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Development and implementation of VOF-PROST for 3D viscoelastic liquid–liquid simulations

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Abstract

We implement a volume-of-fluid algorithm with a parabolic re-construction of the interface for the calculation of the surface tension force (VOF-PROST). This achieves higher accuracy for drop deformation simulations in comparison with existing VOF methods based on a piecewise linear interface re-construction. The algorithm is formulated for the Giesekus constitutive law. The evolution of a drop suspended in a second liquid and undergoing simple shear is simulated. Numerical results are first checked against two cases in the literature: the small deformation theory for second-order liquids, and an Oldroyd-B extensional flow simulation. We then address the experimental data of Guido et al. (2003) for a Newtonian drop in a viscoelastic matrix liquid. The data deviate from existing theories as the capillary number increases, and reasons for this are explored here with the Oldroyd-B and Giesekus models.

Keywords: Drop breakup; Oldroyd-B model; Volume-of-fluid method

1. Introduction

Experimental photographs of a drop of viscous liquid sheared in another in Stokes flow are given in [1–7]. The study of a single drop applies to dilute shear-mixing for which coalescence is negligible [8–13]. The volumes of daughter droplets depend on physical properties and conditions of shear, and affect the rheological properties of the mixture [14–18]. In particular, the gross features of drop size distributions for the case of equal viscosity for Stokes flow have been simulated numerically with a VOF continuous-surface-force (CSF) algorithm [19]. In the context of drop breakup simulations, however, CSF leads to spurious currents and errors, which do not disappear with mesh refinement. Smoothing on a scale large relative to the mesh helps, but is unrealistic in 3D simulations. Smoothing is not needed for the more accurate calculation of interface curvature described in Section 3, the 'parabolic reconstruction of the interface for the calculation of the surface tension force' (PROST) [20].

In this paper, we focus on the development of a viscoelastic liquid–liquid PROST code. A number of experiments have been conducted on the effect of elasticity on the deformation of a drop in a matrix fluid [6,21–23]. They have shown that elasticity affects the amount of drop deformation as well as the angle, which the drop makes with the flow direction. Results reported on experiments in the literature vary in their conclusions. In [21,24], it is reported that viscoelasticity has a major effect on drop elongation, with drop elasticity suppressing deformation and matrix elasticity enhancing it. Numerical computations in [25] show similar trends. On the other hand, recent work by Guido's group [6,26,27] shows that, at low capillary and Weissenberg numbers, drop extension is virtually unchanged by elasticity, in agreement with second order fluid theory, and the main effect of matrix elasticity is to rotate the drop into the flow direction. Outside the range where second order theory is valid, the experiments actually show a decrease in drop deformation when the matrix fluid is elastic. Recent simulations by Yue et al. [28] also show such a decrease at moderate Weissenberg number, while an increase is found at higher Weissenberg number.

We mention in passing that some experiments have also shown new modes of breakup driven by normal stresses, which have no analog in the Newtonian case [29–32]. In these cases, the drop is elastic, and it stretches in the spanwise direction, like a sausage being rolled. This process evolves much more slowly than "ordinary" breakup and seems to be beyond the reach of

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numerical simulations at this point. This effect should not be confused with the minor drop widening in the spanwise direction that is observed in some Newtonian flows [33].

Our computations will focus on the range of parameters covered in the Guido experiments [26]. The results show trends qualitatively consistent with the experiments.

2. Governing equations

We consider shearing flow of a drop surrounded by a matrix fluid. Both liquids are modeled by the Giesekus model. The two liquids may differ in density ρ, solvent viscosity η_s, polymeric viscosity η_p, and relaxation time λ. The total viscosity is denoted $\eta = \eta_s + \eta_p$, and the elastic modulus at time 0 is denoted $G(0) = \eta_p/\lambda$.

The governing equations for the VOF approach are:

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = \nabla\cdot\mathbf{T} - \nabla p + \nabla\cdot(\eta_s(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) + \mathbf{F}, \quad (1)$$

where $\mathbf{T}$ is the extra stress tensor.

