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Numerical study of the rheological characteristics of dispersed systems in shear flow using the boundary element method

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Abstract. Dispersed systems are widely used in chemical, biochemical and pharmaceutical industries. This work is dedicated to the study of the dependence of macroscopic parameters of emulsions, such as effective viscosity, on the microlevel structure and physical properties of emulsion droplets. The numerical approach is based on the accelerated boundary element method in three dimensions. In this paper, we consider the dynamics of two close deformable droplets of equal radius in the volume of a viscous incompressible fluid under the action of a shear flow. Time evolution of minimal distance between droplet surfaces has been considered. A parametric study of the dispersed phase contribution to the stress tensor of a dispersed system as a whole, as well as the first and second differences of normal stresses, is conducted.

Keywords: dispersed systems, shear flow, rheology, boundary element method

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Материалы конференции
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Численное исследование реологических характеристик дисперсных систем в сдвиговом потоке с использованием метода граничных элементов

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Аннотация. Дисперсные системы широко используются в химической, биохимической и фармацевтической промышленности. Данная работа посвящена исследованию зависимости макроскопических параметров эмульсий, таких как эффективная вязкость, от микроуровневой структуры и физических свойств капель эмульсии. Численный подход основан на ускоренном методе граничных элементов. В данной работе рассматривается динамика двух близкорасположенных деформируемых капель равных радиусов в объеме вязкой несжимаемой жидкости под действием сдвигового потока. Рассмотрено изменение минимального расстояния между поверхностями капель во времени. Проведено многопараметрическое исследование вклада дисперсной фазы в тензор напряжений дисперсной системы в целом, а также первой и второй разностей нормальных напряжений.

Ключевые слова: дисперсные системы, сдвиговый поток, реология, метод граничных элементов

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Introduction

The studying of the behavior, dynamics and physical properties of the dispersed systems (emulsions, suspensions, and bubbly liquids) is relevance due to their widespread use in industry [1-3]. Emulsions occur at all stages of production, processing and transportation of raw materials in the oil industry and the ability to predict the values of rheological characteristics is of great importance. Studies performed over many decades have shown that not only the volume concentration of the dispersed phase, but also the droplet size has a significant influence on the rheology of the disperse system [2].

There are also a number of theoretical models for calculating the rheological characteristics of such dispersed systems, but most of them are based on the Einstein formula with various modifications for more concentrated systems, as well as for various nonspherical forms of solid dispersed inclusions. A large number of published works refer to the study of the rheology of suspensions. Dispersed systems consisting of liquid droplets suspended into another liquid have received much less attention, despite the fact that the rheological behavior of emulsions is much more complicated. For example, suspensions at low concentrations of spherical solids behave as Newtonian fluids, while emulsions of deformable particles demonstrate pseudoplastic and viscoelastic properties even at low volume concentrations of the dispersed phase [3]. In [4–5] peculiarities of non-Newtonian flow of suspensions are explained by changes in their structure, in particular, by appearance and destruction of aggregates of particles. The difficulty of developing theoretical models for determining the rheological characteristics of emulsions consisting of liquid deformable droplets of arbitrary size and distribution is due to the fact that it is quite difficult to predict in advance the shape of a deformed droplet, since it will change differently under the combined action of viscous forces and surface tension forces. Therefore, the use of modern computational approaches to direct calculation of the stress tensor components is a convenient and effective tool for conducting studies of the influence of emulsion microstructure on their rheology.

Among numerical methods of emulsion dynamics modeling, the most widely used ones are the finite-difference methods, the finite-element method, the volume of fluid [6] and the boundary-element method (BEM). The above-mentioned approaches are distinguished between each other by the way of representation of the computational domain and mathematical basis. The purpose of this work is to apply the developed software based on the 3D boundary element method to calculate the effect of droplet deformation during interaction in a shear flow on the values of stress tensor components.

Problem Statement and Numerical Implementation

Mathematical model.

