Numerical simulation of the dynamics and calculation of the rheological characteristics of the dispersed systems using BEM

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Abstract. Dispersed systems of various types occupy a significant place in nature, technology, and everyday life. Unfailing interest in this field is shown by researchers from the physics and mechanics, colloid chemistry, micro-manufacturing, and biology, which is due to the variety of phenomena and effects associated with dispersed systems of different nature. High-efficient computational techniques for direct modeling of the dispersed system are required to more accurately determine the rheological parameters of such systems, based on the calculated properties of its components. The present work is dedicated to the numerical investigation of the dispersed system features in a shear flow at low Reynolds numbers using the boundary element method. The results of the simulations and the method details are discussed. Calculations are presented for different types of dispersed inclusions. Viscous droplets and rigid particles of different shapes in a volume of carrier viscous liquid are considered. Furthermore, the standard viscometric functions that characterize the behaviour of an emulsion or suspensions, regarded as a homogeneous medium, are calculated and studied.

1. Motivation

Different types of disperse systems, such as emulsions, suspensions, and bubbly liquids, are widely used in many fields of industry and science, such as medicine, pharmacology, colloid chemistry, micro-manufacturing, oil and gas, food industry, etc. It is known that the structure of multiphase flows is very complex and mostly depends on the streams at the micro level (on the scale of single inclusions). For many years, the rheology of dispersed systems has been evaluated only by experimental or theoretical methods, but in recent years, due to the vast extension and developing of numerical methods and high-performance calculations, direct mathematical modeling of such phenomena has become possible. The research of the dynamics of particles and drops allows elaborating in detail the interface dynamics between two fluids and provides a basis for calculation of the rheological characteristics of the system. The prediction of the water-in-oil emulsion properties is very important for accelerating of oil production from the porous layer, for the separation oil from water and other impurities, for the processing, and transportation of raw materials. The study of the behavior of rigid non-spherical particles is also of great importance for a wide area of technological processes, such as the processing of pulps in the production of paper, polymer composites manufacturing, the production of reinforced plastics, etc.

The calculation of the dynamics of emulsion droplets under the action of various external fields is carried out using various numerical methods for investigation of the continuum mechanics problems, for instance, finite-difference methods [1], finite element method [2], finite volume method, and volume...
of fluid method [3], and boundary element method (BEM). The BEM is appropriate for the study of the
dynamics of the dispersed inclusions with an arbitrary deformation and form in unbounded domains.
BEM for Stokes flow described in [4] was successfully applied for simulation of the dynamics and
interaction of the droplets, bubbles and rigid particles in dispersed flows [5-7]. Therefore, the leading
scientific problem addressed in the present work is the study of the properties of different types of
dispersed systems under imposed simple shear flow using direct numerical simulation based on the
boundary element method.

2. Problem formulation and numerical implementation
In this paper we consider different types of disperse systems: emulsions and suspensions (index 2)
consisting of spherical and non-spherical rigid particles, in an unbounded viscous liquid (index 1) under
imposed shear flow. It is assumed that the processes are isothermal and slow enough and that the
viscosity forces are much more significant than the inertia forces. The intermolecular Van der Waals
forces are not taking into account. In this case, the processes are described by Stokes equations
\[ \nabla \cdot \sigma = -\nabla p + \mu \Delta u_i = 0, \quad \nabla \cdot u_i = 0, \quad i = 1, 2, \]
with the corresponding boundary conditions on the interface surface (\( S \))
\[ u_1 = u_2 = u, \quad f = \sigma_1 \cdot n_1 - \sigma_2 \cdot n_2 = f_1 - f_2 = f_n, \]
\[ f = 2\gamma k + (\rho_1 - \rho_2)(g \cdot x), \quad x \in S \]
where \( u \) and \( \sigma \) are the velocity and the stress tensor, \( \mu \) is the fluid viscosity, \( p \) is the pressure, which
includes the hydrostatic component, \( \rho, \gamma \) and \( g \) are the density, the surface tension, and the gravity
acceleration, respectively, \( f \) is the normal stress, \( n \) is the normal to \( S \) pointed into fluid 1, and \( k \) is the
mean surface curvature. For the carrier fluid the condition \( u(x) \rightarrow u_\infty(x) \) is imposed, where \( u_\infty(x) \)
is a solution of the Stokes equations. The dynamics of the fluid-fluid interface can be determined from the
kinematic condition
\[ \frac{dx}{dt} = u(x), \quad x \in S, \]
where \( u(x) \) is the interface velocity determined from the solution of the elliptic boundary value
problem (1)-(2). The problem is solved using the boundary element method. The surface of each
dispersed inclusion is described by triangular mesh. The boundary integral representation of the velocity
field for the case of dispersed particles in unbounded domain can be found in [4]. More details of the
implementation can be found in our previous works [8, 9].

