

Density effect on the mixing efficiency and flow modes in T-shaped micromixers

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Abstract. Flow patterns and mixing of liquids with different densities in T-shaped micromixers are numerically investigated at Reynolds number range from 1 to 250. The density ratio of the mixing media varies from 1 to 2; its effect on the flow structure and the mixing is studied. The dependences of the mixing efficiency and the pressure difference in this mixer on the density ratio and the Reynolds number are obtained. It is shown that the density ratio has a considerable effect on the flow structure, especially before the transition from the symmetric to the asymmetric flow pattern.

1 Introduction

The miniaturization of technological processes has been actively promoted in recent years in the chemical industry, and thus micro-mechanics has become a rapidly developing and promising research area. Microchannel devices are widely used in various fields of science and technology as microreactors, micro-scale heat exchangers, micro-mixers, 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]. Control over pressure, temperature, reaction time and flow velocities in reactors with small volumes is now realized much easier and more efficiently. This implies the main undeniable advantages of microreactor microsystems: safety of highly exothermic reactions and work with toxic or explosive reagents, possible reactions in supercritical conditions, significant reduction of research costs, as well as implementation and scaling of chemical processes. In this paper a T-shaped micromixer, which is one of the simplest in the manufacture, but at the same time, quite effective form of a microfluidic mixer was considered. Thus, flow regimes depending on the Reynolds number were investigated in many works [4,5]. At that, quite an interesting hydrodynamic phenomenon, namely the flow reversal or engulfment flow regime [5-8] upon reaching the critical Reynolds number of 130-160 was observed in the T-shaped mixer. The aim of the present work is a systematic study of the effects of miscible fluids densities ratio on the flow and mixing regimes in the T-shaped micromixer.

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2 Mathematical model and numerical algorithm

We consider incompressible flows of multi-component Newtonian fluids, which are described using a hydrodynamic approach based on the solution of the Navier-Stokes equations. Currently, numerous experiments show that such description for fluids works well up to the channel size of 1 micron.

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

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

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

The density of the mixture is expressed in terms of the mass concentrations f_i of flow components and partial densities ρ_i in the following way:

$$\rho = \left[\sum_i (f_i / \rho_i) \right]^{-1}$$

Here the evolution of mass concentrations is determined by the equation:

$$\frac{\partial \rho f_i}{\partial t} + \nabla(\rho f_i \mathbf{v}) = \nabla(\rho D_i \nabla f_i) \quad (2)$$

where D_i is the diffusion coefficient of the i -th component.

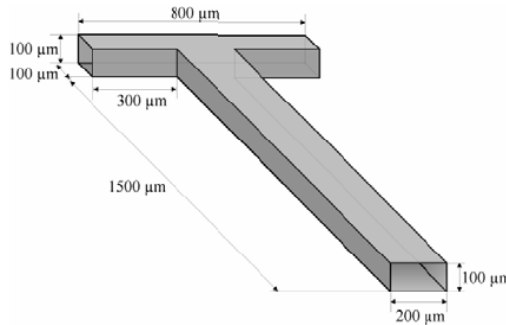


Fig. 1. Geometry of the problem.

In our calculations we used a three-block grid consisting of 9.5 million grid nodes. Preliminary calculations have shown that this level of grid particularization is acceptable in terms of calculation accuracy. The fluid flow rate determined at the inlet of mixer channels was constant with steady-state velocity profile. At the mixing channel outlet, Neumann conditions were set, meaning that the derivative normal to the outlet surface, taken of all scalar quantities, is equal to zero. The walls of the mixer were considered as insulated. For velocity vector components, the no-slip condition was taken as boundary condition on the channels walls. The applicability of this type of boundary conditions for channels with a size of 50 μm had been demonstrated in [1,4].

The channel dimensions are shown in Fig. 1. The channel thickness is 200 μm , while the width of its narrow and wide parts is 200 μm and 400 μm , respectively. In our calculations we determined the pressure drop between one of the mixer inlets and the outlet, as well as mixing efficiency. In the literature, mixing efficiency is usually quantified

using the parameter $M = 1 - \sigma/\sigma_0$, where $\sigma = V^{-1} \int_V (f - \langle f \rangle)^2 dV$ is the root-mean-square deviation of the mass fraction of mixture component f from its average value $\langle f \rangle$, $\sigma_0 = \langle f \rangle \cdot (1 - \langle f \rangle)$ is the maximum root-mean-square deviation, and V is the volume of the computational domain.

