Microfibers formation in two-phase fluid flowing in a channel with the abrupt constriction: Numerical modeling

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Abstract. Numerical modeling was used to study the patterns of droplet deformation in two-phase Newtonian fluids flowing through a three-dimensional rectangular microchannel with a sharp narrowing. The elongation of single droplets of different viscosities was investigated in different channel zones. Calculations were carried out for different confinement parameter—the ratio of droplet diameter to the gap thickness. The increase in this parameter was shown to lead to the substantial increase in the droplet relative elongation. The effect of coalescence to microfiber formation in flowing emulsion was considered.

1. Introduction

The microfibers formation in flowing two-phase fluids (emulsions) is a consequence of the shear-induced droplet elongation. This effect was observed in the extruded incompatible polymer blends [1], emulsions passing the tubular turbulent reactors [2], and microfluidic devices [3]. The current morphology of two-phase fluids depends on the strain rate, rheological properties of the components and interfacial tension, as well as the channel configuration [4].

The analytical description of the droplet deformation behavior could be obtained only for a single droplet in the broad channel in the limits of small or large elongations [5, 6]. Flow of a single droplet and concentrated emulsions in a narrow channel were studied numerically [4, 7, 8]. It was found that walls of the cylindrical or flat capillaries render significant effect on stretching of both Newtonian [9–11] and viscoelastic droplets [10, 12] thus defining largely an ability to microfiber formation.

The droplet deformation properties in a channel with the variable cross-section are determined by the longitudinal velocity gradient at the entrance to the constriction zone and wall effect in a narrow part of the channel. For such a channel configuration, deformation of droplets was investigated experimentally [13, 14] and numerically [15, 16] (see review [17]). The droplet initial diameter was considered equal to or significantly larger than the transversal dimensions of the narrow zone, while coalescence with other droplets was not taken into account. Effects of various factors (ratios of the diameters of the wide and narrow zones of the cylindrical channel, shear rate, initial droplet size, viscosity ratio, and concentration of medium components) on the
coalescence efficiency of microfiber formation in a binary blends of incompatible polymer melts was experimentally investigated in ref. [18]. However, the droplet size was substantially smaller than the capillary diameter and effect of the channel walls was negligible.

In the present paper, the droplet deformation behavior and microfibers formation in two-phase Newtonian fluid flowing through the rectangular three-dimensional channel with an abrupt constriction were investigated by means of numerical simulation. The attention was focused to the confinement effect of the narrow zone of the channel to the flow-induced droplet elongation. The influence of the viscosity ratio of fluid components and some peculiarities of microfibers formation in flowing emulsions are discussed.

2. Model

The flow of a two-phase incompressible fluid in a rectangular channel with a sharp narrowing in figure 1 was studied for the following dimensions: \( H = 0.015 \) m, \( h = 0.001 \) m, \( w = 0.005 \) m. So, the contraction ratio of the channel is equal to \( H/h = 15 \). The short chain length polyisobutylene (PIB) was considered as a continuous phase while polydimethylsiloxane (PDMS) oligomers of different molecular weights—as a dispersed phase (droplets). Both components were considered as Newtonian fluids. The corresponding viscosities (\( \eta_c, \eta_d \)) and densities (\( \rho_c, \rho_d \)) are represented in table 1. The interfacial tension was taken to equal to \( \Gamma = 2.8 \) mN/m. The droplet viscosities (\( \eta_d \)) were taken lower, equal or larger than that of the continuous phase (\( \eta_c \)). Sedimentation was neglected due to the close densities of the continuous and dispersed phases.

The hydrodynamic behavior of a drop is defined by the following parameters: viscosity ratio \( m = \eta_d/\eta_c \), capillary number \( \text{Ca} = \eta_c R \dot{\gamma}/\Gamma \) (\( R \) is the initial droplet radius, \( \dot{\gamma} \) is shear rate), and ratio \( n = 2R/h \) of droplet diameter to height of the channel narrow part, called as confinement parameter. The last one characterizes closeness to walls of the channel: the larger is \( n \) the more substantial is the wall influence. The relative droplet elongation was characterized by the ratio \( L_d/(2R) \), where \( L_d \) is the maximum droplet length.

| Fluid components | Viscosity (Pa s) | Viscosity ratio | Density (kg/m\(^3\)) |
|------------------|-----------------|-----------------|-----------------------|
| PIB              | 101             | 1               | 890                   |
| PDMS30           | 30              | 0.3             | 970                   |
| PDMS100          | 103             | 1.02            | 970                   |
| PDMS500          | 493             | 4.88            | 970                   |
The velocity $u$ and pressure $p$ fields in a two-component medium moving in a channel with the variable section were calculated numerically using OpenFOAM (open source field operation and manipulation) package [19]. The VOF (volume of fluid) method was used to determine the current interface between a droplet and continuous fluid [20]. In this method, the local density and viscosity at each point $x$ of the computational domain were represented as continuous functions $\rho(\alpha) = \rho_d \alpha - \rho_c (1 - \alpha)$ and $\eta(\alpha) = \eta_d \alpha - \eta_c (1 - \alpha)$ of the volume fraction $\alpha(x, t)$ of the dispersed phase. This fraction is equal to 1 in the region occupied by the dispersed fluid, $\alpha = 0$ in the continuous phase, while $0 < \alpha(x, t) < 1$ in a narrow zone $\Omega$ including the interface between the dispersed and continuous phases. Within this representation, the hydrodynamic behavior of two-component medium is described by the unified Navier–Stokes equation

$$\frac{\partial [\rho(\alpha)u]}{\partial t} + \nabla \cdot [\rho(\alpha)uu] = -\nabla p + \nabla \cdot \tau - \Gamma \kappa(\alpha) \nabla \alpha + \rho(\alpha)g$$

