Numerical simulation of a fluid particle rising in non-Newtonian fluids

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Abstract

In this work, a level set method is developed for simulating the motion of a fluid particle rising in non-Newtonian fluids described by generalized Newtonian as well as viscoelastic model fluids. As the shear-thinning model we use a Carreau-Yasuda model, and the viscoelastic effect can be modeled with Oldroyd-B constitutive equations. The control volume formulation with the SIMPLEC algorithm incorporated is used to solve the governing equations on a staggered Eulerian grid. The level set method is implemented to compute the motion of a bubble in a Newtonian fluid as one of typical examples for validation, and the computational results are in good agreement with the reported experimental data. The level set method is also applied for simulating a Newtonian drop rising in Carreau-Yasuda and Oldroyd-B fluids. Numerical results including noticeably negative wake behind the drop and viscosity field are obtained, and compare satisfactorily with the known literature data.

Keywords: Numerical simulation; bubble/drop; level set; non-Newtonian fluid

1. Introduction

As is well known, a large number of investigations concerning various aspects of the bubble or drop motion in non-Newtonian fluids have been reported theoretically and experimentally in the past. The most important results have been well summarized and reviewed by Chhabra [1,2]. Nevertheless, in comparison to the study of bubble or drop motion in Newtonian fluids, various unanswered questions and problems still remain to be considered in non-Newtonian fluid systems due to their inherently complex nature. The studies quoted above are mostly based on experiments, but numerical analysis has become a powerful and useful tool for comprehending and revealing detailed flow structure and mechanism. This is because some essential physical information peculiar to non-Newtonian fluids can be locally obtained and evaluated in detail, which are hard to be estimated using experimental techniques, such as the local effects of shear-thinning on the drop motion.

In this study, we compute the motion of fluid particles freely rising through non-Newtonian fluids. We perform axisymmetric computations using the level set method for tracking the interface. We will also study the local viscosity field formed around a drop and the negative wake behind the drop.

2. Basic equations and simulation methods

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In this study, the motion of a single bubble/drop rising driven by buoyancy in an immiscible quiescent liquid is considered with following assumptions: (1) the fluids in both phases are viscous and incompressible; (2) the two-phase flow is axisymmetric and laminar.

2.1. Governing equations

In the level set formulation, the transient motion of a bubble/drop can be expressed by the continuity and Navier-Stokes equations as follows:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla P + \rho \mathrm{g} + \nabla\cdot\left(\frac{c\mu_N}{\lambda_1}\mathbf{A}\right) + \nabla\cdot\left(2\mu_N\mathbf{D}\right) + \sigma\kappa\nabla H_\varepsilon\left(\phi\right)\mathrm{n} \tag{2}$$

where $\mathbf{u}$ is the velocity, p is the pressure, ρ is the density, σ is the surface tension and $\mathbf{D} = \left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)/2$ is the rate-of-deformation tensor. The viscosity can be described by the Carreau-Yasuda model [3]:

$$\mu_N\left(\dot{\gamma}\right) = \mu_\infty + \left(\mu_0 - \mu_\infty\right)\left[1 + \left(\lambda\dot{\gamma}\right)^\beta\right]^{n-1/\beta} \tag{3}$$

where λ is the inelastic time constant, n is a parameter between 0 and 1 for shear-thinning fluids, μ_0 is the zero shear viscosity, μ_∞ is the minimum viscosity achieved as shear rate approaches infinity. To describe the viscoelastic properties of the fluid, the constitutive equation is by the Oldroyd-B model. The evolution of the configuration tensor $\mathbf{A}$ is given as follows [4]:

$$\frac{\partial \mathbf{A}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{A} = \mathbf{A}\cdot\nabla\mathbf{u} + \nabla\mathbf{u}^T\cdot\mathbf{A} - \frac{1}{\lambda_1}\left(\mathbf{A} - \mathbf{I}\right) \tag{4}$$

Here λ_1 is the characteristic relaxation for a viscoelastic fluid.

