Chemical Engineering Journal 181–182 (2012) 597–606

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Journal

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

Mixing characterization and scaling-up analysis of asymmetrical T-shaped micromixer: Experiment and CFD simulation

Liu Zhendong, Lu Yangcheng*, Wang Jiawei, Luo Guangsheng

State Key Laboratory of Chemical Engineering, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

ARTICLE INFO

Article history:
Received 22 September 2011
Received in revised form
24 November 2011
Accepted 29 November 2011

Keywords:
Micromixing
Microchannel
Villermaux/Dushman method
CFD simulation
Scale up
Reynolds number

ABSTRACT

In this work, an asymmetrical T-shaped micromixer with replaceable channels was used to investigate comparatively the micromixing performance in various micromixing configurations by Villermaux/Dushman method and CFD simulation, and the scale-up strategy of mixing configuration was discussed as well. The results show that both the convergence region and mixing channel contribute considerably to the mixing, and widening the continuous fluid channel of micromixer to several millimeters in individual can still exhibit high micromixing performance as *Re* is above 6000. In an asymmetrical T-shaped micromixer with a constant height of mixing channel, the intensity of mixing (I_M) has a nearly linear relationship with *Re* in the range from 2000 to 10,000 while independent on the width of the mixing channel. Compared with one-dimension scale-up in the vertical direction, one-dimension scale-up in the horizontal direction can benefit from less deterioration to micromixing performance. Adapting for this scale-up strategy, lower mechanical energy dissipation per mass is needed at higher operational capacity. The *Re* can be used as a fundamental criterion for an asymmetrical T-shaped micromixer to adjust the width of mixing channel according to the operational capacity. Our results would be helpful for understanding the mixing phenomena in the asymmetrical T-shaped micromixer and optimizing configuration or operation conditions for micromixer of this kind.

1. Introduction

The conversion and selectivity of chemical reactions in the liquid phase may heavily depend upon mixing [1,2]. Therefore, mixing, in particular micromixing has an intensive influence on many industrial processes such as polymerization [3,4], crystallization and precipitation [5,6]. Indeed, mixing will affect all process parameters including heat and mass transfer, operational cost, process safety and product quality.

According to the scale of dimensions at which mixing takes place, mixing can be classified as micromixing, mesomixing and macromixing [7]. Micromixing refers to mixing at molecular scale. The microreaction technology has been developing rapidly in recent years with a considerable variety of micromixers emerging, promoting the development of miniaturized chemical engineering processes [8–10]. Generally, there are two principles of micromixing: passive micromixing and active micromixing. Different from passive mixing, active mixing applies external energies besides of the mechanic energy of feeds by ultrasound, magnetic field, etc. Some authors have reviewed the characteristics of micromixing and its recent development [7,11,12].

Although miniaturization is the key aspect of micromixer, excessive smallness would bring new problems such as requirements for high-standard fabrication, low processing capacity and high pressure drop [13]. Meanwhile, the concept of numbering-up in microreaction system seems not as promising as expected because of difficulty in distributing flow homogeneously [2]. Thus, the geometric scale-up of micromixer is still worth considering on the basis of exhibiting relatively high-efficient micromixing performance.

Understanding the micromixing performance in the micromixer is very important for the design of these devices and their consequent applications in multi-scale processes. To achieve this goal, several sets of rapid multiple chemical reactions having mixing-sensitive product distributions have been employed to characterize the extent of mixing on the molecular scale [14,15]. Among them, the "Villermaux/Dushman method" has gained wide acceptance. Many authors have studied the micromixing performance in various mixers by this approach [2,16–23].

Another attractive methodology for investigating mixing performance in microreactor is numerical simulation by computational fluid dynamics (CFD), since it can provide local information about fluid flow and reaction species concentration [24]. Generally, two strategies for CFD simulation are used [25]: the first strategy solves momentum equation only, and can give flow characteristics as a means of interpreting mixing performance; the second strategy solves the momentum equation and mass transfer equation, which

* Corresponding author. Tel.: +86 10 62773017; fax: +86 10 62770304.
E-mail address: luyc@tsinghua.edu.cn (L. Yangcheng).

1385-8947/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.cej.2011.11.105

Nomenclature

D_i	the effective diffusivity (m^2/s)
D_i^0	the Fickian diffusivity (m^2/s)
h_c	height of continuous phase plate (mm)
I_S	intensity of mixing
k	the turbulence energy (m^2/s^2)
L	characteristic length (m)
P	pressure (Pa)
Pe	Péclet number
Q_c	flow rate of continuous phase (L/h)
Q_d	flow rate of dispersed phase (L/h)
Q_t	total flow rate (L/h)
R	ratio between Q_c and Q_d
R_i	net reaction rates (mol/m^3s)
Re	Reynolds number
U	averaged velocity (m/s)
w_c	width of continuous phase channel (mm)
w_d	width of dispersed phase channel (mm)
X_S	segregation index
ρ	density of the fluid (kg/m^3)
η	the dynamic viscosity ($N\,s/m^2$)
ε	the dissipation rate of turbulence energy (m^2/s^3)

gives flow and concentration information both. As the most widely used method to investigate micromixing, one methodology among the first strategy involves computationally solving Navier–Stokes equation coupled with tracer's mass transfer equation and characterizing mixing by means of the diffusion efficiency of the artificial diffusive species [26,27]. Recently, Baccar et al. [20] successfully calculated the concentration profiles for chemical species in Villermaux/Dushman competitive reactions in a 2D simplified hollow fiber membrane contactor. However, their method is rather complicated and requires more computing power than aforementioned methods, which hinders its application on full 3D simulation cases.

