Flow morphology of two-phase fluid in co-axial capillaries: Numerical simulation

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Abstract. The dynamic behavior of two-phase Newtonian fluid in co-flow co-axial capillaries was studied numerically. It was found that morphology of the dispersed phase is uniquely described by three non-dimensional parameters as capillary numbers and ratio of Reynolds numbers of the fluid components.

1. Introduction

Micron-sized droplets are in great demand in various research and applications, for example, as chemical microreactors [1, 2], microcontainers for drug delivery targeting [3, 4], in photonic crystals [5], etc. Properties of such objects are depending often on their size. For this reason, generation of the monodisperse microdroplets of a given diameter is one of the important problems. As a rule these droplets could be produced by means of different microfluidic devices [6, 7]. Among them, the co-flow in coaxial capillaries is one of the effective tools of microdroplet production [8–10]. In such a device the polydispersity of the dispersed phase depends crucially on the flow mode. The smallest scatter of droplets in size (<1%) is normally achieved in the dripping mode [10]. On the other hand, in the jetting mode, the droplet size varies in a wide range [11]. The observed flow patterns depend on different factors as flow rates of continuous and dispersed phases, ratio of their viscosities, interfacial tension coefficient, and microchannel geometry. Thus, the determining of conditions under which different flow modes can be observed in the co-flow device belongs to the important fundamental problem.

Up to now, the flow modes were usually classified on the basis of Caᵣ–Caᵢ diagrams, where Caᵣ = ηᵣVᵣ/γ and Caᵢ = ηᵢVᵢ/γ are the capillary numbers of the continuous and dispersed phases, respectively (ηᵣ, Vᵣ and ηᵢ, Vᵢ are viscosities and average velocities in the external and internal capillaries, respectively; γ is interfacial tension coefficient) [12, 13].

For the correct prediction of the flow modes, the similarity of their structure should be met. This implies preservation the dispersed phase morphology at such changes in material and hydrodynamic parameters of fluid phases that leave pairs of the capillary numbers unchanged.

In the present paper, the universality criterion was established for the first time. It was found that fulfillment of this criterion requires accounting for the Reynolds numbers of the continuous and dispersed phases as a restriction for the permitted capillary numbers.
2. Model

Co-flow microfluidic geometry is consists of two coaxial microchannels. The droplet formation occurs due to their detachment or disintegration of jet of the dispersed fluid from the internal capillary due to the interaction with the continuous phase flowing through the external capillary [figure 1(a)]. Due to the cylindrical symmetry of coaxial capillaries, we considered two-dimensional axisymmetric geometry as a computational domain [figure 1(b)]. The inner diameter of the external capillary is \( d_c = 1.06 \) mm while sizes of the inner capillary are described by the internal \( d_{in}^c = 150 \) µm and outer \( d_{out}^c = 360 \) µm diameters.

The velocity \( \mathbf{u} \) and pressure \( p \) fields in a two-phase liquid were calculated numerically using finite-volume-based code OpenFOAM (open source field operation and manipulation) [14]. To track the interface between phases the VOF (volume of fluid) method was used [15]. The local viscosity at each point \( x \) of the computational domain were represented as continuous function \( \eta(\alpha) = \eta_d\alpha + \eta_c(1 - \alpha) \) 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 \( 0 < \alpha < 1 \) in a narrow interfacial zone \( S \). The unified Navier–Stokes equation is integrated simultaneously with the incompressibility condition and the transport equation for \( \alpha \). Considering the two fluids as Newtonian with equal densities \( \rho_c = \rho_d = \rho \), the governing equations can be written as

\[
\rho \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \nabla \cdot \left[ \eta(\alpha) \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right] - \mathbf{F}_s, \tag{1}
\]

\[
\nabla \cdot \mathbf{u} = 0, \tag{2}
\]

\[
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0, \tag{3}
\]

where \( \mathbf{F}_s \) is the interfacial force density which is modeled by the continuum surface force (CSF) method [16]. This force is only active in the interfacial zone \( S \) and calculated as \( F_s = \gamma \kappa \nabla \alpha \), where \( \kappa = \nabla \cdot (\nabla \alpha / |\nabla \alpha|) \) is the curvature of the interface. The stick boundary condition \( \mathbf{u}_w = 0 \) was imposed on the capillaries walls.

The finite volume method [17] was used to numerically integrate the system of differential equations (1)–(3). Separation of velocity and pressure fields was carried out by means of PISO
Figure 2. Development of the dispersed phase morphology at Ca_c = 0.1 and Ca_d = 0.01 for different combinations of the system parameters given in table 1: 1 (a), 2 (b) and 3 (c).

(pressure-implicit with splitting of operators) algorithm. The volume fraction field \( \alpha(x,t) \) of the dispersed phase was used for visualization of interface morphology under the flow. As long as the interfacial zone \( (0 < \alpha < 1) \) is smoothed over several cells, the interface has some finite thickness. The optimized uniform mesh [see figure 1(b)] was used for numerical simulation. An increasing of the number of cells leads to a decreasing of the interface thickness but has almost no effect on the interface shape.

