Three-dimensional simulation of drop motion in channels of different cross-sections

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Abstract. Three-dimensional Boundary Element Method accelerated using a heterogeneous Fast Multipole Method is employed to study two-phase flow in a microchannel of different cross-sections. The flow of a mixture of two Newtonian liquids with equal viscosities and densities is described by Stokes equations. A comparison of the simulation results of the droplet dynamics in cylindrical capillaries with experimental data available in the literature was carried out and showed the qualitative agreement. The deformable droplet motion is considered in a channel with a circle, square, and hexagon cross-sectional shape. The influence of droplet size on a relative velocity in a channel is studied. The applied approach to numerical simulation can be used to solve a wide range of problems related to emulsion flows in microscales.

1. Introduction
Multiphase flows occur in most industrial processes, including fermentation, catalytic processes, oil and gas recovery and processing, and aerobic biotechnological processes. Thus, they are the most technologically significant fluid systems. As a rule, such systems are dispersed and consist of several phases. For example, all types of natural liquid fuels are mixtures of gas, liquid, and solids. In medicine and biophysics, the problem of the deformable droplet flow in microchannels of arbitrary shape is a model of the processes that occur when blood cells move along branched capillary networks. The study of multiphase flows is of great scientific importance. It is the main area in fluid mechanics, which interacts with other physical and mathematical disciplines.

Nowadays, there is a wide range of theoretical and experimental material on the dynamics of dispersed inclusions, developed in the frameworks of both fundamental research, and experiments, as well as various technological developments in the chemical, oil and gas, aerospace, and many other industries where the dynamics of dispersed systems play an important role.

The droplet dynamics under external influences is the subject of a large number of researches. The significant progress was achieved as a result of an avalanche-like growth in the number of studies related to the development of microfluidic technologies and their application in biochemistry, the creation of new materials, design of rapid diagnostic systems, etc. The effects of shear flows and solid flow-restricting walls are one of the main ways of affecting on dispersed systems. Despite a significant number of publications on this subject, the nonequilibrium dynamics of disperse systems in microchannels of complex shapes has not been sufficiently studied even in the case of solid inclusions. At that, the presence of droplets and bubbles considerably complicates the problem due to their deformability and compressibility. Most of the experimental work is devoted to the study of two-phase
flows in rectangular [1] or circular [2, 3] channels. In [4], a model was proposed for determining the pressure drop of a laminar single-phase flow in microchannels of arbitrary cross-section. The model was compared with numerical results for a wide range of cross-sectional shapes, including hyperellipse, rectangular shape with semi-circular ends, trapezoid, sine, rhombic, circular sector, circular segment, annular sector, square duct with two adjacent round corners, and moon-shaped channels.

Numerical methods to simulate the complex three-dimensional flows near deformable droplets were developed in the 80s of the last century, and are widely used and improved at present. These include, for example, the boundary element method (BEM) [5], which is mainly used for flows at low Reynolds numbers (Stokes flow) or potential flow. The flows for which Navier-Stokes equations can be simplified to Stokes equations are typical for microfluidics. There are several publications, in which the BEM is developed in three dimensions, including the computation of droplet dynamics [6]. It should be noted that almost all analytical and numerical studies of Stokes flow of single-phase liquids and emulsions are studied in the context of the plane and circular channels. One reason for this is that the mesh of channel surface when solving a three-dimensional problem even for relatively simple shapes should be pretty large (tens of thousands boundary elements), while such problems were not efficiently solvable about 20 years ago. The current emerging techniques based on algorithmic and hardware accelerations are capable to handle such tasks.

Despite quite extensive research in the field of droplet dynamics in confined geometry conditions, knowledge of the three-dimensional dynamics of deformable droplets in complex microchannels is still limited.