2.2. Level set approach of fluid flow

A smooth scalar function denoted as ϕ is introduced into the formulation of the two phase flow system to define and capture the interface between two fluids, which is identified as the zero level set of the level set function defined on the entire computational domain. The function is chosen as the signed algebraic distance to the interface, being positive in the continuous fluid phase and negative in the bubble or drop. The following Hamilton-Jacobi type evolution equation [5] can be used to advance the level set function exactly as the bubble moves

$$\frac{\partial \phi}{\partial t} + \nabla\cdot\left(\mathbf{u}\phi\right) = \frac{\partial \phi}{\partial t} + \left(\mathbf{u}\cdot\nabla\right)\phi = 0 \tag{5}$$

After introducing the level set formulation, the motion of two separate domains for immiscible two-phase fluids may easily be formulated as a single one.

The curvature of free surface, $\kappa(\phi)$ is expressed as

$$\kappa(\phi) = \nabla \cdot \mathbf{n} = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right) \tag{6}$$

The regularized delta function $\delta_\varepsilon(\phi)$ is defined as

$$\delta_\varepsilon(\phi) = \begin{cases} \frac{1}{2\varepsilon}\left(1+\cos(\pi\phi/\varepsilon)\right) & \text{if } |\phi| < \varepsilon \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

In Eq. (2), $H_\varepsilon(\phi)$ is a smoothed Heaviside function introduced for avoiding the sharp change in pressure and diffusion terms at the interface due to large density and/or viscosity ratios. This is given by

$$H_\varepsilon(\phi) = \begin{cases} 0 & \text{if } \phi < -\varepsilon \\ \frac{1}{2}\left(1 + \frac{\phi}{\varepsilon} + \sin(\pi\phi/\varepsilon)/\pi\right) & \text{if } |\phi| \le \varepsilon \\ 1 & \text{if } \phi > \varepsilon \end{cases} \tag{8}$$

where $\varepsilon \equiv O(h)$ prescribes the finite "thickness" of the interface. In this computation, we take $\varepsilon = h$ generally, where h is equal to the dimensionless uniform mesh size near the interface.

Density and viscosity are written as

$$\rho(\phi) = \rho_G + (\rho_L - \rho_G) H_\varepsilon(\phi) \tag{9}$$

$$\eta(\phi) = \eta_G + (\eta_L - \eta_G) H_\varepsilon(\phi) \tag{10}$$

The fluid relaxation time is assumed to jump across the interface

$$\lambda_1 = \begin{cases} \lambda_{1G} & \text{if } \phi<0 \\ 0.5(\lambda_{1G} + \lambda_{1L}) & \text{if } \phi = 0 \\ \lambda_{1L} & \text{if } \phi > 0 \end{cases} \tag{11}$$

Here λ_{1G} and λ_{1L} are the relaxation time of the fluids inside and outside the bubble, respectively. If the fluid inside (or outside) the bubble is Newtonian, its relaxation time is set to zero. A relaxation time of zero ensures that the fluid relaxes instantaneously and thus behaves like a Newtonian fluid. This allows us to use the same equations for both Newtonian and viscoelastic liquids.

In addition, after certain iteration steps ϕ will no longer remain a distance function (i.e., $|\nabla \phi| \neq 1$) generally, even if Eq. (5) advances the interface at correct velocities. Maintaining ϕ as a distance function is very essential for accurate evaluation of $\mathbf{n}$ and $\kappa(\phi)$. Therefore, a reinitialization procedure for resetting ϕ as an exact distance function should be adopted to keep the interface thickness finite and preserve mass conservation. A reinitialization method proposed by Sussman et al.[6] is often used, which is accomplished by iterating the following equation to steady state:

$$\frac{\partial \phi}{\partial \tau} = \operatorname{sgn}(\phi_0)(1 - |\nabla \phi|) \tag{12}$$

where ϕ_0 is a level set function at any computational time, i.e., $\phi_0(\mathbf{X}) = \phi(\mathbf{X}, \tau = 0)$, τ is the virtual time in a reinitialization step and $\mathrm{sgn}(\phi_0)$ denotes the smoothed sign function with appropriate numerical smearing to avoid any numerical difficulties. The formulation of fluid flow and the procedure of numerical solution have been presented previously by the authors in detail [7], in which another area-preserving reinitialization procedure for ϕ was coupled with Eq. (12) to guarantee the mass conservation by solving a perturbed Hamilton-Jacobi equation proposed by Zhang et al. [8] to pseudo-steady state in each time step. The improved reinitialization procedure can maintain the level set function as a distance function and guarantee the fluid particle mass conservation.

