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Breakup of drops in simple shear flows with high-confinement geometry

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ABSTRACT

The problem of a drop subject to a simple shear flow in high constriction geometry is addressed numerically for different flow conditions. Wall effect on the critical capillary number and drop deformation is analyzed. Under uniform condition, drops in low and moderate Reynolds flows are more stable when the confinement is increased. The critical capillary number is shown to increase for drops more viscous than the medium (viscosity ratio $\lambda = 0.3$) and decreases when the medium is more viscous ($\lambda = 1.9$) or when Reynolds number is increased. A discussion on the accuracy of the numerical method and solutions to typical problems are included for comparison. The drop interface is reconstructed using the piecewise linear interface calculation (PLIC) and transported with the volume-of-fluid (VOF) method, which follows unsplit case-by-case schemes based on the basic donating region (BDR) or the defined donating region (DDR). Surface tension is included with the continuum-surface-force (CSF) model. A high-resolution (SMART) semi-implicit finite-volume discretization is employed in the linear momentum equations. Mass is conserved by following an implicit pressure-correction method (SIMPLEC). The normal vector of the interface is computed from height functions using least squares fitting. The advantage of the DDR scheme lies in its volume-conserving capabilities which have not been exploited in recent investigations.

1. Introduction

Problems involving particle deformation and breakup are commonly observed in many industrial applications and natural processes, leading to vigorous theoretical and experimental research activity in a variety of fields. Fundamental studies in drop dynamics allowed for the understanding of principal mechanisms and the effect of properties, forces and geometry on the deformation. Herein, the scope is limited to the numerical analysis of drop deformation and breakup in simple shear flows using the volume of fluid (VOF) method and the effect of inertia.

When viscous drops are subject to initial deformations, the interface motion behaves like a linear or a damped oscillator, for large values of the Reynolds number, *Re*, and low *Re*, respectively. When external forces are present, like in shearing flows, the motion of the drop is governed by *Re*, capillary number, *Ca*, viscosity ratio, $\lambda = \eta_d/\eta_m$, density ratio, $\gamma = \rho_d/\rho_m$, confinement geometry, among others. In the case of simple shear flows, drops can adopt steady-state shapes or break up into daughter drops, depending on the competing effect of surface-tension, inertia and viscous forces. Typical parameters of interest are the Taylor deformation, *D*, given by $D = (L - B)/(L + B)$, where *L* and *B* are the half-length and half-breadth of the drop; orientation angle θ, which is measured between the drop semi-major axis and the horizontal; critical conditions for breakup or fragmentation; number of satellites; and mechanisms. These parameters are very well documented in the literature [5,6,9,16,21,34,40,47,53,54]. When inertia is present, the drop is expected to break at lower *Ca*.

The numerical study of these and other problems have been performed in the past using several techniques: boundary integral method (BIM), level set (LS) [49], VOF, front tracking (FT) [51], smoothed particle hydrodynamics (SPH), lattice Boltzmann (LB) and hybrid methods like the coupled level-set and VOF (CLSVOF) [48], and the particle-level-set (P-LS) [11], among others. Each method has its own limitations and improvements, normally related to implementation time, accuracy of the solution, mass conservation capabilities and minimal resolution of the subgrid structures. Rider et al. [43] concluded that a level-set methodology does not guarantee volume conservation in highly distorted flows, giving rise to unacceptable errors. Front-tracking methods are very accurate, but they exhibit loss of mass due to non-solenoidal velocity projections; accurate advection of the front points tends to minimize the error produced by changes in the total mass. Furthermore, changes in mass were found to be unacceptably high

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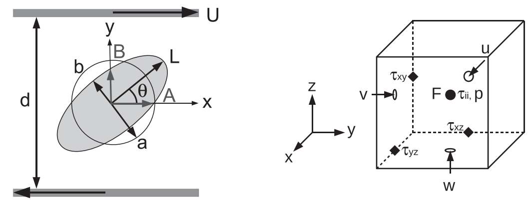
for long-term simulations involving many bubbles or drops where the resolution of each particle is relatively low [50]. Additional techniques aimed at improving computational performance have been successfully applied to compute the surface-tension force and other properties across the interface, like the multi-level methods, formulations based on adapted grids, and the use of unstructured meshes.