2. Problem statement and numerical approach

The present study is related to the simulation of the flow of a mixture of two Newtonian liquids of equal viscosities and densities of a droplet structure in a channel. The processes are considered under isothermal conditions at low Reynolds numbers (Re < 1) and moderate Strouhal numbers (St ≤ 1). Thus, the fluid flow is described by Stokes equations with following boundary conditions for the velocity \( \mathbf{u} \) and traction \( \mathbf{f} = \sigma \cdot \mathbf{n} \) on the fluid-fluid interface \( S_d \)

\[
\mathbf{u}_1 = \mathbf{u}_2 = \mathbf{u}, \quad \mathbf{f}_1 = \mathbf{f}_2 - \mathbf{f}_f, \quad \mathbf{f} = \gamma (\nabla \cdot \mathbf{n}(\mathbf{x})) + (\rho_2 - \rho_1)(\mathbf{g} \cdot \mathbf{x}), \quad \mathbf{x} \in S_d,
\]

where \( \sigma \) is the stress tensor, \( \mathbf{n} \) is the unit normal to \( S_d \) directed into carrier fluid, \( \mathbf{x} \) is the radius vector, \( \gamma \) is the surface tension, \( \rho \) is the density, \( \mathbf{g} \) is the gravity acceleration, index 1 is used for ambient fluid parameters, and index 2 is used for the liquid inside droplets. We consider the periodic channel flow with the period \( L \) in \( x \) direction under following conditions: the no-slip condition is assumed on the channel side surface, the periodicity flow conditions are assumed on the inlet and outlet cross-sections, and given pressure drop \( \Delta p \) on the considered channel length \( L \).

In this work, we used the efficient numerical approach based on the BEM accelerated heterogeneous Fast Multipole Method (FMM), developed in our previous work [6]. To solve large scale problems, a flexible version of the general minimal residual method (fGMRES) solver is applied. A low-accuracy FMM is used in the inner fGMRES loop as a preconditioner, while the outer iteration utilized the more accurate FMM. The calculations are performed on the workstation equipped with a graphics card using CPU/GPU parallelism that allows conducting one direct three-dimensional simulation of the deformable drop dynamics in the channels of different shapes in the Stokes regime for a reasonable time. More detailed information about implementation features can be found in [6].

3. Results and discussion

In this work, we study the motion of a single deformable droplet in a channel under constant pressure drop \( \Delta p \) along the length \( L \). Droplet dynamics in a channel is characterized by several dimensionless parameters, namely, the ratio of droplet radius to the channel radius, \( a/R \); liquid viscosities ratio,
\( \lambda = \mu_2 / \mu_1 \); Reynolds number, \( \text{Re} \); and the parameter taking into account the surface tension of the drop, for instance, we are using \( K = Ra \left| \frac{p_\infty}{\gamma} \right| \frac{p_\infty}{\gamma} = \Delta p / L \). The numerical results were performed for dimensionless time \( t' = t_{\text{nondim}} = \gamma / (\mu_1 a) \), where \( \mu_1 \) is the viscosity of carrier liquid.

First of all, the relevance of the applied numerical approach was confirmed by comparison with several experiment data for droplets in a cylindrical channel. In experimental work [2] the results of the study of the deformable droplet motion with a radius comparable to the cylindrical channel radius are represented. The authors considered the case of viscous Newtonian liquid droplets and viscoelastic liquid droplets suspended in the volume of a viscous liquid with the same density. The data of similar experimental work for the mixture of two Newtonian liquids are also available in [3]. The following parameters determining the process in case of two viscous liquids were considered in the above-mentioned works: \( a / R \), \( \lambda \), \( \text{Re} \); parameter characterizing the degree of deformability of droplets at small Reynolds numbers, reflecting the influence of viscous forces as compared to surface tension forces, \( \Gamma = \mu U_{ch} / \gamma \), where \( U_{ch} = \left| \frac{p_\infty}{\gamma} \right| R^2 / (8 \mu_1) \) is the average cross-section velocity of a viscous liquid in a cylindrical channel. To conduct the comparison among several experimental cases of a mixture of two Newtonian fluids (drops of silicone oil in glycerol-water solution, two data sets were chosen from work [2]. Corresponding physical and dimensionless parameters are represented in Table 1 and the first two rows in Table 2. Also, we consider two cases from the experimental work [3] with dimensionless parameters listed in the last two rows of Table 2.