2.3 Computational scheme

The control volume formulation with the power-law scheme and the SIMPLEC algorithm are used to solve the governing equations and the level set evolution equations. A staggered grid is used and the different dependent variables are approximated at different mesh points. In order to ensure variables more accurately interpolated and revolved, a double fine grid is also applied. The detailed numerical method and technique are described in [7]. A 5th order weighted ENO scheme for discretization of the constitutive equations is applied to achieve higher order accuracy in space, and a third-order Runge-Kutta scheme in time is used to avoid any instability and divergence in temporal integration of configuration tensor evolution equations.

In the initial set-up, the spherical bubble with radius R is set in the middle of the z-axis and the computational domain $\Omega = \left\{ (x,y) \middle| 0 \le x \le 40R, 0 \le y \le 15R \right\}$ is widely enough to avoid wall effect. Regarding the boundary conditions, the outflow boundary is set at the top wall and the no-slip condition is applied for side wall. The configuration tensor for the Oldroyd-B model on the solid wall is expressed in terms of the velocity gradient through solving the momentum and constitutive equations:

$$A_{xx} = 1 + 2\lambda_1^2 \left(\frac{\partial u}{\partial y}\right)_w^2, \quad A_{xy} = \lambda_1 \left(\frac{\partial u}{\partial y}\right)_w, \quad A_{yy} = 1, \quad A_{\theta\theta} = 1$$

The initial value of $\boldsymbol{A}$ is taken as $\boldsymbol{I}$, implying the Oldroyd-B fluid is in a relaxed state.

3. Numerical results and discussion

3.1 Bubble rising in Newtonian fluids

In order to test the accuracy of our fluid flow solver, in particular the numerical treatment of the free-surface boundary conditions. We conducted three case studies and compare the results of the present method with those published literature.

The first validation case is to simulate a bubble rising in Newtonian fluids. The physical properties of air bubbles are $\rho_g = 1.2\ \mathrm{kg/m^3}$ and $\eta_g = 1.8 \times 10^{-5}\ \mathrm{Pa \cdot s}$.

The comparisons of steady-state cases in Figure 1, and Figure 2 indicate good agreement between computational and experimental results. These simulations suggest that our method is effective for investigating the motion of a bubble with very steep gradients in density and viscosity across interface under the laminar flow conditions using an Eulerian grid. The method provides the basis for further investigation of non-Newtonian fluids.

a) calculated shape b) measured shape [Bhaga和Weber, Fig.3(b)][9]

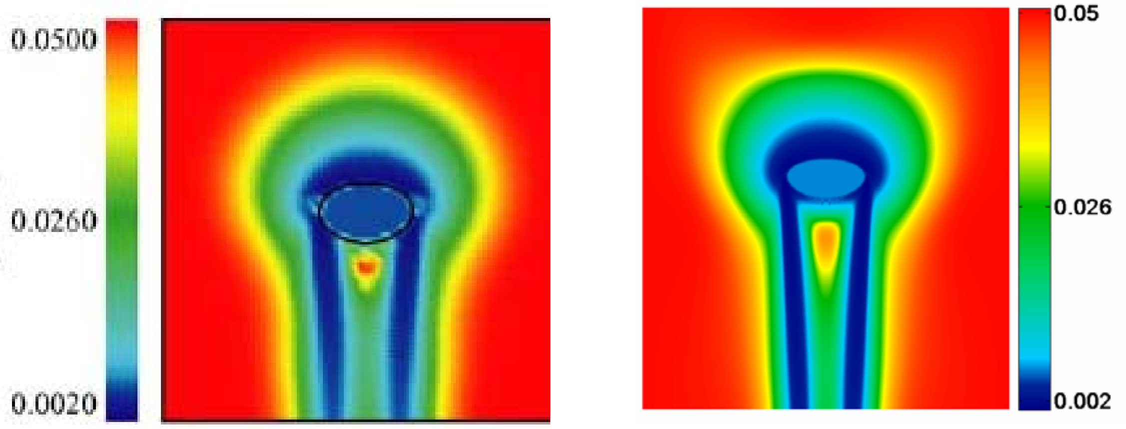
Fig.1. Comparison of the shape of a 9.3 cm^3 bubble in a sugar solution with high viscosity at steady state (E=116, M=266, Re=3.57)