2.1. Calculation of the rheological characteristics
There are several theoretical models for calculation of rheological characteristics, for instance, the
relative viscosity, but most of them are valid for small concentrations and undeformable spherical
particles. A large number of published papers are related to the study of the rheology of the dispersed
systems [10-12]. A comprehensive review of the fundamental rheology of dilute disperse systems is
presented in [13]. The theoretical model constructing for calculation of the rheological characteristics
of the dispersed system consisting of deformable liquid droplets of arbitrary size or rigid particles of
different non-spherical shapes is very complicated. The existing models are usually restricted by the
assumptions of the small deformation of the particles, near-spherical shapes or small volume
concentrations.

In this work we used the numerical approach which allows one more detailed research and direct
calculation of the rheological properties of dispersed systems [14]. It has been derived that if the
dispersed phase is also a Newtonian fluid and the motion occurs at low Reynolds numbers, then stress tensor $\Sigma$ for the dispersed system in a shear flow $u_\infty = (Gy, 0, 0)$ is defined as

$$\Sigma_y = -\delta_y P + \mu \left( \frac{\partial u_j}{\partial x_j} + \frac{\partial u_i}{\partial x_i} \right) + \alpha \Sigma_{ij}^d, \quad \Sigma_{ij}^d = \frac{1}{V_2} \int \left[ f(x_j, x_j - \mu_1(1 - \lambda)(u_j n_j + u_i n_i) \right] dS,$$

where $\alpha$ is the volume concentration of dispersed phase, and $G$ is the shear rate, $i, j = 1, 2, 3$. The first two terms in the right side of the equation (4) is the contribution of the continuous phase, the last integral expresses the contribution of the dispersed phase in the stress tensor of the whole system and its value depends on the microstructure of the considered system. Based on the variables in formula (4), it is seen that the geometry of the inclusions (their deformation and orientation in the flow) significantly affects the stress tensor of the dispersed system.

If the velocity and traction on the surface of each particle are defined, then using formula (4), the following rheological characteristics can be calculated

$$\mu_{eff} = \mu_1 + \alpha \Sigma_{ij}^d / G, \quad N_1 = \alpha \left( \Sigma_{ij}^d - \Sigma_{ij}^d \right), \quad N_2 = \alpha \left( \Sigma_{ij}^d - \Sigma_{ij}^d \right),$$

where $\mu_{eff}$ is the effective viscosity, and $N_1, N_2$ are the first and second normal stress differences. For Newtonian fluids, the viscosity does not depend on the shear rate, and the normal stresses differences are zero. When the system shows a non-Newtonian behavior the changing of system viscosity while changing $G$ is observed. Furthermore, for example normal stresses differences appear in polymer melts and solutions due to the elasticity of the polymer chains which extend downstream.

3. Results and discussion

In the frame of this work we consider different types of the dispersed systems under an imposed shear flow (figure 1). We calculated the contribution of a single droplet to the stress tensor of the emulsion for different values of the ratio of viscosities and capillary number, $Ca = \mu_1 a G / \gamma$, where $a$ is the droplet radius. Then the obtained results were compared with the numerical results and theoretical expressions available in the literature. Good agreement has been found in all cases. The validation of applied approach is represented in more detail in our previous work [9].

![Figure 1](image_url)

**Figure 1.** Triangulation of the considered inclusions of different shapes (from the left to the right): stable deformable shape of droplets for $\lambda = 0.5$ and $Ca = 0.1$, $\lambda = 0.5$ and $Ca = 0.5$, particles $L / R = 2$ and $L / R = 5$.

