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Dimensionless number for identification of flow patterns inside a T-micromixer

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ABSTRACT

Results are presented from a numerical study examining the flow dynamics of the liquid phase inside T-type micromixers. The main aim of the study was to determine an identification number for the differentiation of the different flow regimes in the liquid phase in T-type micromixers. The critical value for the identification number at which the transition from vortex flow to engulfment flow occurs was obtained. The results were used to optimize the geometrical parameters and the operating conditions to achieve high mixing performance for the liquid phase in T-type micromixers. The model results were found to be consistent with experimental data for different T-mixers available in the literature.

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1. Introduction

Microreaction technology has opened up new perspectives for the chemical industry. In general, microdevices offer fundamental advantages compared with conventional macroscale systems due to their small characteristic dimensions. Apparent advantages of microreactors are highly efficient micromixing, a high area-to-volume ratio, efficient heat transfer ability, the avoidance of hot spots by effective temperature control, and high operational safety (Engler et al., 2004; Ehlers et al., 2000).

The performance of most microchemical processes strongly depends on the efficiency and rate of the mixing, especially when dealing with fast reactions (Mengeaud et al., 2002). Optimization of the mixing part is therefore important to enhance the efficiency of a microprocess (Mengeaud et al., 2002). Over the past decade micromixers based on various principles have been developed and investigated. Each of these micromixer types has a different capacity, mixing speed, and operating requirements. Consequently, some micromixers are more suitable for certain applications than others. Multilaminated mixers employ the principle of minimizing diffusional distance between fluids by splitting and arranging the streams into a single multilaminated channel (Bessoth et al., 1999; Ehrfeld et al., 1999; Erbacher et al., 1999). The thickness of each fluid layer is greatly reduced, allowing a faster mixing. In the other common category of micromixers a transversal component of the velocity is generated to increase the interfacial area across which diffusion takes place. This flow phenomenon can be achieved using helical channels (Liu et al., 2000), bas-relief structure on the channel (Stroock et al., 2002), or electricokinetic instability (Oddy et al., 2001). A comprehensive overview over micromixers with different working principles can be found in Hessel et al. (2005).

Although much work has been done to develop micromixers based on a wide variety of fundamental principles, detailed mixing characterization in a T-micromixer has yet to be explored (Wong et al., 2004). In T-micromixers complete mixing of the gas phase can be ensured by molecular diffusion mechanism at low Reynolds number. This fact can be attributed to the large molecular diffusion constant of gas phase. Gobby et al. (2001) studied the mixing characteristics of two gases in a T-micromixer using computational fluid dynamics simulations. They investigated the effects of the fluid speed, the aspect ratio of the mixer, the angle between the inlet channels, and the throttle on the mixing length.

Such a configuration is also applicable to liquids at high Reynolds number regimes as demonstrated by Bökenkamp et al. (1998) and Hoffmann et al. (2006). Applying two T-mixers connected by a channel, Bökenkamp et al. achieved complete mixing between liquid samples with a mixing time as short as 110 μs for Reynolds numbers larger than 1000. Hoffmann et al. performed experimental investigation of liquid mixing in T-shaped micromixers at Reynolds numbers higher than 150 but within the laminar flow regime. Employing the microlaser-induced fluorescence (μ-LIF) technique, they highlighted the convective effects and concluded that rapid mixing is achievable despite the laminar flow conditions. In addition they showed

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that the hydrodynamics and the corresponding mass transfer is a three-dimensional problem in the studied range of Reynolds numbers.

Recent work on liquid mixing with T-shaped micromixers carried out by Engler et al. (2004) and Bothe et al. (2006) highlighted the three laminar flow regimes in the mixing channel namely, stratified flow, vortex flow, and engulfment flow. At very low Reynolds numbers where the flow is in the stratified regime, the mixing is entirely due to molecular diffusion between the layers of different concentrations. Owing to the small diffusion coefficient of liquids, the resulting species distribution consists of two completely segregated regions. For moderate Reynolds numbers (vortex flow) an increase in the mixing efficiency sets in, indicating that the flow patterns change and convective mass transfer promotes mixing. However, the main mixing principle is still diffusion. It was shown that improved mixing performance was achieved with the third flow regime, engulfment flow, which occurs at higher Reynolds numbers. This improved mixing was attributed to the creation of secondary flow and the generation of vortices due to the separation of boundary layers around the sharp bends at the junction. The generated vorticity increases the contact area of the components and reduces the mixing distance in the T-micromixer where, due to the very small dimensions, mixing by turbulence is not feasible. Since diffusion over small distances is fast, rapid and efficient mixing is achieved.

With this knowledge it is clearly essential to work in the engulfment flow regime to ensure fast and efficient mixing of liquids in a T-micromixer, owing to the small molecular diffusion coefficient of liquids. Key questions are under what conditions flow in a T-micromixer could become engulfment, and more importantly, what is the identification number for the differentiation of the different flow regimes.

