Chemical Engineering & Processing: Process Intensification 124 (2018) 11–23

Contents lists available at ScienceDirect

Chemical Engineering & Processing: Process Intensification

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

Analyzing mixing quality in a T-shaped micromixer for different fluids properties through numerical simulation

A.S. Lobasov[a,b,*], A.V. Minakov[a,b]

[a] Siberian Federal University, Krasnoyarsk, 660074, Russian Federation
[b] Institute of Thermophysics SB RAS, Novosibirsk, Russian Federation

ARTICLE INFO

Keywords:
Hydrodynamics
Numerical simulation
T-shaped micromixer
Microagitator
Mixing
Viscosity
Temperature
Rheology
Pressure drop

ABSTRACT

Microreaction engineering enables new strategies in process intensification. A precise analysis of local mass transfer and hydrodynamics in micromixers for different flow regimes are strongly needed for a complete understanding the processes occurring. One of the simplest in the manufacture, but at the same time, quite effective T-shaped micromixer was used for numerical investigation and analyzing the mixing quality and flow regimes as well as the influence of different fluids properties on this parameters. It was numerically revealed that the viscosities and the densities, as well as the initial temperatures and the rheology of mixing fluids have significant effects on the flow regimes and the mixing efficiency of two fluids. In this study viscosities and densities ratios of mixing fluids ranged from 1 to 2; the coefficient n in power-law model of non-Newtonian fluids ranged from 0.3 to 1; the initial temperatures difference of two fluids was varied up to 40 °C. Mixture components concentration as well as pressure and velocity fields distribution in the micromixer was obtained. The dependence of fluids mixing efficiency and the pressure drop, as well as a map of flow regimes and mixing modes on the Reynolds number and properties of miscible fluids was numerically established.

1. Introduction

The miniaturization of technological processes is being actively promoted in recent years in the chemical industry, and thus micromechanics has become a rapidly developing and promising research area. Microchannel devices are widely used in various fields of science and technology as microreactors, microscale heat exchangers, micromixers, etc. Many studies have noted that the use of microdevices allows significantly enhancing the physicochemical processes in comparison to classical space consuming reactors [1–3]. It can be confidently predicted that the situation in the chemical laboratories will change radically in the near future toward a significant improvement in the productivity and efficiency of synthesis processes through a substantial miniaturization of instruments and apparatuses. Control of pressure, temperature, reaction time and flow velocities in reactors with small volume is carried out much easier and more efficiently. Thus, the main undeniable advantages of microreactor microsystems are safety of carrying out highly exothermic reactions and working with toxic or explosive reagents, carrying out reactions in supercritical conditions and significantly reducing the cost of research, as well as implementation and scaling of chemical processes.

However, despite the obvious benefits of microchannel technology, there are a number of specific problems. Most microchannel devices that used in chemistry and biology require fast and effective mixing of substances [1–5]. At the same time, the flow in microchannels is predominantly laminar and mixing occurs through diffusion, and thus very slowly. Therefore, the design and optimization of micromixers with the shortest mixing time is an actual problem in the development of microchannel devices.

The T-shaped micromixers (Fig. 1) are the simplest in the manufacture in terms of their underlying geometry. The first study of T-shaped micromixer [6] shown very high stirring rates obtaining in such configuration of micromixers. Flow regimes at low Reynolds numbers have been systematically studied previously in many works [6–8]. Apparently, first studies of fluids mixing processes in T-shaped micromixer at moderate Reynolds numbers were conducted in [9]. The effective mixing rate in the T-shaped micromixer at a certain inlet flow velocities was obtained experimentally for the first time in that work. The most comprehensive experimental study of mixing in T-shaped micromixer at moderate Reynolds numbers (100–400) was carried out in [10].

A number of experimental and theoretical works [11–14] should be also mentioned. They present calculations of some flow regimes in T-shaped micromixers with different cross sections. The existence of a

* Corresponding author at: Siberian Federal University, Krasnoyarsk, 660074, Russian Federation.
E-mail address: perpetuityrs@mail.ru (A.S. Lobasov).

https://doi.org/10.1016/j.cep.2017.11.004
Received 6 April 2017; Received in revised form 12 October 2017; Accepted 8 November 2017
Available online 23 November 2017
0255-2701/

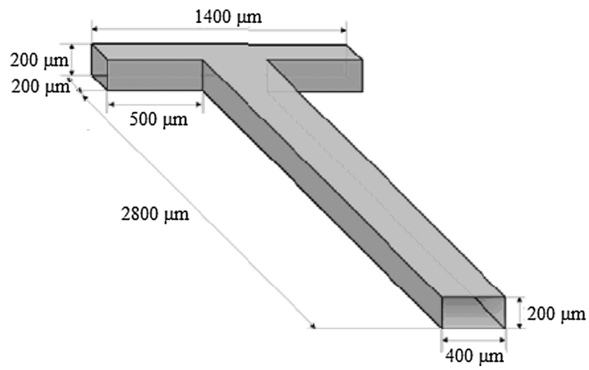

Fig. 1. Geometric configuration of the task.

certain critical Reynolds number, at which Dean vortices in the T-shaped micromixer lose their symmetry was shown experimentally.

A more detailed study of this effect was carried out in a series of works [15–17]. Flow regimes and mixing modes in the water-water system in the T-shaped micromixer were investigated within a wide range of Reynolds number from 1 to 1000, using numerical simulation, micro Particle Image Velocimetry (μ-PIV), and micro Laser Induced Fluorescence (μ-LIF) measurements.

