Initial temperatures effect on the mixing efficiency and flow modes in T-shaped micromixer

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Abstract. Flow patterns and mixing of liquids with different initial temperatures in T-shaped micromixers are numerically investigated on the Reynolds number range from 1 to 250. The temperature of the one of mixing media was set equal to 20ºC, while the temperature of the another mixing media was varied from 10ºC to 50ºC; its effect on the flow structure and the mixing was studied. The dependences of the mixing efficiency and the pressure difference in this mixer on the difference in initial temperatures of miscible fluids and the Reynolds number were obtained. It was shown that the presence of a difference in initial temperatures of miscible fluids leads to a shift of flow regimes and the flow and mixing of two fluids with different initial temperatures can be considered as self-similar pattern with regard to the reduced Reynolds number.

1. Introduction

The miniaturization of technological processes has been actively promoted in recent years in the physical and 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, significantly 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 mixers was considered. Thus, flow regimes depending on the Reynolds number in such micromixers 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 equal to 130-160 was observed in the T-shaped mixer. The aim of the present work is a systematic study of the effects of difference in the initial temperatures of miscible fluids on the flow and mixing regimes in the T-shaped micromixer.

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:

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

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

Here ρ is the fluid density, p is the pressure, $\mathbf{v}$ is the velocity, and $\mathbf{T}$ is the tensor of viscous stresses. The evolution of mass concentration is determined by the equation:

$$\frac{\partial \rho f}{\partial t} + \nabla(\rho f \mathbf{v}) = \nabla(\rho D \nabla f) \tag{2}$$

where D is the diffusion coefficient and f is the mass fraction of the passive component.

The energy conservation equation is considered as follows:

$$\frac{\partial}{\partial t}(\rho E) + \nabla(\mathbf{v}(\rho E + p)) = \nabla(\lambda \nabla T) \tag{3}$$

where $E = h - p\rho^{-1} + 0.5v^2$, λ is the thermal conductivity coefficient and h is the enthalpy, which determined by equation:

$$h = \int_{T_0}^{T} C_P dT \tag{4}$$

The mixture temperature T is calculated in each point from equation (4) by using the mixture enthalpy h found by equation (3). The viscosity coefficient and the density of the mixture as well as the thermal conductivity coefficient and the specific heat capacity are dependent on the temperature and are determined by using the well-known thermophysical properties [9-11] of pure water. The specific heat capacity of the pure water is defined in the form of a fourth-degree polynomial of temperature.

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 figure 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 each of the mixer inlets and the outlet, as well as mixing efficiency. In the literature, mixing efficiency is usually quantified using the parameter $M = 1 - (\sigma/\sigma_0)^{1/2}$, 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.
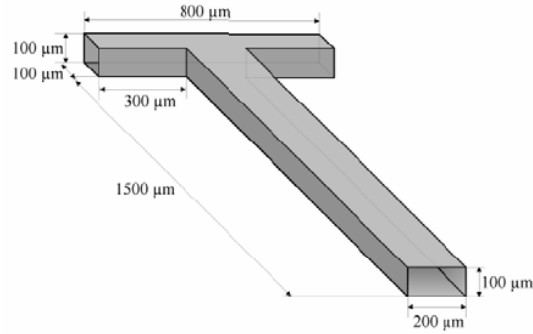
Figure 1. Geometric configuration of the task.

3. Results and discussion

The thermal mixing of Newtonian fluids in T-shaped micromixer was studied. The effect of different initial temperatures of the fluids at the inlets on the flow regimes was investigated. The temperature of one of the fluids was set equal to 20°C, while the temperature of other fluid tinted with rhodamine varied and was equal to: 10°C, 30°C, 40°C, and 50°C. Pure water with the well-known temperature-dependent thermophysical properties [9-11] was used.

The change in the flow regimes in the microchannel is characterized by the Reynolds number, determined as $Re = \rho U d_h / \mu$, where $U = Q (2\rho H^2)^{-1} = Q_{in} (\rho H^2)^{-1}$ is the superficial velocity in the mixing channel, $H = 200$ μm is the channel height, $d_h = 267$ μm is the hydraulic diameter.

Fluids have different thermal properties at various fluid temperatures at the channel inlet. Mainly the mixing mode of two fluids in micromixer will be influenced by the fluid viscosity and density. As shown in [5], increasing the viscosity of one of the fluids shifts the region of transition from steady symmetrical vortex flow to the engulfment regime and increasing the density of one of the fluids causes the appearance of asymmetry in the flow of this fluid relative to the other. Both of these effects manifest themselves in the case of mixing of two fluids with different temperatures at the inlet to micromixer. The fluid with a greater viscosity starts gradually "flowing around" the fluid with a lower viscosity, as it was shown for the case of different viscosities. However, since densities of fluids are also different, therefore, with the increase in Reynolds number, the fluid with a higher density starts in turn "flowing around" the fluid with a lower density, as was shown above for the case of different densities. In addition, it was shown that the beginning of the engulfment regime depends only on the viscosity ratio and does not depend on the density ratio. Further, with the increase in Reynolds number the engulfment flow regime begin and continue to develop. This is accompanied by increase of the vortices size, the interface area and, accordingly, the mixing efficiency.