The dynamics of two closely spaced droplets of one Newtonian liquid (index 2) in an unbounded volume of a viscous incompressible fluid (index 1) in a shear flow is considered. It is assumed that the flow is sufficiently slow, therefore inertial effects can be disregarded. The processes are considered for small Reynolds numbers ($Re \ll 1$), at moderate Struhal numbers $St \sim 1$, in isothermal conditions ($T = const$), and without taking into account the interaction forces between dispersed inclusions (Van der Waals forces).

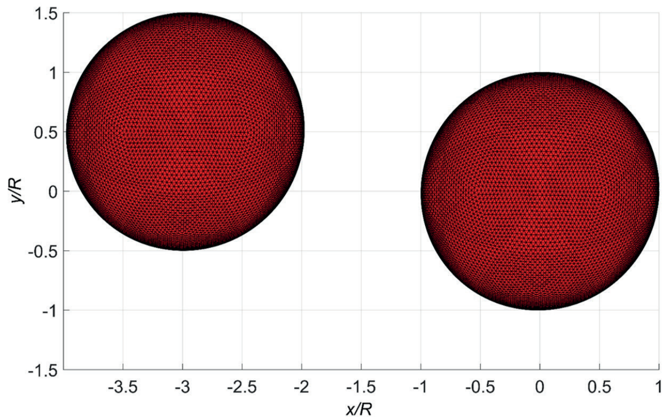

Fig. 1. Discretization of two closely spaced droplets at an initial moment in the *xOy* plane

The dynamics of the considered system are described by the Stokes equations

$$\nabla \cdot \boldsymbol{\sigma}_i = -\nabla p_i + \mu_i \nabla^2 \mathbf{u}_i = 0, \quad \nabla \cdot \mathbf{u}_i = 0, \quad i = 1,2\ , \tag{1}$$

where $\boldsymbol{\sigma}$ is the stress tensor, p is the pressure, μ is the dynamic viscosity, $\mathbf{u}$ is the velocity vector.

The problem is solved under the following boundary conditions. The velocities at the interface are equal and the traction is given

$$\mathbf{u}_1 = \mathbf{u}_2 = \mathbf{u} \tag{2}$$

$$\mathbf{f} = \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{f}_1 - \mathbf{f}_2 = f\mathbf{n},\ f = \gamma(\nabla \cdot \mathbf{n}) + (\rho_1 - \rho_2)(\mathbf{g} \cdot \mathbf{x}), \quad \mathbf{x} \in S, \tag{3}$$

where $\mathbf{n}$ is the normal to the surface that is directed into the dispersion medium (liquid with index 1), γ is the surface tension coefficient, ρ is the liquid density, $\mathbf{g}$ is the gravity vector, $\mathbf{x}$ is the radius vector of the considered point, S is the drop surface. The constant velocity is specified at the infinity, $\mathbf{u}_1(\mathbf{x}) \to \mathbf{u}_\infty(\mathbf{x})$.

The dynamics of the fluid-fluid interface can be determined from the kinematic condition

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}), \quad \mathbf{x} \in S. \tag{4}$$

The numerical method for solving the problem is based on the boundary element method. The BEM is well applicable for studying the motion of droplets with arbitrary deformation and for simulation of large volume liquid-liquid systems in infinite domains, because the requirement to completely discretize the three-dimensional domain is eliminated. Only the surfaces of the considered objects are covered by triangular mesh (Fig. 1). The BEM for the flows in the Stokes regime is described in [7] and has been successfully employed to calculate the dynamics and interaction of droplets, bubbles, and solid particles in disperse flows [8–12].

Calculation of the rheological characteristics.