The flow structure and its influence on mixing mode was investigated, five different flow regimes were revealed, and dependences of friction coefficient and mixing efficiency on the Reynolds number were obtained. Dramatic increase in mixing efficiency at transition from symmetric to asymmetric mode for stationary flow regime was noted. The laminar-turbulent transition area was investigated and good qualitative and quantitative agreement with the results of field experiments was obtained.

A systematic study of the viscosity effect on mixing modes in the T-shaped micromixer was carried out in [18], where the significant effect of viscosities ratio on the flow structure before and after the transition from symmetric to asymmetric flow regimes was shown. The self-similar behavior of the asymmetric flow regime is established.

Also a comprehensive investigation of mixing of binary fluids with composition-dependent viscosity in a T-shaped micro-device was carried out in [19]. In that study, it was shown that in the case of a positive fluidity of mixing, the onset of the engulfment regime is accompanied by a sharp increase of the degree of mixing, with the critical Re decreasing as the fluidity of mixing increases. This research was developed in [20], where unsteady mixing of binary liquid mixtures with composition-dependent viscosity was studied. It was shown that a viscous layer forms at the confluence of the inlet flows when the viscosity of the mixture is larger than that of the pure components. It tends to keep the two streams separated, resulting in a shift of the engulfment regime towards larger Reynolds numbers.

Water-ethanol mixing in T-shaped microdevices was investigated numerically in [21] and experimentally in [22] taking into account both density and viscosity variations. The results were compared with studies of water-water mixing. In both research works, it was shown that at smaller Reynolds number there is no vortex formation for either cases, and at larger Reynolds numbers, mixing of water and ethanol may take considerably longer, as the onset of engulfment is retarded and occurs at larger Reynolds number.

In addition to micromixing of Newtonian fluids, the problem of non-Newtonian fluids mixing (blood, polymer solutions, suspensions) is relevant as well. A study of non-Newtonian fluids mixing in serpentine and T-shaped micromixers was carried out in [23]. The Reynolds number ranged from 10^{-2} to 10^{2}. A blood, whose viscosity was given by Casson and Carreau-Yasuda non-Newtonian blood viscosity models, served as a non-Newtonian fluid. It was shown that the efficiency of mixing in T-shaped mixer decreases with the increase in the Reynolds number due to the corresponding increase in the Peclet number. In the serpentine micromixer the mixing efficiency originally decreased and then sharply increased upon reaching the region of transition from symmetric to asymmetric mode at stationary flow.

The effect of non-Newtonian fluid characteristics, specifically the effect of shear-thinning on the critical Reynolds number through the use of the power-law model in the power-law index range from 0.5 to 1 was investigated in [24]. It was shown as a result that, depending on the exact choice of Reynolds number, it would be possible to claim that shear-thinning either promotes or inhibits the bifurcation to asymmetric flow.

Thus, flow regimes depending on the Reynolds number were investigated in many works [18–21,24–29]. At that, quite interesting hydrodynamic phenomenon, named flow reversal or engulfment flow regime upon reaching the critical Reynolds number was observed in the T-shaped mixer. This critical Reynolds number differs for different mixtures, also it strongly depends on the channel geometry, e.g., for water-water mixing in the T-channel, shown in Fig. 1 the critical Reynolds number is equal to 140–150. The aim of the present work is to carry out systematic investigation of the effects of miscible fluids properties on the flow regimes and the critical Reynolds number in the T-shaped micromixer.

2. Mathematical model and numerical algorithm

Incompressible flows of multi-component and generally non-Newtonian fluids, which are described using a hydrodynamic approach based on the solution of the Navier-Stokes equations were considered in this work. Currently, in numerous experiments was shown that such description for fluids works well for the channels sizes up to 1 μm.

In general, the Navier-Stokes equations system has the following form:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho v) = 0$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla(\rho \mathbf{v}\mathbf{v}) = -\nabla p + \nabla \mathrm{T} + \rho g \tag{1}$$

Here ρ is the fluid density, p is the pressure, $\mathbf{v}$ is the velocity, and $\mathbf{T}$ is the tensor of viscous stresses, $\mathbf{g}$ is the gravity vector.

The widely known approach [30,31], in which the medium is considered as a nonlinear viscous fluid characterized by the effective fluid viscosity $\mu(\dot{\gamma})$ depending in general on shear rate, was used for the simulation of non-Newtonian flows. At that, the viscous tension tensor is defined as $\mathbf{T} = \mu\varepsilon$, while components of the strain velocity tensor ε can be written as:

$$\varepsilon_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}.$$

Shear rate $\dot{\gamma}$ is the second invariant of the strain velocity tensor:

$$\dot{\gamma} = \sqrt{\frac{1}{2}\sum_{i \neq j} \varepsilon_i \varepsilon_j}.$$

The considered medium may be both Newtonian viscous fluid and non-Newtonian viscoplastic fluid, whose behavior is described by the most common “power-law” rheological fluid model.

The effective viscosity depending on the rheology of the medium is given by:

$\mu(\dot{\gamma}) = k$ for Newtonian medium (k is the molecular viscosity of the fluid),

$\mu(\dot{\gamma}) = k\dot{\gamma}^{n-1}$ for the power-law model, where n and k are coefficients of the model.

The effective viscosity of the mixture is determined through the mass fraction of its components f and effective viscosities of pure components $\mu_{1,2}$:

$$\mu = f\mu_1 + (1 - f)\mu_2$$