The total stress tensor is $\underline{\tau} = -p\mathbf{I} + \mathbf{T} + \eta_s[\nabla\mathbf{u} + (\nabla\mathbf{u})^T]$. The body force is equal to the interfacial tension force:

$$\mathbf{F} = \sigma\tilde{\kappa}\mathbf{n}\delta_s, \quad (2)$$

where σ denotes the surface tension coefficient, $\mathbf{n}$ the normal to the interface, δ_s the δ-function at the interface, and $\tilde{\kappa}$ the curvature $-\nabla\cdot\mathbf{n}$. [34].

The constitutive equation for the Giesekus model is:

$$\lambda\left(\frac{\partial \mathbf{T}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{T} - (\nabla\mathbf{u})\mathbf{T} - \mathbf{T}(\nabla\mathbf{u})^T\right) + \mathbf{T} + \lambda\kappa\mathbf{T}^2 = \lambda G(0)(\nabla\mathbf{u} + (\nabla\mathbf{u})^T). \quad (3)$$

The interface is represented as the surface where a color function:

$$C(\mathbf{x}, t) = \begin{cases} 0 & \text{in the matrix liquid} \\ 1 & \text{in the drop} \end{cases} \quad (4)$$

jumps in value. C is advected by the flowfield. In $\mathbf{F}$, $\mathbf{n} = \nabla C/|\nabla C|, \delta_s = |\nabla C|$. The numerical implementation of the surface tension force will be described later.

2.1. Boundary conditions

The drop is initially spherical with radius a. The walls are located at $z = 0, L_z$, and move horizontally with speeds $\pm U_0$. The boundary conditions at the upper and lower walls impose a shear rate of:

$$\dot{\gamma} = U'(z) = \frac{2U_0}{L_z} \quad (5)$$

in the matrix liquid. Spatial periodicity is imposed in the x and y directions. Additional boundary conditions are not needed for the extra stress components. The computational domain $0 \le x \le L_x, 0 \le y \le L_y, 0 \le z \le L_z$ is chosen so that we minimize the effect neighboring drops and that of the walls. Typically, the distance between the walls is eight times the drop diameter, the spanwise period is four times the drop diameter, and the period in the flow direction is chosen dependent on drop extension. We have found, in these and prior (Newtonian) simulations, that the influence of the boundaries is negligible under these circumstances.

2.2. Initial conditions

The initial flow field is simple shear for both the drop and the matrix fluids. This is $(U(z), 0)$, satisfying $U(z) = U_0(2z - L_z)/L_z$. The stresses are set equal to the values which would prevail in the corresponding steady shear flow with the given shear rate.

This initial condition, used in most of the computations below, corresponds to a drop being placed into a pre-existing shear flow. Alternatively, we can consider a shear flow started up with the drop in place; the difference is that the viscoelastic stresses are initially zero. We shall see some differences between the two cases, as discussed in Section 4.1 below. Even in these comparisons, we took the initial velocity field to be linear and did not consider any transient propagation of shear waves starting from the walls.

2.3. Parameters

The dimensionless parameters are the viscosity ratio (based on total viscosities) $m = \eta_{drop}/\eta_{matrix}$, a capillary number $Ca = a\dot{\gamma}\eta_{matrix}/\sigma$ which measures the competition between the viscous force causing deformation versus capillary force keeping the drop together, a Reynolds number $Re = \rho\dot{\gamma}a^2/\eta_{matrix}$, a Weissenberg number $We = \dot{\gamma}\lambda$ and retardation parameter $\beta = \eta_s/\eta$.

3. Viscoelastic PROST algorithm

A rectangular Cartesian staggered mesh is used. Fig. 1 shows a typical staggered grid cell on which the unknowns are evaluated at different locations as indicated. The u-velocity is centered at the back face, the v-velocity at the left side face, and the w-velocity is centered at the bottom face of the cell. The pressure $p_{i,j,k}$ and the color function $C(i, j, k)$ are located at the center. The diagonal components of the extra stress tensor take values at the center of the cell, while each off-diagonal component is at the mid-point of an edge.

There are two primary features to the solution method: the calculation of the interfacial tension force and the time-integration of the governing equations.

3.1. Calculation of the interfacial tension force

The body force for a grid cell cut by the interface includes the interfacial tension force. When such an interface cell shown in Fig. 2 is encountered in PROST (parabolic reconstruction of the surface tension force), a quadratic surface is fitted through