In this paper, we used the approach [13, 14] based on the proposition that the stress tensor of the system $\sum$ is calculated as a stress tensor $\mathbf{T}$ averaged over the isolated volume of the dispersed medium V

$$\sum = \frac{1}{V} \int_V \mathbf{T} dV. \tag{5}$$

It was deduced that if the dispersion phase is also a Newtonian fluid and the motion occurs at small Reynolds numbers, then for an emulsion in shear flow $\mathbf{u}_\infty(\mathbf{x}) = (Gy;0;0)$ the stress tensor is defined as

$$\sigma_{ij} = -\delta_{ij} p + 2\mu_1 e_{ij} + \alpha \Sigma_{ij}, \tag{6}$$

$$\Sigma_{ij} = \frac{1}{V_2} \int_S \left[f_i x_i - \mu_1 (1 - \lambda)(u_i n_j + u_j n_i) \right] dS, \quad i, j = 1,2,3, \tag{7}$$

where α is the volume concentration of the dispersed phase, $\lambda = \mu_2/\mu_1$ is the viscosity ratio of the liquid inside droplet volume and outside.

The geometry of the droplets, i.e. their deformation and orientation in space, has a significant influence on the emulsion stress tensor. Based on the calculated velocities and the traction on the surface of each droplet contained in the emulsion volume, one can determine the effective viscosity, first and second differences of normal components of the stress tensor using the following formulae

$$\mu_{eff} = \mu_1 + \alpha \Sigma_{12}^d / G, \tag{8}$$

$$N_1 = \alpha\left(\Sigma_{11}^d - \Sigma_{22}^d\right), \tag{9}$$

$$N_2 = \alpha\left(\Sigma_{22}^d - \Sigma_{33}^d\right), \tag{10}$$

where μ_{eff} is the effective viscosity of the emulsion, N_1 and N_2 are the first and second normal stress differences correspondingly, the index d denotes the contribution to the stress tensor components from the drops.

To validate the method for determining the rheological characteristics of dispersed systems, the calculated contribution of a single drop to the emulsion stress tensor was compared with the numerical results reported in the literature [15]. The comparison for several values of capillary numbers and for $\lambda = 6.4$ and $\lambda = 1$ were shown a good coincide of the results and were discussed in more details in our previous work [12]. Furthermore, we tested this approach for case of non-spherical rigid particles [10] and for calculation of effective viscosity of suspension with spherical rigid particles and monodispersed and polydispersed emulsions [12].

We consider the dynamics of two closely spaced droplets with high discretization containing N_Δ = 20480 triangular elements on the each droplet surface (Fig. 1). The combination of parameters that describes the deformation of droplets and it's orientation in the shear flow of a viscous incompressible fluid includes the viscosity ratio λ, and the capillary number $Ca = \mu RG/\gamma$, where R is droplet radius, G is shear rate. The calculations have been performed for a range of Ca capillary numbers Ca = [0.25, 0.5] and viscosity ratio λ = 5. Initially, droplets have a spherical shape and equal size. We consider two values of the distance between coordinates of droplet mass centers along y-axis $dy = 1R$, $dy = 0.7R$, and the distance along x- and z-axes is the same for all cases: $dx = 3R$, $dz = 0$. Under the action of constant shear flow the droplets deform and move and also the distance between droplets' surfaces changes Fig. 2 demonstrates the variation in time of the minimum distance between the droplet surfaces in cases $Ca = 0.3$ (b) and $Ca = 0.25$ (a) ($t = t_{nondim} = \gamma t_{dim}/(\mu_1 R)$ is the dimensionless time, t_{dim} is the dimension time). At the initial moment, the distance between droplet surfaces was $h_{min} = 1.08R$ and $h_{min} = 1.16R$.