Furthermore, the difference in the fluids densities may cause some changes in flow and mixing patterns due to the influence the natural convection in non-zero gravity case. There is the dimensionless number that expresses the ratio of the buoyancy term to the flow shear term and called the Richardson number (Ri). In thermal convection problems, Richardson number represents the importance of natural convection relative to the forced convection. The Richardson number in this context is defined as $Ri = g\beta(T_h - T_c)LU^{-2}$, where g is the gravitational acceleration, β is the thermal expansion coefficient, T_h is the hot fluid temperature, T_c is the cold fluid temperature, L is the characteristic length, and U is the characteristic velocity. The Richardson number can also be expressed by using a combination of the Grashof number and Reynolds number, $Ri = Gr\,Re^{-2}$. The Grashof number (Gr) is a dimensionless number in fluid dynamics and heat transfer which approximates the ratio of the buoyancy to viscous force acting on a fluid. For pipes and channels the Grashof number is defined as $Gr = g\beta(T_h - T_c)L^3\nu^{-2}$, where ν is the kinematic viscosity. Typically, the natural convection is negligible when $Ri < 0.1$, forced convection is negligible when $Ri > 10$, and neither is negligible when $0.1 < Ri < 10$. In our case the maximum temperature difference was 30°C ($T_h = 50°C$, $T_c = 20°C$). In these conditions the average thermal expansion coefficient $\beta_{av} = 3.155$ K^{-1},

the average kinematic viscosity $v_{av} = 0.781 \cdot mm^2/s$ and $L = h = 200$ μm. Eventually, Gr = 1.218 and the Reynolds number in the calculations was ranged from 10 to 300, so the Richardson number was ranged from $1.353 \cdot 10^{-5}$ (for Re = 300) to 0.01218 (for Re = 10). Based on this, the natural convection can be neglected.

The distribution of temperature and concentration of mixing components in various sections of the mixer for $\Delta t = 10$ºC and different Reynolds numbers is shown in figure 2. As is obvious, the distributions of concentration and temperature are not absolutely identical. The thickness of the mixing layer of temperature field is considerably higher than that of the concentration field. This is due to the different scales of the heat conduction and diffusion processes. Thus, the case of variable-temperature fluid cannot be considered absolutely identical to the cases of variable viscosity and density of mixing media.
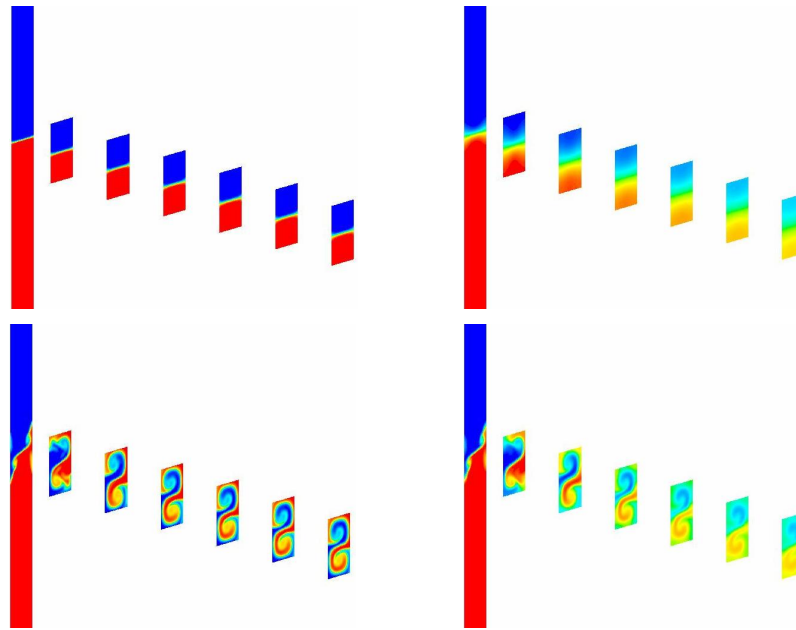

Figure 2. Concentration (left) and temperature (right) distribution at Re = 10 (upper) and Re = 150 (lower)

Figure 3a represented mixing efficiencies depending on the Reynolds number for different initial temperatures of the fluids. Analysis of the calculation results shows that change of flow regime at the Reynolds number equal to 162 occurs at a temperature difference equal to -10°C, while at Re = 126 for $\Delta t = 10$ºC, at Re = 118 for $\Delta t = 20$ºC, and at Re = 114 for $\Delta t = 30$ºC. Certainly, this is largely due to the viscosity effect. An interesting effect can be obtained if the reduced Reynolds number is calculated using the arithmetic mean value of $\mu_m = 0.5 \cdot (\mu_0 + \mu_1)$, where μ_0 is the viscosity of water at 20°C, while μ_1 is the viscosity of water at some other temperature. Different ways of defining the effective viscosity and their influence on the obtained results were considered in [5]. Using this method of defining the reduced Reynolds number, it is possible to plot a dependence of two fluids mixing efficiency on this number (see figure 3b). It is obvious that the transition occurs at reduced Reynolds number equal or close to 145 and the mixing efficiency is approximately the same for all studied cases.

