

Contents lists available at ScienceDirect

Chemical Engineering Journal

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Design method for micromixers considering influence of channel confluence and bend on diffusion length

Nobuaki Aoki, Ryota Umei, Atsufumi Yoshida, Kazuhiro Mae*

Department of Chemical Engineering, Graduate School of Engineering, Kyoto University, Kyoto-daigaku Katsura, Nishikyo-ku, Kyoto 615-8510, Japan

ARTICLE INFO

Article history: Received 25 March 2010 Received in revised form 12 August 2010 Accepted 16 August 2010

Keywords: Micromixer Diffusion length Energy dissipation rate Confluence Bend Computation fluid dynamics

ABSTRACT

In micromixers, fluids deform through convection generated by variations in the shape of a channel, e.g., channel confluence and bend. This deformation enhances the mixing performance of the micromixer. In this study, we consider the effect of deformation on mixing performance in terms of a reduction in diffusion length, which is equivalent to the size of the fluid segments formed through fluid deformation. Based on improvements in the mixing rate through convection, we establish a design method that enables a micromixer to achieve a desired rapid mixing rate. For this purpose, we correlate the mixing performance of micromixers having various channel shapes and fluid velocities with the diffusion length; the equivalent mixing rate is obtained using computational fluid dynamics (CFD) simulations. The results of the CFD simulations reveal that the combination of fluid collision and channel bend after the development of the velocity profile of confluent flow is effective at enhancing the mixing rate. To establish a design method for a micromixer, we define and employ the energy dissipation rate based on the pressure drop profile in microchannels. The relationship between the segment size and the energy dissipation rate based on channel shape has been derived and integrated into the design method.

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1. Introduction

Microreactors are miniaturized reactors that have microchannels of characteristic dimensions in the submillimeter range [1]. Some micromixers, which are mixers containing submillimeter mixing chambers, can be used as a reactor especially for reactive mixing. The reactor miniaturization provides improved mass- and heat-transfer rates and thus enables us to proceed with reactions under conditions controlled more precisely as compared to conventional macro-scale reactors, which leads to the possibility of improved yields and selectivities of desired products [2]. Enhancing mixing performance in microreactors is also essential to produce desired products in high yield and selectivity by precisely controlling reactor operations. The selectivities of desired products for very fast multiple reactions have been improved using micromixers, which are miniaturized mixing devices [3]. Micromixers are, thus, important components of microreactors used to control reactor operations. Many mixing principles have been developed for enhancing mixing performance in micromixers [4]. Many other principles have been derived by focusing on reducing the diffusion length between reactants. This is because mixing in microreactors is mainly driven by molecular diffusion and reactor miniaturization

leads to low Reynolds numbers in reactor channels. In micromixers, splitting reactant fluids into small fluid segments is a method to reduce diffusion length and thus enhance mixing performance. Three principles are mainly used to split reactant fluids into small fluid segments. The first principle is to divide reactant fluids into many fluid segments using the channel geometry of micromixers. One mixing method that uses this mixing principle splits reactant fluids into many laminated fluid segments by the geometry of the inlet channels that lead into the mixing chamber. Examples of micromixers using this mixing method include the interdigital mixer [5] and the multi-stream mixer with focusing after confluence [6,7]. When only this mixing principle is used, it is necessary to shorten the diffusion length by channel reduction to achieve fast mixing. However, channel reduction also leads to a high-pressure drop in the channel and thus a limited flow rate, resulting in a low productivity and operability. Another principle that enhances mixing performance is therefore needed for industrial production where high throughput is to be achieved.

The second principle used to split reactant fluids into small fluid segments is the collision of reactant fluid streams for applying shear to the streams. The collision deforms fluids and shortens the diffusion length between the fluids. As a result, the mixing performance is improved. To evaluate the mixing rate quantitatively, we can consider the enhancement of mixing performance in terms of a reduction in diffusion length (fluid segment size). Collision of two fluid streams at a channel confluence is the simplest method for this mixing principle. T- and Y-shape microchannels are exam-

^{*} Corresponding author. Tel.: +81 75 383 2668; fax: +81 75 383 2658. *E-mail address:* kaz@cheme.kyoto-u.ac.jp (K. Mae).

^{1385-8947/\$ -} see front matter © 2010 Elsevier B.V. All rights reserved. doi:10.1016/j.cej.2010.08.084

Table 1Physical properties of fluids A and B.

Density, ρ	$1.0 imes 10^3$	kg/m ³
Viscosity, μ	$1.0 imes 10^{-3}$	Pa s
Diffusivity, D _{AB}	$1.0 imes10^{-9}$	m ² /s

ples of micromixers that use this mixing principle and have been employed in investigations on the relationship between design factors such as channel sizes and flow rates in the mixers, flow pattern, and mixing performance in the micromixers [8–10].