3. Results and discussion

At the first stage, a series of numerical experiments was conducted to verify the invariance of the flow morphology with respect to such variations in viscosities \( \eta_c \) and \( \eta_d \), average velocities \( V_c \) and \( V_d \), and interfacial tension \( \gamma \) which preserve the prescribed values of capillary numbers of Ca_c and Ca_d of the fluid components. For this purpose, three combinations of \( \eta_c, \eta_d, V_c, V_d \), and \( \gamma \) corresponding to Ca_c = 0.1 and Ca_d = 0.01 were considered (table 1, combinations 1–3).

Figure 2 shows the corresponding morphologies of the dispersed phase at different moments representing flow patterns before the droplet detachment \( (t_1) \), at breakup \( (t_2) \), and just after droplet detachment \( (t_3) \). It is seen that the observed morphologies of the dispersed phase are dissimilar for each combination considered. In particular, a typical dripping mode can be observed in the case of combination 2 [11, 12, 18], figure 2(b). However, flow patterns corresponding to combinations of the characteristics 1 and 3 differ from the dripping mode, figure 2(a, c). In the first case, a few submicron satellite droplets are observed just after detachment of the main droplet, figure 2(a, t_3). This type of flow patterns could be recognized as a transition between the dripping and tip-streaming flow modes [18, 19]. For the third combination, the droplet detachment occurs at rather large distance from the internal capillary tip, figure 2(c, t_2). This is a sign of the jetting flow mode [11,12]. Thus, the couple Ca_c and Ca_d of capillary numbers is not sufficient to determine unambiguously the flow mode of a two-phase fluid in the co-axial capillary arrangement.

We found that the relative inertial and viscous forces applied to the continuous and dispersed phases should be taken into account while studying the resulting morphology of the dispersed phase. This is determined by the ratio \( R = Re_c/Re_d \) of the corresponding Reynolds numbers \( Re_c = \rho V_c d_c / \eta_c \) and \( Re_d = \rho V_d d_d^n / \eta_d \) in the external and internal capillaries. It can be
Table 1. Combinations of material and hydrodynamic characteristics corresponding to $Ca_c = 0.1$ and $Ca_d = 0.01$.

| Combination | $\eta_c$ (Pa s) | $\eta_d$ (Pa s) | $V_c$ (m/s) | $V_d$ (m/s) | $\gamma$ (N/m) | $r$ |
|-------------|-----------------|-----------------|-------------|-------------|----------------|-----|
| 1           | 0.1             | 0.1             | $10^{-2}$   | $10^{-3}$   | 0.01           | 10  |
| 2           | $10^{-2}$       | $10^{-3}$       | 0.2         | 0.2         | 0.02           | 0.1 |
| 3           | 0.1             | $10^{-3}$       | $10^{-3}$   | $10^{-2}$   | 0.001          | 0.001|
| 4           | $1.58 \times 10^{-2}$ | $5 \times 10^{-3}$ | $3.16 \times 10^{-2}$ | $10^{-2}$ | 0.005          | 1   |
| 5           | 3.16            | 1               | $6.32 \times 10^{-4}$ | $2 \times 10^{-4}$ | 0.02           | 1   |
| 6           | 10              | 3.16            | $10^{-4}$   | $3.16 \times 10^{-5}$ | 0.01           | 1   |

Figure 3. Development of the dispersed phase morphology at $Ca_c = 0.1$, $Ca_d = 0.01$ and $r = 1$ for different combinations of the system parameters given in table 1: 4 (a), 5 (b) and 6 (c).

represented as $R = r \left( d_c/d_d^{in} \right)$, where $r = V_c \eta_d/V_d \eta_c$. Here we considered the specified capillary diameters with a constant ratio $d_c/d_d^{in} \approx 7$. By this reason, we could restrict our attention to $r$ parameter.

Figure 3 shows flow patterns of two-phase fluids at $r = 1$ and capillary numbers $Ca_c = 0.1$ and $Ca_d = 0.01$ corresponding to combinations 4–6 of different material and dynamic parameters presented in table 1. The similar morphology of the dispersed phase is clearly observed during the droplet formation for each combination of the parameters. The only difference is in the processing times appearing due to the distinction in the average fluids velocities $V_c$ and $V_d$ in the external and internal capillaries. This finding proves that the additional restriction accounting for the relative value of Reynolds numbers of fluids running in the external and internal capillaries has to be used to ensure the universality of the dispersed phase morphology at the given pair $Ca_c$ and $Ca_d$ of capillary numbers.
4. Conclusion
Numerical modeling of two-phase liquids operating in coaxial capillaries allows us to conclude that the morphology of the dispersed phase is uniquely determined by three dimensionless values \( C_a = \eta_c V_c / \gamma \), \( C_d = \eta_d V_d / \gamma \) and \( r = V_c \eta_d / V_d \eta_c \), which include material and dynamic characteristics of the phases.

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