As one of the simplest configurations for micromixing, T-shaped micromixers have been widely used and studied [28]. In general, there are two types of T-shaped micromixers. One is symmetrical T-shaped micromixer with two parallel inlets. The other is asymmetrical T-shaped micromixer with two perpendicular inlets. The former type has been received more extensive investigations [29–31]. Though viscous force dominates in microscale devices due to relatively large surface-to-volume ratio, it is reported that vortices can easily form in symmetrical T-shaped micromixer and enhance the mixing efficiency. The mixing in symmetrical T-shaped micromixer at sufficiently high Reynolds numbers (above approximately 150, depending on the geometry) is proved to be a combination of convection and diffusion effects by experiments and simulations [2,32].

Based on their efforts, a consensus on mixing in micromixer has been reached that rapid micromixing could hardly be achieved in laminar flow regime where Fickian diffusion limits the mixing process. For low and moderate Reynolds numbers (typically from 0.1 to 1000 as reported in literature), it is difficult to attain turbulent flow in T-shaped micromixer. Rapid mixing is still probable by the generation of secondary flow, swirling flow and vortices in the micromixer [33]. With the increase in Reynolds number, chaotic flow phenomena and further turbulence could be generated. Therefore, at high Reynolds numbers, convective transport should be considered in design and optimization of micromixers. Accordingly, turbulence model should be introduced in CFD simulations of micromixers [34,35].

Up till now, the mixing performance in the asymmetrical T-shaped micromixer with two perpendicular inlets has not been fully investigated. Although the asymmetrical T-shaped micromixer seems easy for application in large-scale process by stacking, the design is still lack of dimensional scaling up strategy of channel considering on the effect of channel sizes on micromixing performance. In this work, a novel micromixer with replaceable channel plates was used to investigate what is the general factor that gives decisive influence on micromixing in asymmetrical T-shaped configurations with different dimensions and how to accommodate for operational capacity by adjusting channel configuration properly. Under this motivation, our paper was organized as following. Firstly, the influences of various factors such as flowrates and mixer's feature dimensions on micromixing were comparatively assessed by Villermaux/Dushman method. Secondly, since mixing is a multi-scale process and it is important to resolve the flow and concentration fields on the microscale, CFD simulation was conducted to calculate the concentration profile of a tracer and characterize the mixing quality by a normalized index, the intensity of mixing. As the Reynolds numbers in the micromixer were relatively high (generally above 1500 under operational conditions discussed below in this paper), a widely accepted turbulence model, the k-ε model was used to describe turbulent flow in the micromixers. Finally, possible mechanisms of these influences on micromixing were analyzed, and the scaling-up strategy and optimization of operational conditions were briefly discussed from the view point of robust application as well.

2. Experimental approaches

2.1. Micromixer with adjustable channels

In this work, we designed a novel micromixer with replaceable channel plates. As shown in Fig. 1, the micromixer consisted of four parts: the continuous fluid plate, the dispersed fluid plate, and two cover plates. All the parts were made of stainless steel (type 304). The height of the continuous fluid plate (h_c), the width of the continuous fluid channel (w_c), and the width of the dispersed fluid channel (w_d) could be adjusted separately to form the mixing region of various sizes, as shown in Fig. 2(a).

To better discuss the mixing phenomena happened in the micromixer, we define two separate mixing regions: the convergence region and the mixing channel, as depicted in Fig. 2(b).

2.2. Villermaux/Dushman method

Micromixing efficiency was studied by Villermaux/Dushman method based on a competitive parallel reaction system. The reaction formulas are shown as follows:

$$H_2BO_3^- + H^+ \rightarrow H_3BO_3 \quad \text{(i)}$$

$$5I^- + IO_3^- + 6H^+ \rightarrow 3I_2 + 3H_2O \quad \text{(ii)}$$

$$I_2 + I^- \leftrightarrow I_3^- \quad \text{(iii)}$$

Reaction (ii) is fast but is much slower than reaction (i). Both reactions compete for sulphuric acid in defect stoichiometrically. In perfect mixing condition, the sulphuric acid is instantaneously dispersed in the reactive medium and consumed by borate ions according to reaction (i). In other cases, local over-concentrated acid, resulted from that the characteristic dissipation time of the acid aggregates is in the same order as or longer than the characteristic reaction time of reaction (ii), can react with surrounding iodide and iodate to yield iodine. The iodine can further react with iodide ions to triiodide according to the quasi-instantaneous equilibrium shown as reaction (iii). I_3^- concentration can be easily measured by an UV spectrophotometry at 286 nm.