The third principle commonly applied is channel bend. Channel bend also deforms fluids and shortens the diffusion length between fluids. Previous investigations based on experimental and simulation results reveal that channel shapes of bend and curve after fluid collision enhance mixing performance [11,12].

However, most previous investigations considered only the qualitative effects of channel shape on mixing. For the versatile use of micromixers in industrial production, a method to design channels in accordance with the kinetics of the reaction system is needed. Quantitative relationships between mixing rate and design parameter of microchannels utilizing convection are required for this purpose. In this context, we correlate the mixing performance of microchannels having various channel shapes and fluid velocities with the diffusion length, which gives the equivalent mixing rate using computational fluid dynamics (CFD) simulations. To establish a design method, we also propose an index to express the effects of both channel shapes and operating conditions on mixing performance and integrate the index into the design method.

2. Simulation method

2.1. Geometry of microchannels

The three-dimensional laminar flow and the finite-rate model of Fluent 6.3 were used in the CFD simulations. We simulated mixing between fluids A and B having the same physical properties with each inlet velocity v in the microchannels. Table 1 lists the physical properties of fluids A and B.

As explained in Section 1, mixing can be enhanced by convection due to channel confluence and bend. To examine the effects of channel shapes on mixing rate, we simulated various sizes of microchannels with combinations of channel confluence and bend. Fig. 1(a) and (b) shows schematics of micromixers that include these channel shapes. The micromixer containing only channel confluence is called the Tmixer and the mixer with both channel confluence and bend is referred to as the TLmixer. The channel sizes d_x , d_y , and d_z (µm), and the channel length between the points for channel confluence and bend *X* (mm) and bend angle θ (°) are considered as design parameters. In the simulations, the relationship among the channel sizes was fixed as $d_x = d_z = d_y/2$.

Table 2

Design	parameters	of r	nicron	nixers	emplo	ved	in	CFD	simu	lations
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Shape	Notation	<i>X</i> (mm)	θ (°)
Tmixer	T133, 167, 200	-	-
TLmixer	TL67, 133, 167, 200	1	90
TL-Xmixer	TL167-0.1, 0.2, 0.33, 0.5, 1, 2	Χ	90
T- θ mixer	TL133-30°, 60°, 90°, 120°	1	θ

Table 2 lists the micromixers used in this investigation. The mixer names represent the design parameters. We name micromixers using the shape of mixer (T or TL), the channel hydraulic diameter *D*, the channel length between the points of channel confluence and channel bend, and the bend angle. The definition of *D* is given by

$$D = \frac{2d_x d_y}{d_x + d_y} \tag{1}$$

The TLmixers include a bend of 90° at X = 1 mm after the channel confluence (see Fig. 1(b) for the definition of the length of X). The TL-Xmixers include a bend of 90° at X mm after the collision. In the T- θ mixers, the channel bends with an angle of θ at 1 mm after the collision. Therefore, TL133 and TL133-90° have the same shape, and TL167 and TL167-1 also have the same shape.

The intensity of convection depends on the inlet velocity. For this reason, we considered the inlet velocity to be a design parameter and investigated the effects of velocity on mixing enhancement for each shape. The range of inlet velocity v is between 0.6 and 2 m/s, and the corresponding Reynolds number is between 120 and 300.

In addition, we simulated mixing in a multi-lamination mixer (MLmixer). In the MLmixer, the flow rate is so low that only molecular diffusion promotes mixing. Under such conditions, the mixing rate in the MLmixer depends on the fluid segment size W (μ m), namely the diffusion length. As shown in Fig. 1(c), the multi-lamination of fluids in the ML mixer is expressed by periodic boundaries in the width and depth directions. For the Tmixer and TLmixer, each fluid deforms through channel confluence and channel bend as shown in Fig. 2. We considered the effect of this deformation in terms of a reduction in diffusion length. By obtaining the MLmixer fluid segment size, which gives the corresponding mixing rate for the Tmixer or TLmixer, we can quantify the enhancement in mixing achieved through channel confluence and bend in terms of a reduction in the diffusion length W.

2.2. Evaluation of mixing performance

We evaluate the degree of mixing in a plane perpendicular to the axial direction of the microchannel using the mixing ratio δ . The definition of δ is given by

$$\delta = \frac{\sigma}{\sigma_0} \tag{2}$$



Fig. 1. Schematic of micromixers: (a) Tmixer, (b) TLmixer, and (c) MLmixer.

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