Chinese Journal of Chemical Engineering 24 (2016) 711–718

Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

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

Fluid Dynamics and Transport Phenomena

Simulation of the mixing process in a straight tube with sudden changed cross-section☆

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ARTICLE INFO

Article history:
Received 17 March 2015
Received in revised form 22 July 2015
Accepted 2 September 2015
Available online 28 January 2016

Keywords:
Mixing
Intensification
Simulation
Sudden change in cross-section
Vortex

ABSTRACT

In this work, we revised the expression of mixing intensity to describe the mixing output through a cross section in a flow system by considering heterogeneity of flow field, and carefully investigated the mixing process along a straight tube with expanding/contracting cross section by simulation method. The simulation results show that a sudden expansion of cross section has remarkable mixing intensification effect within a limited period (on the sub-second scale) or tube-length (on the millimeter scale), corresponding to the generation of considerable local vortices determined by both the flow capacity and the ratio of cross section change; a sudden contraction of cross section has instantaneous but weak mixing intensification effect; through introducing a local expansion structure with proper length, as the combination of sudden expansion and sudden contraction, their mixing intensification effects could be superposed. Besides, the rationality and importance are experimentally verified to explore the time profile of mixing intensity and carry out the vortex analysis by simulation for enhancing the selectivity of a complicated reaction system. These progresses may lead to more meaningful quantitative description of mixing process in a flow microreactor for some specific chemical processes.

1. Introduction

Microfluidics focuses on the effective manipulation of fluids at microscale, which are concerned in varieties of research fields such as DNA sequencing, synthesis, reaction and analysis, environmental monitoring, and so on [1–6]. Microfluidic technologies are drawing close attentions from both industry and academia [7–9], and some microfluidic technologies have been used at industrial scale [10,11]. As a well-known representative, microreactor is commonly featured with excellent heat and mass transfer as well as precise control of residence time [12–14]. On the demands of chemical process intensification towards continuous production in modern chemical industry, the microreactor has potential advantages including small hold-up of chemical reagent, low equipment and energy costs [15], precise process control, high productivity, enhanced reaction selectivity, and inherent safety [16].

Since microreactor is of kernel components in integrated microfluidic systems [17], enhanced micromixing is an essential function of micromixer. Many chemical processes following reactant mixing are accompanied with relatively slow side step [18], for which the time duration before achieving good micromixing may have significant influence on the product quality. Nanoparticle preparation by precipitation is such an example. Using microreactor with high mixing performance can shorten the duration of insufficient micromixing and inhibit unexpected nanoparticle growth and aggregation [19]. The mixing performance of an equipment, dependent on both geometric structure and operating conditions, is a hotspot in microchemical engineering [20].

A number of methodologies have been exploited and developed for characterizing the mixing performance of micromixer, which can be summarized into two categories: experimental method and simulation method [21–24]. The "Villermaux/Dushman" reaction system is the most widely accepted experimental method, where the distribution of products from an instantaneous reaction and another rapid reaction in parallel reflects the rate of mixing on the molecular scale [25,26]. Investigations on various micromixers using this method have shown that the micromixing can be distinctly enhanced after passing through some specially designed structures, like the branch, combination [27], sudden expansion [28], contraction [29], wavelike microchannels [30] and small tubular turbulent apparatuses with star-shaped diaphragms [31]. Considering the expenditure in manufacture and flow distribution control, a straight single channel/tube with sudden changed (expanded/contracted) cross section is a good choice for practical use [32–35]. Common experimental methods are difficult to reveal the temporal and spatial profiles of the mixing status along flow direction. Viewed from this point, the simulation methods (such as computational fluid dynamics, Lattice-Boltzmann method) providing the local three-dimensional flow information are powerful tool to understand the details of mixing process [36,37]. For the commonly used T-mixer, researchers identified by simulation various flow patterns, such as vortex flow, engulfment flow

☆ Supported by the National Natural Science Foundation of China (21176136, 21422603) and the National Science and Technology Support Program of China (2011BAC06B01).
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http://dx.doi.org/10.1016/j.cjche.2016.01.011
1004-9541/

and unsteady flow, and reveal their dependence on the Reynold number and geometrical parameters [38–43]. However, what happens along a straight single channel/tube with sudden changed cross section is still less reported, and its exploration is quite necessary for developing easy-to-access microreactor.

In this work, we investigated the mixing process along a straight tube with expanded/contracted cross section by numerical simulation. The mixing intensity of fluid across a cross section was newly defined as an index of mixing status, and the spatial/temporal profile of which, along the flow direction, was evaluated to determine the effect scope of a sudden cross section change in mixing enforcement. The relationship between the effect and the geometrical parameters was revealed as a guidance for realizing good match between mixing process and chemical process. These progresses may lead to more meaningful quantitative description of mixing process in a flow system and more precise structure design of microreactor towards some specific chemical processes.

2. Simulation Methods

2.1. Simulation conditions

Computational fluid dynamics (CFD) simulation is used to obtain the numerical solution to the equations of momentum and mass transport to describe the mixing process. Herein, an incompressible fluid was assumed, all the simulation cases corresponded that $Re \ll 2000$ and $Pe \gg 1$, so a direct numerical simulation was exploited and solved by COMSOL 3.4. The following are main equations.