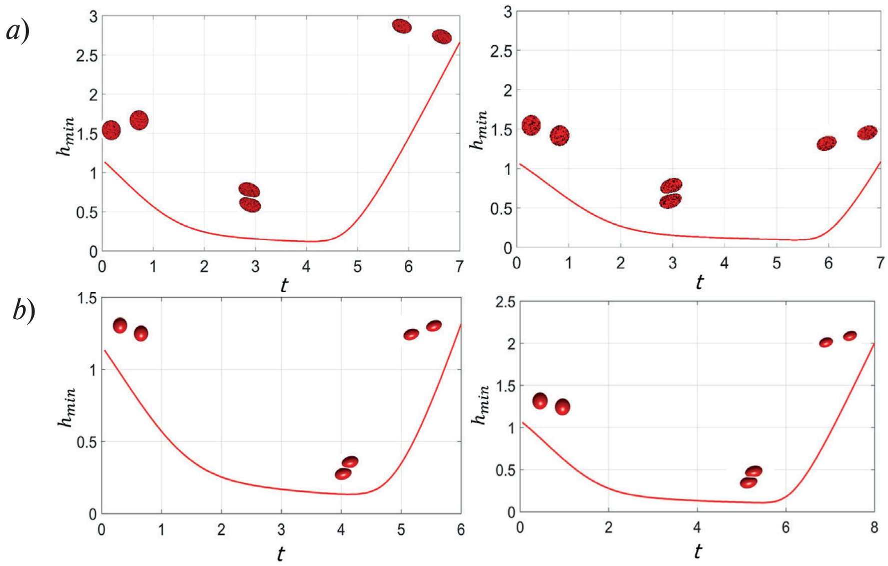

Fig. 2. Time evolution of the minimum distance between the droplets surfaces Ca = 0.25 (a), Ca = 0.3 (b), λ = 5, $dy = 1R$ (left column) and $dy = 0.7R$ (right column)

Fig. 2 demonstrates the time evolution of the distance between droplet surfaces. The general behavior of the curves is similar for all considered cases. When the drops move in the flow relative to each other, they approach each other up to some minimum values of the distance between the surfaces. The graph shows a zone of close contact of the drops, when the value h_{min} is minimal and changes insignificantly, and the drops have the maximum effect on the deformation and dynamics each other. The drops coalescence does not occur, and after the end of the close contact zone, the distance between droplets increases. One can see from the Fig. 2 that the smaller the initial distance, the longer the zone of close contact between the drops for both values of the capillary number.

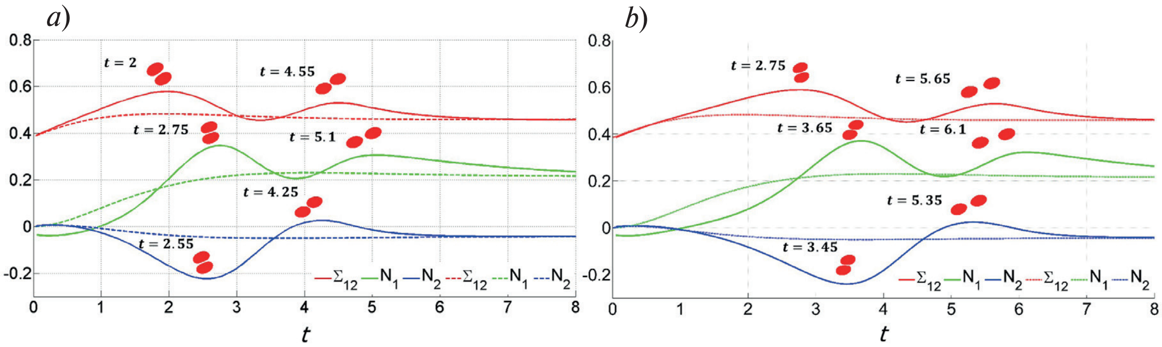

Fig. 3. Time evolution of rheological characteristics of the system in time at Ca = 0.25, λ = 5, dy = 1R (a) and dy = 0.7R (b); solid lines – contribution values of one droplet in case of two close droplets, dashed lines – contribution values of one single droplet in shear flow

