3D simulation of single bubble dynamics in a microchannel with a complex cross-sectional shape

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Abstract. The relevance of a study of bubbly liquid dynamics in porous media is due to a wide range of their use in technological and industrial processes. This work is dedicated to the numerical study of the dynamics of single incompressible bubbles in a viscous fluid flow in a microchannel with a cross-section in the shape of a deltoid. This geometry is due to the similarity with the domain between closely packed cylindrical fibers, forming a porous medium, for example, in the manufacturing of composite materials. In the present study for solving the considered problems, the boundary element method (BEM) was chosen as a basis of the numerical approach, since all calculations were associated only with boundaries. BEM is effective in studying 3D problems in the domains with complex geometry and modelling objects with arbitrary deformation. The influence of the initial radius of the bubble, its position relative to the channel centerline on the bubble deformation, relative velocity of the mass center of the bubble to the average flow velocity in the channel is considered.

1. Introduction
The topicality of the detailed study of the bubbly liquids behavior in the elements of a porous medium is caused by the need to solve applied and fundamental problems. As a rule, these problems arise in the oil and gas industry, manufacturing of composite material, and developing medical, bio, micro, and many other technologies. At the micro-level, bubbly liquids are considered in more detail from the point of view of the dynamics and interaction of single deformable bubbles in various domains. The macroscopic behavior of complex systems is the result of processes occurring at the micro-level at the scales of individual microparticles and their aggregates.

The features of the geometry of the pore channels have a significant impact on the ongoing processes. Nowadays, various micromodels of a porous medium representation are considered. Capillary representation is porous medium modeling as a network of microchannels of complex shapes with various structural features. Structural representation is modeling of the pore space in which the fluid flows by distributing rigid elements of various shapes in a particular region.

There are a number of works devoted to the numerical study of dispersed system flow and viscous fluid flow in the channels of various shapes, which are based on the using of different numerical approaches. However, the channel geometry is mostly limited to some simple cases: a cylindrical channel, rectangular or square channel, and two parallel planes. Moreover, only few numerical simulations are carried out for dispersed flow in channels with a nontrivial cross-section in the three-dimensional case.
The boundary element method (BEM) is applicable for the study of motion of the deformable bubbles, since it is effective for the 3D modelling of the flow of a large volume of dispersed systems (bubbly liquids, emulsions, suspensions) in unbounded domains, and in the domains with complicated geometry. One of the advantages of the BEM is that it allows making a significant breakthrough in specific directions.

The study of limiting regimes – Stokes [1] and potential flow [2] – is important since the bubble dynamics is defined by the force acting from the compressible gas, surface forces, and the force acting from the incompressible liquid. The relative contribution of viscous, non-stationary, and inertial forces from the liquid is determined by Reynolds number and Strouhal number. Authors of the present paper successfully applied the BEM for potential flow to simulate bubble cluster dynamics in the presence of an acoustic field [3]. At a low Reynolds number and moderate Strouhal number, the liquid motion is described by the Stokes equation. For example, this regime can occur in a high viscous oil with bubbles. In the present study, we consider the 3D dynamics of single incompressible bubbles in a part of capillary micromodel using the BEM for Stokes flow.

2. Problem formulation and numerical implementation
The periodic creeping flow of viscous liquid (index 1) with an incompressible bubble (index 2) in a channel under constant pressure drop in Cartesian coordinates is considered. Since the motion is slow, the viscous forces resulting from the fluid flow are more significant than the inertia forces related to the acceleration or slowdown of the fluid's particles. This fact allows completely neglecting the inertial terms in the calculations. All processes are studied under isothermal conditions, without taking into account the intermolecular Van der Waals forces. It is assumed that the dynamic viscosity and density of the gas can be neglected compared to the corresponding parameters of the carrier liquid. In this case, we consider the model of viscous liquid motion, which is described by the Stokes equations. The problem was solved under the following boundary conditions: on the interface boundary the equal velocities inside and outside are considered, and the traction is known. For the channel flow, we consider no-slip condition on the side boundary and periodic conditions for inlet and outlet cross-section. A more detailed representation of the considered problem statement can be found in [4].