a) simulation b) experiment [Bhaga和Weber, Fig.3(e)][9]

Fig.2. Comparison of the shape of a 9.3 cm^3 bubble in a sugar solution with low viscosity at steady state (E=116, M=1.31, Re=20.4)

3.2 Drop rising in a shear-thinning non-Newtonian fluid

The second validation case is to simulate a Newtonian drop rising in shear-thinning non-Newtonian fluids. Ohta et al. [10] investigated the Newtonian drop (silicone oil) flow in a shear-thinning fluid (sodium acrylate polymer, SAP) with the Carreau-Yasuda model and the VOF (Volume-of-Fluid) method. In this work the level set method for tracking the interface is used to simulate the motion of a drop in non-Newtonian liquids and the predictions are compared with the results of Ohta et al. [10]. Figure 3 compares the predicted viscosity distributions with those in [10] for a drop rising in a SAP solution. It can be verified that the computed viscosity distributions by VOF and the present level set method agree well qualitatively with each other.



(a) VOF[10] (b) Level set

Fig. 3. Comparison of the viscosity distribution (in unit of Pa·s) and shape of a drop rising in Carreau-Yasuda shear-thinning solution (n=0.25, $\lambda = 0.89$ s, $\eta_0 = 0.05$ Pa·s, $\eta_d = 0.006$ Pa·s and d_e=10.7 mm)

Scrutinizing the VOF results in Figure 3, some flow structures of minor scale are observed around the drop surface. It is some kind of so-called "parasite" flows [11], probably arising from inaccurate account for the interfacial force. However, neat flow structure is obtained from our simulation without any interfacial disturbance. In our method, the “parasitic” surface flow is suppressed by adopting a double fine grid for simulating the motion of drops and bubbles and advancing the deformable interface for each time step starting from the interface instead of the boundary of computational domain [7].

3.3 drop rising in a shear-thinning viscoelastic non-Newtonian fluid

The third validation case is to simulate a Newtonian drop rising in a shear-thinning viscoelastic non-Newtonian fluid. An adequate understanding of the flow pattern around a single drop in a non-Newtonian fluid is a prerequisite to studying further phenomena like interaction and coalescence between drops or bubbles. In Figure 4, the flow fields around an individual drop in these fluids has very peculiar features: the flow in the front of the drop is very similar to that in Newtonian case; in the central downstream wake, the motion of the fluid is surprisingly downward; finally, a hollow coneic zone of upward flow begins on the sides of the drop. The real shape of the drop is also plotted in Figure 4. Li et al. [12]. gave the new insights into the flows of shear-thinning viscoelastic non-Newtonian fluids around bubbles (or drops) by means of the PIV measurements in Figure 5. The complete flow field around bubbles shows three distinct zones: a central downward flow behind the bubble, a conical upward flow surrounding the negative zone, and an upward flow zone in front of the bubble. The numerical result of the negative wake is in good agreement with experiments.