The changing of the contribution from two droplets in the rheological functions of the system was investigated. The case when the droplets are a sufficient distance apart, matches the case of dilute emulsion so that the droplets do not influence each other, hence the rheological characteristics of the emulsion do not change in time. However, when considering two close droplets, the influence of the droplets on each other can be observed as in case of more concentrated emulsions, resulting in changes in rheological functions over time. Fig. 3 demonstrates the time evolution of the rheological characteristics (contribution to the effective viscosity of the system $\sum_{12}$, the first difference of normal stresses N_1, the second difference of normal stresses N_2) calculated for one of the two interacting droplets (solid lines) and for the single droplet with the same parameters in shear flow (dashed lines). The curves on Fig. 3 demonstrate that the contribution to the components of the stress tensor for interacted droplets differs significantly from the case of well-separated droplets. When the droplets are far enough, their influence on deformation on each other is minimized, and rheological characteristics take constant values. The values of the first and second normal stress difference are indicators of the non-Newtonian behavior of the system and are most different from zero when the droplets are close enough to each other and affect each other, which corresponds to the case of concentrated emulsions.

Furthermore, the effect of droplet deformability on the calculated values of the contributions to the components of the stress tensor was considered. The calculations of $\sum_{12}$, N_1, N_2 were conducted for different values of capillary numbers Ca = [0.25, 0.5] in case of two droplets with

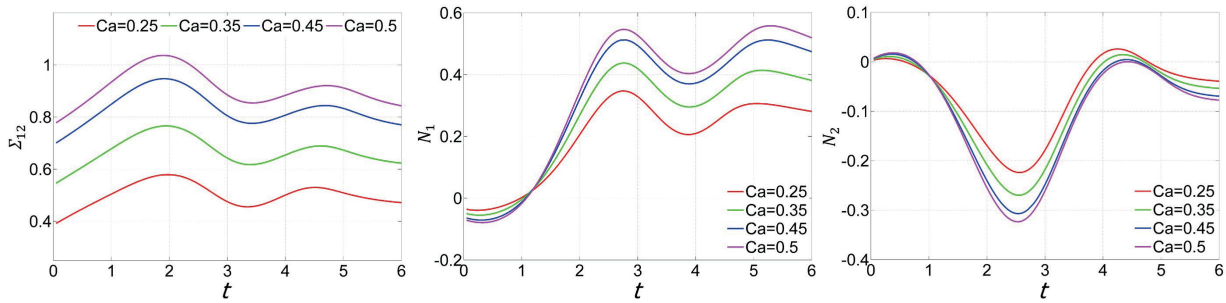

Fig. 4. Time evolution of rheological characteristics of the system in time at different Ca, λ = 5, h_{min} = 1.16R

initial distance between the surfaces $h_{min} = 1.16R$ and for $\lambda = 5$. Fig. 4 demonstrates the time evolution of the rheological characteristics of the system for droplets with different *Ca*. The graphs show that as *Ca* and droplet deformability increases, the droplet contribution to the system stress tensor increases.

Conclusion

The possibility of applying the computational approach based on the accelerated three-dimensional boundary element method to the problems of calculating the components of the stress tensor of various types of disperse systems is demonstrated. The dependence of rheological characteristics of the emulsion on its microstructure (relative position and deformability of the droplets) has been investigated. Numerical experiments of the study of the dynamics of two closely spaced droplets in a shear flow have been performed in cases of $Ca = [0.25, 0.5]$, $\lambda = 5$, and different distance between droplets. Reducing this distance increases the contribution to the effective viscosity of the dispersed systems as a whole. The results of calculations of the values of the first and second normal stress differences showed that in the case of more concentrated emulsions, when the droplets actively interact with each other, there will be appear the non-Newtonian effects. It is shown, that the highest values of the stress tensor components correspond to the most deformable drops. The study of changing rheological characteristics at close contact between droplets shows that the properties of the emulsion flow in different areas, for example in microchannels, at dense packing of particles, i.e. when the contact surface between droplets significantly increases, is determined not only by the position and dynamics of droplets in the flow, but also by the nature of interaction between droplets at their close contact. Thus, direct numerical simulation of the emulsion flow consisting of deformable droplets can be utilized for a more complete and reliable description of the rheological features depending on the microstructure.

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