Table 1. Physical parameters to compare with experimental data [2].

| Case | 1 (a) | 4 (a) |
|------|-------|-------|
| \( a = 3.63 \cdot 10^{-3} \) m, \( R = 5 \cdot 10^{-3} \) m, \( \gamma = 3.63 \cdot 10^{-3} \) N/m, \( \rho_1 = \rho_2 = 1.089 \cdot 10^{-3} \) kg/m\(^3\), \( U = 3.9 \cdot 10^{-3} \) m/s |
| \( \mu_1 = 0.425 \) Pa \cdot s, \( \mu_2 = 0.865 \) Pa \cdot s |

Table 2. Dimensionless parameters to compare with experimental data [2, 3].

| Case | \( a / R \) | \( \lambda \) | \( \Gamma^{-1} \) | \( \text{Re} \) | \( K \) |
|------|------------|----------|---------|---------|---------|
| 1 (a) [2] | 0.726 | 2.04 | 13.3 | 0.05 | 0.437 |
| 4 (a) [2] | 0.726 | 0.19 | 13.3 | 0.05 | 0.437 |
| 1 [3] | 0.95 | 0.99 | 20 | 0.025 | 0.38 |
| 2 [3] | 0.95 | 0.99 | 10 | 0.05 | 0.76 |

In computational experiments, the surface of the channel and drops were covered by meshes with \( N_{\text{Channel}} = 11000 \) and \( N_{\text{Drop}} = 5120 \) triangular elements, respectively. The simulation was carried out until the droplets reached their stable deformed shape in a flow. The comparison of the stable shape of the droplet is shown in Figure 1 for cases considered in [2] and in Figure 2 for data [3]. As it is seen from the figures, we obtain a good qualitative agreement.

Figure 1. Comparison (middle column) of the numerical simulation results (right column) with the experimental data [2] (left column), the cases 1(a) (top row) and 4(a) (bottom row).
Figure 2. Comparison of the results of numerical simulation (right column) with the experimental data [3] (left column), cases 1 and 2 respectively are shown from top to bottom.

Furthermore, we compared the calculated relative velocity of the mass center of the droplet in channel flow $U_{rel} = U_{dr}/U_{ch,average}$ with experimental data [2]. The calculated values: 1.43 and 1.51, experimental values: 1.46 and 1.56, and relative errors: 2% and 3.2% for cases 1(a) and 4(a).

In [7], the authors obtained a formula to determine the relative velocity of droplets in the Poiseuille flow using the reflection method. This relation (2) is valid for small droplets on the channel centerline with the same density as the carrier fluid.

$$\frac{U_{dr}}{U_{ch}} = 2 - \frac{4\lambda}{3\lambda + 2} \left(\frac{a}{R}\right)^2 + O((a/R)^3). \tag{2}$$

We carried out the comparison of the relative velocity of a drop calculated using (2) with the results of numerical simulation for the cases with $\lambda = 0.99$ and $\lambda = 2.04$ but for small ratios of the droplet and channel radii $0.1 < a/R < 0.6$. The curves in Figure 3 show better consistency for the smaller value of $a/R$ for both $\lambda$.

Figure 3. Relative droplet velocity on a channel centerline: calculations square symbol – $\lambda = 2.04$, circle symbol – $\lambda = 0.99$, theory [7] – lines.