3 Results and discussion

The effect of density on flow regimes in the microchannel was studied. Water, tinted with rhodamine was supplied through one of the channel inlets. Fluid with viscosity and diffusion coefficient similar to those for pure water but with a changed density was supplied at the same flow rate through another inlet to the mixer. We have performed three series of calculations with densities 1.25, 1.5 and 2 times greater than the density of water. Because of this fact the viscosities of both fluids were set constant and equal to $\mu = 0.001 \text{ Pa}\cdot\text{s}$ in such methodical research. The change in the flow regimes in the microchannel is characterized by Reynolds number, determined as $\text{Re} = \rho U d_h / \mu$, where $U = Q/(2\rho H^2) = Q_{in}/(\rho H^2)$ is the superficial velocity in the mixing channel, $H = 200 \text{ }\mu\text{m}$ is the channel height, and $d_h = 267 \text{ }\mu\text{m}$ is the hydraulic diameter.

Increasing the density of one of the miscible fluids leads to significant changes in the flow pattern. For very small (less than 10) Reynolds numbers the flow structure and mixing of fluids with different densities is in general similar to the flow of two identical fluids. Therefore, the mixing efficiency in this regime slightly depends on the density of fluids (see Fig. 2a). The increase of Reynolds number in the channel causes formation of vortices, and the difference in densities starts its effect. It is clear that in contrast to the case of equal densities of miscible fluids, the interface between media is not flat. Fluid with a higher density pushes a less dense fluid from channel walls and somewhat envelops it. When fluids density ratio increases, this effect is amplified; that results in an increase of the interface area of miscible fluids and consequently the enhancement of the mixing efficiency in this regime (see Fig. 2a).

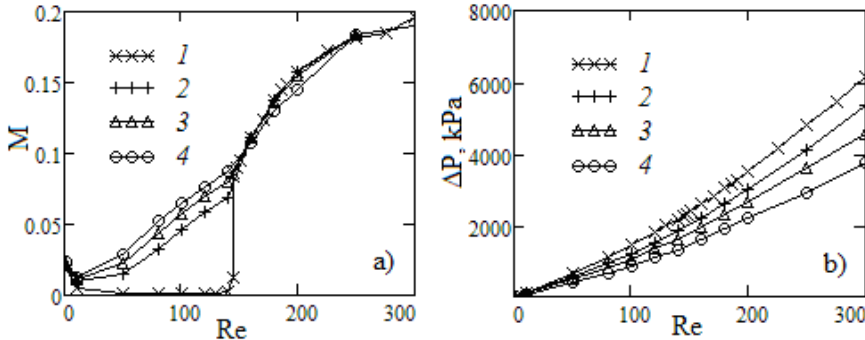


Fig. 2. Mixing efficiency (a) and pressure drop between the mixer inlet and the outlet (b) depending on Reynolds number: $\rho/\rho_0 = 1$ (1), 1.25 (2), 1.5 (3), 2 (4).

In addition, an interesting behavior is observed in horseshoe vortices (Dean vortices), which are generally preserved when increasing the density of one of the fluids. Though the increase in density ratio leads to appearance of asymmetry with respect to the central axis of the channel. The horseshoe vortex in the mixing channel is growing faster in a fluid with a lower density than in the fluid with a greater density. And the larger the density ratio the more pronounced this process. A similar asymmetry is observed in the region of secondary vortices formation at the junction of inlet channels and the mixing channel. At that, the

Dean horseshoe vortex, which is located in the more dense fluid, changes significantly with increasing the density of this fluid, in contrast to the vortex located in the water. With further increase in the Reynolds number we observed flow reversal and the beginning of engulfment regime. In the course of numerical simulations analysis, it was revealed that this transition occurs within the region of Reynolds numbers from 144 to 144.5, regardless of the density ratio at the inlet of the T-shaped channel. Flow reversal and transition from symmetric to engulfment flow regime are accompanied by a sharp increase in the mixing efficiency. In addition, the mixing efficiency jump in the transition region becomes almost unpronounced up to its complete nonoccurrence, as it is observed for mixing of fluids with density ratio equal to two (Fig. 2a).

Also, we analyzed a pressure drop between the mixing channel inlet and outlet. Fig. 2b presents the pressure drop between the inlet to the mixing channel with a more dense fluid and the outlet from the T-shaped microchannel. As is obvious, similarly to the case of $\rho/\rho_0=1$, the pressure drop in fluids with higher density is not characterized by any peculiarity in the transition region from the symmetric flow regime to the asymmetric pattern. It is interesting that with increasing density the pressure drop decreases.

4 Conclusions

The conducted numerical simulation allowed identifying the following regimes for incompressible fluid flow in T-shaped micromixers: stationary vortex-free flow; stationary symmetric vortex flow; intermittent transition from symmetric to asymmetric flow (engulfment flow); and stationary asymmetric vortex flow. It is shown that the change in the density of one of the miscible fluids does not result in a shift of flow regimes. However we observed a significant flow asymmetry in the region before its transition to the engulfment flow mode. It is established that in the symmetric flow region, the mixing efficiency increases with the increase in density ratio because of the same reason. This is caused by an increase in the interface between miscible media due to the flow around a more dense fluid over the less dense fluid.

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