Navier–Stokes equation and the continuity equation describing the momentum and mass transfer:

$$\rho\frac{\partial \boldsymbol{u}}{\partial t}+\rho\boldsymbol{u}\cdot\nabla\boldsymbol{u}=\nabla\cdot\left(-P\boldsymbol{I}+\mu\left(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^{\mathrm{T}}\right)\right)+\boldsymbol{F} \quad (1)$$

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

where ρ is the fluid density, $\boldsymbol{u}=(u, v, w)$ the flow-velocity field, P the fluid pressure, $\boldsymbol{I}$ the unit matrix, μ the dynamic viscosity of fluid, and $\boldsymbol{F}=(f_x, f_y, f_z)$ the volume force affecting the fluid. In this work, we also assume that (1) the reference fluid is water with ρ of 1000 $\mathrm{kg\cdot m^{-3}}$ and μ of 0.001 Pa·s; (2) $\boldsymbol{F}$ is zero as neglecting volume forces.

The convection–diffusion equation describing mass transfer:

$$\frac{\partial c}{\partial t}+\nabla\cdot(-D\nabla c)+\boldsymbol{u}\cdot\nabla c=R \quad (3)$$

where c is the concentration, D the diffusion coefficient, and R the reaction rate. The default settings include $D=2\times10^{-9}$ $\mathrm{m^2\cdot s^{-1}}$ and $R=0$ (no chemical reaction is involved).

Staring from a T-junction for initiating mixing, three typical geometries are introduced in simulation and illustrated in Fig. 1, corresponding to sudden expansion, sudden contraction, and their combination. The three branches of the tee are the same in diameter. The length of the mixing tube before the cross section changing is 20 mm, guaranteeing a nearly fully developed flow after the collision of two flows at T-junction. The other geometric sizes were set according to the objective of simulation and illustrated case by case.

The boundary conditions were set as follows: (1) the no slip and no flux boundary conditions were applied on the tube walls; (2) the velocity through the cross section of each inlet was uniform; (3) the gauge pressure at the outlet was 0 ($P=0$ Pa); (4) the two feeds had the same physical properties except for solute concentration; and (5) the concentration of two feeds was 20 $\mathrm{mol\cdot L^{-1}}$ and 2 $\mathrm{mol\cdot L^{-1}}$, respectively.

The *physics-controlled mesh* was adopted and the element size is *normal*. The mesh was *tetrahedral*. The convergence test was conducted to ensure the accuracy. In detail, we selected several meshes, from *coarser*, *coarse*, *normal*, *fine* to *finer*, to calculate the profile of mixing intensity (I_M, described later). Taking a 20 mm length straight tube (i.d. 0.45 mm) as an example, Fig. 2 shows calculation results (I_M of fluid at the end cross section of the tube) using various types of mesh. As seen, the results corresponding to the *normal* mesh (70 triangles in the cross section, cell size in flow direction 0.076–0.25 mm, 95381 cells) and *fine* mesh (104 triangles, 0.038–0.20 mm, 219073 cells) almost coincide with each other, deviating apparently from those corresponding to the *coarse* mesh (40 triangles, 0.11–0.38 mm, 50927 cells) and the *coarser* mesh (40 triangles, 0.15–0.49 mm, 25997 cells). From

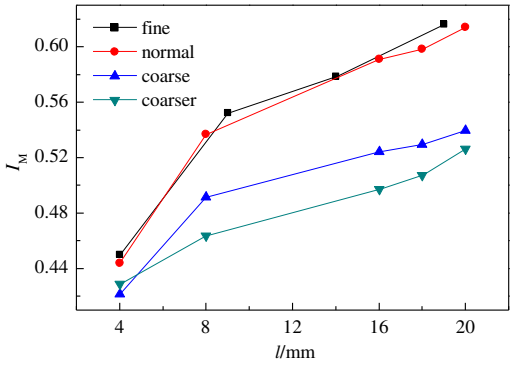

Fig. 2. The comparison of simulation results using various meshes. The flow velocity at each inlet is 0.1 $\mathrm{m\cdot s^{-1}}$.

this point of view, the requirement of grid (mesh) independence could be met for using *normal* mesh to characterize I_M. On the other hand, using *normal* mesh could evade the difficulty in convergence at high velocity or critical cross section change as using mesh with higher precision.

2.2. Index for characterizing mixing status

Based on Danckwerts' intensity of segregation [44], the mixing intensity (I_M) is commonly used to quantify the mixing efficiency, and defined as

$$I_M=1-\sqrt{\frac{\delta^2}{\delta^2_{max}}} \quad (4)$$

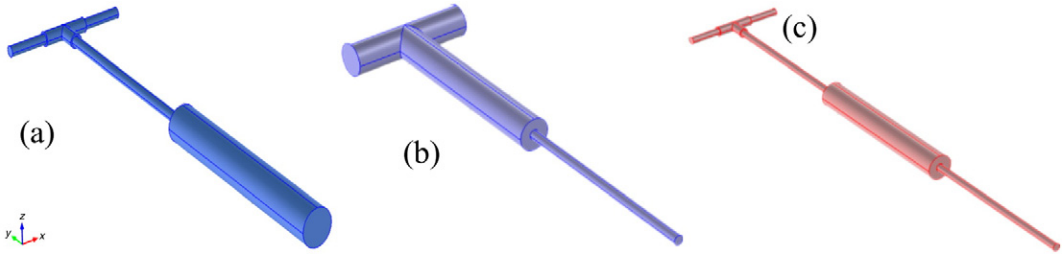

Fig. 1. Straight tube with (a) suddenly expanded cross-section, (b) suddenly contracted cross-section, or (c) their combination.