The kinematic condition for the bubble surface dynamics

\[ \frac{dx}{dt} = u(x), \quad x \in S, \] (1)

where \( u(x) \) is the interface velocity, determined from the solution of the problem stated above, \( x \) is the radius-vector of the considered mesh point, and \( S \) is the bubble surface.

During the evolution of the interface, the mesh nodes move according to the kinematic condition (1), which for a few initial time steps is solved using the 4th order Runge-Kutta scheme, while the 6th order Adams-Bashforth-Moulton (ABM) predictor-corrector scheme was employed for the later time. Adams method and the associated ABM method provide high accuracy integration and economy because they require one (Adams) or two (ABM) estimation of the right-hand side for a single time step. However, these methods require an initial approximation that must be performed with reasonable accuracy. For this purpose, in this work, we use the Runge-Kutta 4 order accuracy. The time step was chosen according to the stability condition [4].

The problem was solved using the BEM, described in more detail in [1, 4]. Such approach allows one to effectively simulate the three-dimensional dynamics of inclusions with arbitrary deformation in complex domains. The surface of bubbles, channel side, inlet and outlet cross-section of the channel is discretized by the triangular meshes (Figure 1).

3. Results
We consider the processes occurring in a narrow space between close-packed filaments of the circular cross-section of the radius \( R \) (Figure 1). This type of channel form describes the deltoid with the corresponding parameters. This geometry is due to the similarity with the space between the
cylindrical fibers forming a porous medium in the manufacturing of composite materials. First of all, the corresponding channel triangulation with \(N_\Delta = 10328\) triangular elements is developed.

**Figure 1.** Schematic representation of the domain between the closely packed fibers (on the left) and triangulation of the deltoid cross-section channel (on the right), \(N_\Delta = 10328\), \(L/R = 2\).

Calculations were carried out to study the dynamics of incompressible bubbles in a viscous fluid flow in a complex-shaped channel under a constant pressure drop \(\Delta p\) over the length of the channel fragment \(L\). The influence of the initial bubble radius, its position relative to the channel centerline on the bubble deformation, and the velocity of the center of mass relative to the channel's average flow velocity were considered. The calculations were conducted for the following set of dimensional parameters: \(\mu = 0.3 \text{ Pa} \cdot \text{s} \), \(\mu_\perp = 0 \text{ Pa} \cdot \text{s} \), \(\rho = 1.1 \times 10^3 \text{ kg/m}^3 \), \(\gamma = 0.05 \text{ N/m} \), where \(\mu\) is the dynamic viscosity, \(\rho\) is the density, and \(\gamma\) is the surface tension. The radius of the individual fibers, between which we are considering the flow, was \(R = 2.3 \times 10^{-3} \text{ m}\). The pressure drop was \(\Delta p = 0.5 \times 10^5 \text{ Pa}\) set on the length \(L = 1.1 \times 10^{-1} \text{ m}\). The bubble surface was covered by a mesh with a number of triangular elements \(N_\Delta = 1280\). All results are presented in dimensionless form and for moments of dimensionless time \(t = t_{\text{dim}} / (\mu a)\), where \(t_{\text{dim}}\) is the dimensional time, and \(a\) is the bubble radius.

The calculations were carried out with the same physical parameters mentioned above for different bubble radii \(a = 0.06R\), \(a = 0.07R\), \(a = 0.08R\), \(a = 0.09R\), \(a = 0.1R\), and \(a = 0.11R\). Initially, a spherical bubble was placed on the channel centerline \(y = 0\), \(z = 0\), so there was a distance from the centerline \(\Delta h = 0\).

Figure 2 shows the results at various dimensionless time for two bubble sizes \(a = 0.06R\) and \(a = 0.11R\), including visualization of the initial position of the bubble in the channel cross-section, a comparative analysis of the bubble shape (calculations for each bubble were carried out separately, and the shapes are combined on one figure for convenience visualization). It can be seen that for a given pressure drop in the considered time range, the bubble shape is almost the same as spherical regardless of the radius. It is possible the spherical shape of bubbles of the considered size is due to its position on the centerline in creeping flow for a given channel geometry.

