilitate mixing in laminar pipeline flow, in-line devices or static mixers are inserted into the channel. The best designs of such devices create a high degree of plug flow, thus decreasing temporal inhomogeneities, whilst achieving homogenisation in the radial direction, which increases the spatial homogeneity (Etchells and Meyer, 2004). The design of micromixers, which are comparatively similar devices at a much smaller scale, can be looked at in the same manner, whereby the aim is to provide sufficient spatial and temporal mixing as fast as possible.

A number of methods are commonly used in order to characterise both the spatial and temporal mixing performance of large-scale static mixing devices, for example:

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the coefficient of variation and the intensity of segregation (Hobbs and Muzzio, 1997, 1998a,b; Mickaily-Huber et al., 1996; Rauline et al., 2000; Zalc et al., 2002), Poincaré sections (Hobbs and Muzzio, 1998a,b), striation thickness (Fourcade et al., 2001) and residence time distributions (Hobbs and Muzzio, 1997; Nauman et al., 2002; Visser et al., 1999). These can be implemented experimentally and/or numerically—the numerical approaches have been detailed in Aubin et al. (2003).

Over the past few years, a number of studies using different types of micromixers have been carried out with the aim of characterising the mixer performance using various experimental techniques, such as fluorescent microscopy and special chemical reactions, as well as CFD simulations to trace particle trajectories (Beebe et al., 2001; Bertsch et al., 2001; Ehrfeld et al., 1999; Lui et al., 2000; Stroock et al., 2002a,b). As we discussed in a previous paper (Aubin et al., 2003), these methods are indirect and enable mainly qualitative comparisons of micromixers but they do not give quantitative data, such as mixing times or mixing lengths. Furthermore, they rarely make use of the characterisation methods that have been developed for macro-scale static mixers. In Aubin et al. (2003), we have used a numerical approach for quantifying the mixing quality in micromixers, which is based on a spatial analysis method that has previously been used for assessing the performance of macro-scale static mixers. This statistical approach employs quadrat analysis of Lagrangian particle trajectories whereby two-dimensional planes in the mixer are divided into equal sized quadrats and the number of particles within each quadrat is recorded. At each plane, the variance of particle distribution with respect to an ideally homogenised distribution is calculated. This in turn gives an idea of the channel length necessary to obtain a particular degree of mixing. Although the methodology described above is useful for quantifying the rate at which particles are spread throughout the mixer, it is highly dependent on the size and number of quadrats used, as well as the number of particles traced (Lui et al., 1994). If the quadrats are too large, the technique will quantify mixing only on a coarse scale and thus small scale flow patterns that are smaller than the quadrat size will be filtered out. On the other hand, if the quadrats are very small, a very large number of particles would be required, which would demand an extremely long computational time. In Aubin et al. (2003), the micromixer geometries investigated gave strikingly different flow patterns and therefore the quadrat size and particle number that were employed were sufficient for the comparison of the two mixers. In the current study, the differences between the various micromixer flow patterns are much smaller and a higher degree of resolution is thus required for better quantification.

In our previous paper, we characterised the mixing quality in a diagonally grooved micromixer (DM) and a staggered herringbone micromixer (SHM) using computational fluid dynamics (CFD). It was shown that the SHM mixes much more efficiently and in a shorter time than the DM. In the current study, we have decided to study numerically the effect of different geometrical parameters of the SHM on the mixing quality, with the aim of improving the mixer design. We present an alternative method for quantifying the level of spatial homogenisation in micromixers, which is based on a statistical method called nearest-neighbour analysis. A measure of the reduction in maximum striation thickness as a function of mixer length is also used to quantify distributive mixing. Temporal mixing is then assessed by the determination of residence time distributions. Lastly, the effect of the various geometrical modifications on the pressure drop is examined.

Sections 2–4 describe the various micromixer geometries investigated, as well as the numerical and characterisation methods employed in this work. A detailed analysis of the results is then presented in Section 5 and the conclusions are given in Section 6.

2. Mixer geometry

The mixer geometries used in this study are based on that proposed by Stroock et al. (2002a) and have an off-centred herring bone pattern in the channel floor (Fig. 1), which creates a transverse velocity component in the flow field. The mixer is composed of several mixing cycles, whereby a mixing cycle comprises two sequential regions of grooves, i.e., two half-cycles. The direction of asymmetry of the herringbones switches with respect to the centreline of the channel every half cycle. The mixer consists of a rectangular channel ($w = 200\,\mu\text{m}$, $h = 77\,\mu\text{m}$, $L = 0.01\,\text{m}$) with grooves of depth, d_g, and width, W_g, which have a wave vector of $2\pi/100\,\mu\text{m}^{-1}$. In this work, the groove depth, the groove width and the number of grooves per cycle, N_g, were varied in order to understand their effect on the mixing quality. Table 1 presents the different cases investigated and the values of the geometrical parameters.

3. Numerical methods

The numerical simulation of the flow and mixing in the micromixers has been performed using ANSYS-CFX5 (ANSYS, 2003). This is a general purpose commercial CFD package that solves the Navier–Stokes equations using a finite volume method via a coupled solver. The analysis procedure has been carried out in two steps. Firstly, the velocity and pressure fields in the mixer are solved. These values are then used to calculate particle trajectories within the flow field.

3.1. Flow computation

A mesh composed of approximately 1 330 000 hexahedral elements (1 500 000 nodes) was used. A preliminary grid convergence study was carried out in order to verify