and the continuity condition

$$\nabla \cdot u = 0,$$

where $\tau$ is the stress tensor of Newtonian fluid defined as $\tau = 2\eta(\alpha)D$, where $D$ is the strain rate tensor with components $D_{ik} = (\partial u_i/\partial x_k + \partial u_k/\partial x_i)/2$. The third and fourth terms in the right-hand side of equation (1) corresponds to the capillary force [21] ($\kappa = \nabla \cdot (\nabla \alpha / |\nabla \alpha|)|\Omega$ is the interface curvature at arbitrary point) and gravitation force ($g$ is gravitational acceleration vector) densities, respectively. The volume fraction of the dispersed phase obeys the continuity equation

$$\frac{\partial \alpha}{\partial t} + \nabla (\alpha u) = 0.$$

Equations (1)–(3) were solved numerically using the finite-volume method and the adaptable mesh. The velocity and pressure fields were calculated by means of PISO (pressure-implicit with splitting of operators) algorithm. The position of the droplet interface in the computational cells was restored at each integration time step. More details on evaluation of performance of the OpenFOAM solver can be found in reference [22]. The periodic boundary conditions for the fluid velocity and pressure were imposed on the lateral faces of the computational domain (see figure 1).

3. Results

The axial flow velocity $u_x$ of the continuous phase increases sharply at the entrance to a narrow part of the channel and then levels off. Figure 2 shows this effect in the non-dimensional form as a dependence of $u_x/U_0$ versus $x/h$ ($U_0$ is the average fluid velocity in the constriction zone). The step-up of the axial velocity results in jumping of its longitudinal gradient $\partial u_x/\partial x$ in the same area (see the inset in figure 2). It is reasonable to expect that such a flow pattern at the entrance to a narrow passage zone would contribute to a drastic droplet elongation.

The question arises of how the structure of the flow affects the deformation of the droplet at various values of the viscosity coefficients and the retention parameter $n = 2R/h$. The answer is presented in figure 3 which shows that the channel constriction (or enlargement of the initial droplet diameter) results in the increase in droplet deformation. Specifically, at $n = 0.2$ (the case of the broad channel) the droplet relative elongation $L_d/(2R)$ grows gradually within the narrow zone. Then its shape restores partially due to the capillary forces. However, increase in the confinement parameter up to $n = 0.8$ leads to the significantly longer droplets at the same capillary number $Ca = 3$. It should be noted that maximum elongation $L_{d,\text{max}}$ of a droplet is reached just after the entry to the narrowing. After that the elongation becomes smaller. This kind of transient behavior is originated by droplet oscillations similar to those observed in
Figure 2. Variation of dimensionless velocity $u_x/U_0$ along the symmetry axis of the channel. The inset represents its longitudinal gradient.

Figure 3. Relative lengthening of a single drop along the channel with a sharp narrowing at retention parameters $n = 0.2$ (1) and 0.8 (2) for the viscosity ratios $m = 0.3$ (dotted lines), 1.02 (dashed lines), and 4.88 (solid lines).

a simple shear flow [9]. The found decrease in the oscillation magnitude with increase in the confinement parameter $n$ agrees with previous results [23].
Figure 4. Dependence of the relative maximum length of a single droplet on the confinement parameter $n$ at different viscosity ratios $m = 0.3$ (dotted lines), 1.02 (dashed lines), and 4.88 (solid lines).

Figure 5. Formation of microfibers in 5 vol% emulsion flowing from the wide to narrow part of the channel at $n = 0.4$ (a) and 0.8 (b). Viscosity ratio is $m = 1.02$.

It is seen that the larger is the viscosity ratio $m$, the larger is the relative elongation of a droplet. This phenomenon is due to the fact that in the elongational flow, which is formed at the entrance to the narrow part of the channel (see figure 2), with a given longitudinal velocity gradient $\varepsilon_{xx} = \partial u_x / \partial x$, a more viscous drop is affected by a higher tensile stress $\tau_{xx} \propto \eta_d \varepsilon_{xx}$. Similar result was obtained by Taylor [5] in a limit of small $\varepsilon_{xx}$. The effect becomes more noticeable at larger confinement parameter $n$ (figure 4). It was found that for all $m$ values the maximum droplet elongation $L_{d,\text{max}}$ is reached approximately at the $n \approx 0.4$. The further increase in $n$ does lead to a visible growth in the droplet length.

However, the maximum elongation of a single droplet with the initial diameter $2R$ comparable with the gap size $h$ is not sufficient to generate longer microfiber. The only way to do that
is to increase concentration of the dispersed phase thus contributing to the droplet coalescence and longer fibers formation. To study this effect, the numerical modeling of 5 vol.% emulsion was carried out for different confinement parameters \( n \) at the matched viscosities of the fluid components. Figure 5 shows two snapshots corresponding to \( n = 0.4 \) [figure 5(a)] and 0.8 [figure 5(b)]. The microfibers are formed in both of the cases. They become longer at larger confinement parameter \( n \). This effect is due to the growing of coalescence probability of droplets with narrowing of a gap and agrees with experimental data [18].

4. Conclusions

Effect of the abrupt constriction of the channel to droplets elongation at different viscosity ratios and confinement parameters was investigated numerically. The increase in \( n \) at a fixed capillary number results in a significant increase in droplet elongation. It becomes larger with increase in the viscosity ratio \( m = \eta_d/\eta_c \). The maximum elongation of a single droplet approximately levels off at \( n > 0.4 \). Increase in concentration of the dispersed phase leads to formation of microfibers owing to the droplets coalescence. The microfibers grow with increase in confinement parameter.

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