Furthermore, the changing in the velocity of the center of mass of the bubble relative to the average channel flow velocity \(U_{ch} \approx U_c / U_{ch}\) is considered. The average velocity \(U_{ch}\) was calculated from a numerical experiment for the flow of a viscous fluid without the bubble in the same channel. Figure 3 shows the graphs of the relative velocity \(U_{rel} \approx U_{rel} / U_{ch}\) as a function of dimensionless time for all considered radii of bubbles. There are no significant fluctuations of velocity in time since the bubbles remain almost spherical. The bubbles move with constant velocity. In addition, as the bubble size increases, its velocity decreases, but it does not exceed the maximum channel flow velocity \(U_{\text{max}} = 2U_{ch}\) in all cases.
Figure 2. Simulation results for bubble dynamics for $a=0.06R$ (top row) and $a=0.11R$ (bottom row). Initial position of the bubble (left column) and bubble motion at different dimensionless time, from left to the right $t=0$, $t=2$, $t=4$ (right column).

Figure 3. Relative velocity of the center of mass of the bubble.

Then we considered the dynamics of bubbles of the radius $a=0.07R$ with the same physical parameters. The bubbles were located at some equal distance from the channel centerline $\Delta h = 0.1R$. 
but in three directions from the centerline in the plane \(yz\). Accordingly, the initial coordinates of the center of mass: \(y = 0.1R, z = 0\); \(y = -0.0481R, z = -0.0833R\); \(y = -0.0481R; z = 0.0833R\).

Figure 4 presents the results of these series calculations. In contrast to the cases for bubbles located on the channel centerline, in this case, the bubbles have significant deformations consistent with the channel cross-sectional shape features. The asymmetry of the velocity field explains the variation in the bubble shape and even in their inclination relative to the flow direction for different positions of the bubble center of mass. The features of time changes of the relative velocity of the center of mass of the bubble with different initial positions are shown in Figure 5. In all cases, the relative velocity increases in time, and in the considered time interval, the velocity increases by 11.5% on average. In the case of a bubble located on the channel centerline of the same radius, there is a small change in the relative velocity in time of about 4%. Also, the velocity value for a bubble with \(\Delta h = 0\) exceeds the velocity for all variants of the bubble positions with \(\Delta h = 0.1R\). It should be noted that, despite the equal distance from the centerline of all cases, the values of the relative velocity of the center of mass differ (Figure 5). Furthermore, some fluctuations are noticeable on the graphs, which are caused by an asymmetric deviation from the spherical shape.

**Figure 4.** Simulation results for bubble dynamics for \(a = 0.07R, y = -0.0481R, z = -0.0833R\) (top row) and \(y = -0.0481R, z = 0.0833R\) (bottom row). Initial position of the bubble (left column) and bubble motion at different dimensionless time, from the left to the right \(t = 0, 2, 4\) (right column).
Figure 5. Relative velocity of the center of mass of the bubble with equal radius $a = 0.07R$ with different initial position of the bubble.

Conclusions
The features of single incompressible bubble dynamics in viscous fluid flow in microchannels with a cross-section in the form of the deltoid have been studied. To conduct the calculations, we implemented the program code based on the boundary element method for the Stokes equations. A triangulation for channels of non-trivial geometry was implemented as well. The influence of the initial bubble radius, its position relative to the channel centerline on the bubble deformation, and the relative center of mass velocity has been considered for the constant pressure drop and viscosity of the surrounding liquid. It is shown that with increasing bubble size, its relative velocity decreases. The deformation of bubbles located at some equal distance from the channel centerline but in three different directions in the plane $yz$ differs significantly. The behavior of the relative velocity changes has been studied for the bubble positions. In the future, it is planned to modify the software for calculating bubble dynamics in the channel in the presence of an acoustic field, which can be used to study a broad class of phenomena associated with the bubbly liquid flow in porous materials.

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