The contribution of one inclusion to the stress tensor components of the system is calculated using the formulas $\Sigma_{ij} = \Sigma_{ij}^d$, $N_1^d = \Sigma_{ij}^d - \Sigma_{ij}^d$, and $N_2^d = \Sigma_{ij}^d - \Sigma_{ij}^d$. First of all we consider the case of the deformable single emulsion droplet with a center at the origin, placed in a stationary uniform shear flow, for different values of capillary numbers and set of a values of $\lambda = \mu_2 / \mu_1$. There were $N = 642$ calculation points and $N_\Delta = 1280$ triangular elements on the drop surface. The contribution of a single drop to the components of the stress tensor of the emulsion was calculated for stable deformable shape in shear flow for each specific pair of parameters ($Ca, \lambda$). The rheological characteristics (contribution
to the effective viscosity and normal stress differences) are presented in Figure 2 for \( \lambda = 0.5 \) and \( \lambda = 5 \) as functions of \( Ca \). As it is seen, \( \Sigma_{12} \) is positive for all values of \( Ca \) and \( \lambda \). First and second normal stress differences are not equal to zero and grow in absolute value with increasing \( Ca \), which is equivalent to an increase in the deformability of the drop.

![Figure 2](image1)

**Figure 2.** The dependence of rheological characteristics for single droplet on \( Ca \) for \( \lambda = 0.5 \) (left) and \( \lambda = 5 \) (right).

![Figure 3](image2)

**Figure 3.** The dependence of \( \Sigma_{12} \) for single droplet on \( Ca \) (left) and \( \lambda \) (right).

In figure 3 the values of the contribution of single deformable droplet to effective viscosity \( \Sigma_{12} \) is presented as a function of \( Ca \) and \( \lambda \). For different \( \lambda \) the influence of the presence of droplets on the effective viscosity varies. For \( \lambda > 1 \) the value of \( \Sigma_{12} \) grows faster and more linear, in the case of \( \lambda < 1 \) there is a non-linear behavior of the curves. Thus, the presence of deformable droplets affects the effective viscosity of the disperse system as a whole and the behavior of rheological functions significantly depends on the ratio of viscosities and capillary numbers.
Then, the numerical experiments were conducted for the case of non-deformable single particle in shear flow \((Ca \ll 1 \text{ and } \lambda \gg 1)\). The considered particle had the form of a capsule; the ratio of the length of the cylindrical part of the capsule to the radius \(L / R\) was varied. The distribution of the velocity components on the particle surface in several dimensionless times \(t = \frac{n_{\text{ord}}}{\mu} \gamma_{\text{dim}} / \mu_{\text{a}}\) is shown in figure 4 for \(L / R = 5\), \(N_{\Delta} = 3368\). It is seen that the velocity distribution over the surface of the particle changes in time and causes the particle to rotate in the shear flow. Also, the rheological characteristics were calculated for the cases of \(L / R = 2\), \(N_{\Delta} = 1928\) and \(L / R = 5\), \(N_{\Delta} = 3368\). Figure 5 shows the changing in time of the contribution to the first and second normal stress differences. The values of \(N_{1}^{d}\) and \(N_{2}^{d}\) almost match and change in time depending on the rotation of the particle. The contribution to the effective viscosity as a function of time is shown in figure 6. The behavior of the curves depends on the geometry of the particles, i.e. the greater the relation \(L / R\), the greater the absolute values of all characteristics. As it is seen from figures 5, 6 the orientation of the particles in the flow significantly affects the values of rheological parameters. Thus, the observations show the strong dependence of the rheology of suspensions and emulsions on the microstructure of the considered system.
Figure 5. First and second normal stress differences for single nondeformable particle for $L/R = 2$ (left) and $L/R = 5$ (right).

Figure 6. Contribution to the effective viscosity from single particle for $L/R = 2$ (left) and $L/R = 5$ (right).

Conclusions
The application of the BEM-based approach for 3D calculation of the dynamics of dispersed inclusions in shear flow has been presented. The rheological characteristics of the dispersed systems for wide range of viscosity ratio and capillary number have been considered. It served to study the changes of different rheological characteristics in time, as well as the dependence on the physical parameters in a range that remains uncovered by various theoretical models, which are often limited by the assumption of monodispersity of the systems, non-deformability or spherical shapes of the particles.

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