Several researchers (Engler et al., 2004; Soleymani et al., 2008) have reported that the flow patterns in a T-micromixer depend strongly on both the volume flow rates and the geometrical parameters of the mixer such as the aspect ratio and mixing angle. This indicates that the appearance of vortices depends not only on the Reynolds number, but also on another dimensionless group accounting for the geometrical parameters.

Over the past decade, computational methods have proven to be an effective tool to design and develop microprocesses which has opened up the possibility of proofing the feasibility of processes in microreaction devices or optimizing these devices on a computer with minimum expenditure of time and money. In this current work the flow dynamics of the liquid phase inside T-type micromixers was studied by means of computational fluid dynamics. The aim was to determine an identification number for the differentiation of the different flow regimes and to find out the critical value for the identification number at which the transition from vortex to engulfment flow occurs.

2. Methodology

As shown in Soleymani et al. (2008) the flow patterns and development of vortices in a T-micromixer (Fig. 1) of dimensions $A \times B \times C$ depend strongly on both the volume flow rates and the geometrical parameters of the mixer such as the aspect ratio of the inlet channel (B/C) and the aspect ratio of the mixing channel (A/C). A and B are the width of the mixing channel and inlet channels in μm, respectively. C is the depth of all channels in μm. The above mentioned dependence parameters can be grouped together as

$$f\left(Re, \frac{B}{C}, \frac{Dh_{\mathrm{in}}}{Dh}, \frac{A}{C}\right) = 0 \tag{1}$$

where Re is the Reynolds number in the mixing channel. Dh_{in} and Dh are the hydrodynamic diameters of the inlet channels and mixing channel, respectively. The identification number K, a dimensionless number describing the flow regime inside the T-micromixer, is then expressed as

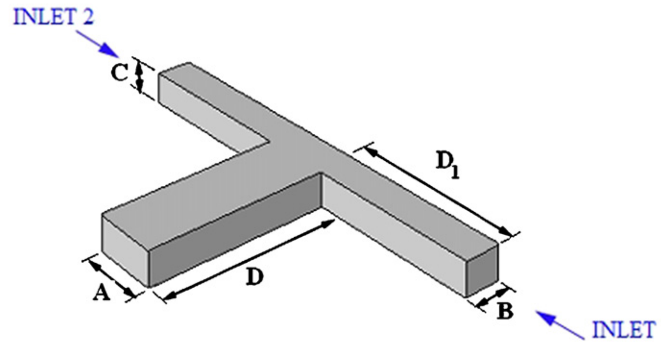

Fig. 1. Schematic picture of the T-mixer with dimensions

$$K = Re^{\alpha}\left(\frac{B}{C}\right)^{\beta}\left(\frac{Dh_{\mathrm{in}}}{Dh}\right)^{\gamma}\left(\frac{A}{C}\right)^{\varsigma} \tag{2}$$

To obtain the constants of the identification number K in Eq. (2) (α, β, γ, and ζ), a set of numerical type simulations was performed for 30 different mixers. The beginning of the engulfment regime was measured since this can be clearly distinguished from the vortex regime.

2.1. Determination of the onset of engulfment flow regime

It has been shown (Bothe et al., 2006) that at high flow velocities, breaking up of the symmetry in the flow field occurs. This results in the so-called engulfment flow, which is characterized by some fluid from one side reaching beyond the centerline of the T-micromixer to engulf fluid from the other side. It has been shown (Soleymani et al., 2008) that improved mixing performance is achieved with engulfment flow. Fig. 2 presents the path lines at the entrance of the mixing channel for both the vortex and engulfment flow regimes in a 600 × 300 × 300 micromixer. It can be seen that for vortex flow the symmetry plane perpendicular to the inlet channels is preserved while for engulfment flow the axial symmetry breaks up. The beginning of the breaking up of the axial symmetry is interpreted as the beginning of the engulfment regime and it is defined as the point where the first streamlines intersect both the symmetry planes of the T-micromixer.

For each mixer, the mass flow rate was changed once the transition from vortex to engulfment flow could be observed. Fig. 3 describes the procedure used to determine the transitional velocity.

3. Simulation method

In principle, information on flow and mixing in a T-micromixer can be observed via a numerical solution of the Navier–Stockes equation and the convection–diffusion equation for the concentration field. However, numerical errors due to the discretization of the convective terms in the transport equation of concentration fields introduce an additional, unphysical diffusion mechanism. This so-called numerical diffusion limits the accuracy of the numerical prediction. It is particularly important in liquid mixing at high flow rates with characteristic diffusion constants in the order of $10^{-9}\ \mathrm{m^2\,s^{-1}}$, which induce cell Peclet numbers that are too high for convection–diffusion calculations. Here the cell Peclet number, a dimensionless group determining the strength of numerical diffusion, is defined as UL_C/D_0, where U is the local flow velocity, L_C and D_0 are the extension of a computational cell and diffusion coefficient, respectively. It was

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