In this study, we consider the influence of cross-sectional channel shape on the droplet motion. A high-quality triangulation of circular, hexagon, and square-shaped channels with $N_{\text{c,Channel}} = 20420$, $N_{\text{h,Channel}} = 23112$, and $N_{\text{s,Channel}} = 15408$, respectively, is used (Figure 5). Computational experiments were conducted for a single initially spherical droplet on the channel centerline at constant pressure drop and different dimensionless parameters $0.2 \leq a/R \leq 0.9$, $0.15 \leq K \leq 0.675$, $L/R = 5$, $\lambda = 1$, $\epsilon = 1$.\n
where \( R \) is the radius of cylindrical channel and the that of the inscribed circle in the polygon of the other channels cross-section. We calculated the relative velocity of the droplet mass center in channel flow for each cross-sectional shape. The average velocity \( U_{ch} \) was calculated for the single-phase flow in the same channel. Figure 4 shows the graphs of the relative velocity \( U_{rel} \) as a function of the ratio \( a/R \). The difference in the curve behavior appears due to the variation of cross-sectional shape and associated changing in the velocity field (Figure 5). As follows from the relation (2), the relative velocity of a drop always exceeds the average flow velocity in the channel, and as the droplet size increases, its velocity decreases. It was confirmed by many experimental observations, in which the relative velocity was greater on the average. Calculations for all considered cases also confirm these observations.

Figure 4. The relative velocity of the drop on a channel centerline.

Figure 5. Triangulation of the considered channels, velocity field distribution for single-phase flow in channel cross-section, droplet shape, and contour in the plane \( y = 0 \) \( a/R = 0.9 \).
The deformation of droplets of a radius comparable to the radius of the channel is of great interest. The stable deformable drop shapes with velocity distribution on the surface are represented in Figure 5 for different cross-sections at $a/R = 0.9$. Despite contours of the drops in the plane $y = 0$ looks similar, one can see a significant discrepancy in the velocity distribution on the drop surface and in the three-dimensional drop shape due to the influence of close channel walls.

![Image](image_url)

**Figure 6.** Influence of droplet on the normal stress vector on the channel side wall, $a/R = 0.9$.

Furthermore, we studied both the influence of the presence of the channel walls on droplet motion characteristics and also the impact of a droplet on stress tensor on the channel surface. The normal stress vector on the channel side wall was calculated for viscous fluid flow without droplet and in the presence of large droplets for all cross-sectional shape variations. The absolute values of the difference between the found values are presented in Figure 6. We consider the hexagonal shape of the cross-section as a transition from a cylindrical to a channel with a square cross-section. It is seen that the influence on the normal stress vector is characterized by the deviation of the cross-sectional shape from the circle.

**Conclusions**
The detailed study of multiphase flow in microchannels is of great interest for both scientific and industrial fields. In the present work, the deformable droplet dynamics simulation in periodic channel flow was carried out in three-dimensional case using the accelerated boundary element method. The efficiency of the used approach is confirmed by a successful comparison with experimental data published in the literature for drops in a cylindrical channel. The influence of cross-sectional channel shape (circle, hexagon, and square) on the droplet deformation and relative velocity of the mass center was investigated. It was shown that the velocity distribution on the droplet surface substantially depends on the channel shape, as well as the distribution of normal stresses over the channel surface when a droplet with a radius comparable to the channel radius moves near the wall.

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**References**
[1] Sarrazin F, Loubiere K, Prat L, Gourdon C, Bonometti T, Magnaudet J 2006 *AIChE Journal.* 52(12) 4061–70
[2] Ho B P, Leal L G 1975 *J. Fluid Mech.* 71(2) 361–83
[3] Olbricht W L, Kung D M 1992 *Phys. Fluids* 4(7) 1347–54
[4] Bahrami M, Yovanovich M M, Culham J R 2007 *Int. J. Heat and Mass Transfer* 50 2492–502
[5] Pozrikidis C 1992 Cambridge (Cambridge University Press) p 259
[6] Abramova (Solnyshkina) O A, Pityuk Y A, Gumerov N A 2013 *Proc. IMECE 2013* IMECE2013-63193
[7] Hetsroni G, Habel S, Wacholder E 1970 *J. Fluid Mech.* 41(4) 689–705