Besides, the pressure drop between the micromixer inlet and mixing channel outlet was analyzed. In figure 4a shown the dependence of the pressure drop between the micromixer outlet and the inlet, where was supplied the water at a temperature of 20°C on Reynolds number. It is obvious that the differences between them are not very significant. When considering the pressure drop between the micromixer outlet and the inlet, where was supplied the water at the varied temperature depended on the Reynolds number, more substantial difference between results was obtained for different cases

(figure 4b). It is apparent that these curves are arranged in order of increasing the initial inlet temperature of the fluid. This behaviour is easy to explain, since the pressure drop is proportional to the fluid viscosity and density, therefore the increase of the inlet fluid temperature leads to decrease in pressure drop.
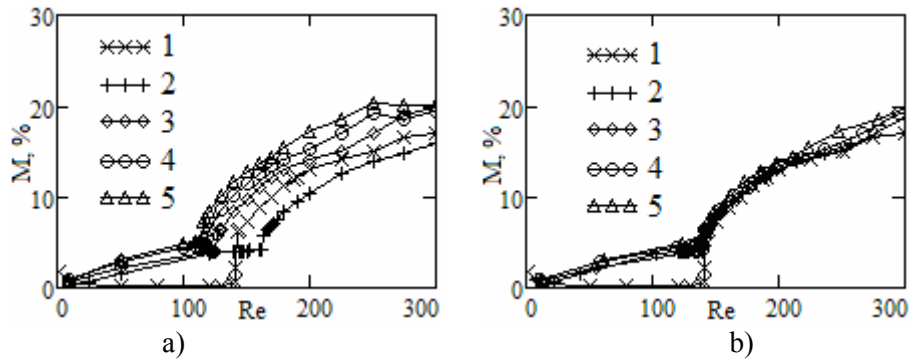

Figure 3. Mixing efficiency versus Reynolds number and reduced Reynolds number:
$\Delta t = 0^{\circ}C$ (1); $\Delta t = -10^{\circ}C$ (2); $\Delta t = 10^{\circ}C$ (3); $\Delta t = 20^{\circ}C$ (4); $\Delta t = 30^{\circ}C$ (5)
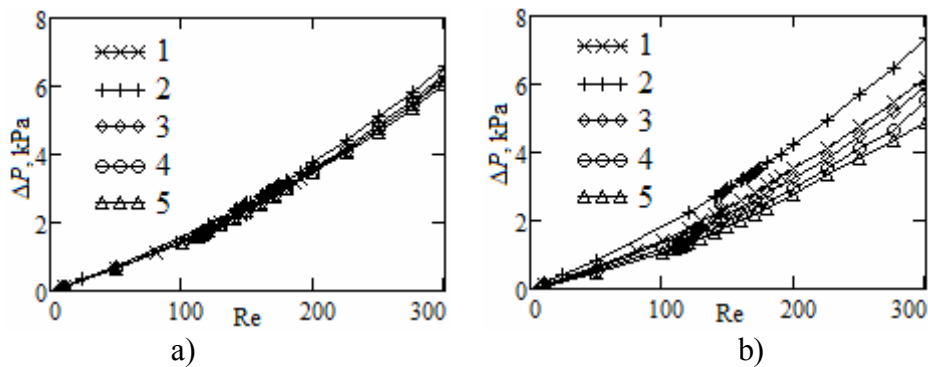

Figure 4. Pressure drop versus Reynolds number:
$\Delta t = 0^{\circ}C$ (1); $\Delta t = -10^{\circ}C$ (2); $\Delta t = 10^{\circ}C$ (3); $\Delta t = 20^{\circ}C$ (4); $\Delta t = 30^{\circ}C$ (5)

4. Conclusions

The conducted numerical simulation allowed identifying following regimes for incompressible fluid flow in T-shaped micromixer: 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 presence of a difference in initial temperatures of miscible fluids also leads to a shift of flow regimes. The simultaneous effect of differences in the viscosities and densities due to different initial temperatures of the fluids on the mixing efficiency was revealed. It was also shown that the flow and mixing of two fluids with different initial temperatures can be considered as self-similar pattern with regard to the reduced Reynolds number. Besides, the considerable effect of the difference in initial temperatures of miscible fluids on a pressure drop between the outlet and inlet of micromixer, through which water with variable temperature was supplied was revealed.

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