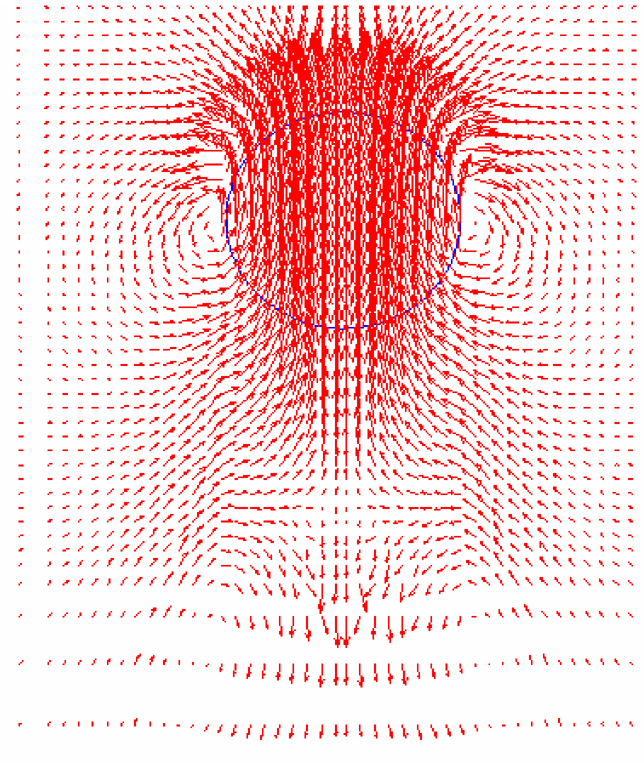


Fig. 4. Simulation results: flow field and shape of a drop rising in shear-thinning viscoelastic solution ($n = 0.25$, $\lambda = 0.89$ s, $\eta_0 = 0.05$ Pa·s, $\lambda_1 = 3.0$ s, $c = 8.0$, $\eta_d = 0.012$ Pa·s and $d_e = 3.06$ mm)

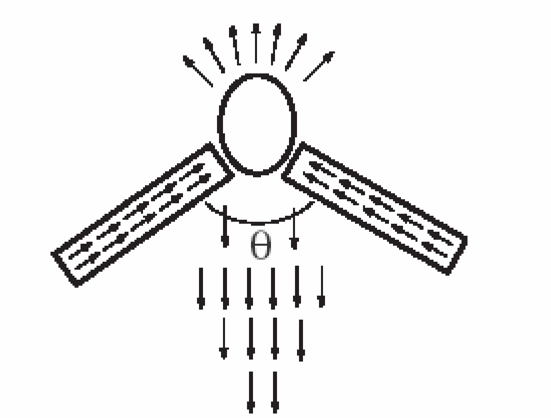


Fig. 5. Schematic representation of the flow field around a drop (or bubble) rising in a shear-thinning viscoelastic fluid. The θ angle is defined as the opening angle of the upward cone[12]

4. Concluding remarks

In this work, an improved level set method based on a staggered Eulerian grid is used to simulate the motion of deformable fluid particles. The proposed method is applied to simulate the rising of a single fluid particle in viscous Newtonian and non-Newtonian liquids. For the motion of bubbles in purely viscous liquids, the current computational scheme shows good numerical stability in simulation of realistic gas/liquid systems. The comparison of simulation with the present and literature experiments shows satisfactory agreements. The newly proposed algorithm is applied to simulate the rising Newtonian drop in shear-thinning non-Newtonian solutions. The comparison of simulation with the available literature results shows satisfactory agreements. The numerical scheme is then used to compute the Newtonian drop rising in shear-thinning viscoelastic non-Newtonian fluids within the framework of an Oldroyd-B model to take into account the viscoelasticity of the fluid. Theoretical flow fields are numerically obtained and compare satisfactorily with experimental measurements for the main features such as the negative wake.

Further theoretical and experimental investigations should be conducted in order to gain new insights into the relationship between the negative wake and the fluid's viscoelasticity. It will also be interesting to couple the level set method with other viscoelsticity models for numerical experiments for studying the bubble's or drop's shape evolution. This is the avenue we are currently exploring.

Acknowledgements

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