Despite all the advances in volume-tracking methods (VOF), there are several disadvantages. For example, traditional and high-order/high-resolution techniques used to solve the advection equation have been shown to degrade the interface thickness and shape, regardless of the order of the scheme [24,25,43], unless special downwinding schemes or interface reconstructions are employed, like in the flux-corrected transport (FCT) algorithm of Rudman [44] or the piecewise parabolic method (PPM) of Miller and Colella [33]. Low-order VOF methods suffer from the so-called "flotsams" or "wisps", which are lumps of dispersed or matrix fluid not fluxed properly. This problem has been mitigated by using redistribution algorithms [17].

The surface-tension force acting on an interface has been successfully implemented with the continuum surface force model (CSF) of Brackbill et al. [4], where the interfacial force is expressed as a force per unit volume. The extent of this force is determined by a discrete delta function which smooths the jump conditions ideally present across an interface. The CSF method yields a continuous pressure distribution across the interface characterized by first-order convergence in space, meanwhile the sharp surface-tension force (SSF) method [14] yields a sharp jump which shows second-order convergence in space. However, both methods show the same error of the spurious currents, which are artificial vortex-like structures created by large body forces that increase flow acceleration. These structures have a larger impact on the region with lower density and may disrupt the interface, conducing to a failure of convergence, even on grid refinement. The spurious currents also depend on other parameters: they reduce slightly when the time step Δt is reduced; they increase slightly when the density ratio ρ_{out}/ρ_{in} is increased; and they reduce considerably by increasing the internal fluid density, following $u \sim \sigma \Delta t E(\kappa)^2/\rho_{in}$, where E is the error in curvature. In the static-drop problem, the magnitude of the spurious currents at the interface depends on fluid properties, $u \simeq C\sigma/\eta$, and the curvature model, but not on the surface-tension model (CSF or SSF), meanwhile the error in pressure depends primarily on the surface-tension model. The constant of proportionality C adopts values of 0.01 in the VOF method of Lafaurie et al. [26], 10^{-4} in the parabolic reconstruction method of Renardy and Renardy [41] (both with uniform properties), and 10^{-5} in the connected marker method of Tryggvason and coworkers [45] (Tryggvason, unpublished lecture notes).

Several multi-dimensional fluxing schemes have been proposed. The first-order defined donating region (DDR) method of Harvie and Fletcher [18] is a piecewise linear scheme that integrates cell boundary fluxes geometrically and provides exact mass conservation. The second-order methods of Puckett et al. [38] and Rider and Kothe [42] increased the complexity by extending the donating region to adjacent cells. Another fluxing strategy is the Stream scheme of Harvie and Fletcher [17], which is a fully multidimensional boundary flux integration technique based on the calculation of the volume of several streamtubes crossing a control surface. The Stream scheme is first to second-order in the single-vortex test, depending on the reconstruction method. Several multidimensional schemes require volume redistribution to conserve mass. High-order multidimensional fluxing schemes have been achieved, like the fourth-order DRACS (donating region approximation by cubic splines) method of Zhang [55].

Among methods that reconstruct an interface following case-by-case procedures are the linear 2D method FLAIR Ashgriz and Poo [2] and the second-order 2D method of Kim and No [23]. Second-order case-by-case reconstructions are in general avoided because of the excessive amount of cases. In 3D, the parabolic reconstruction of surface tension (PROST) method of Renardy and Renardy [41] is second-order and predicts drop deformation and breakup accurately.



(a) Drop deformation (b) Variables in a typical cell

Fig. 1. Problem description and discretization.

When comparing PLIC-based methods, accuracy is determined by the error in the reconstruction step (calculation of the interface normal vector) and the fluxing. A sufficient condition to reconstruct smooth interfaces with second-order accuracy is for the algorithm to reproduce linear/planar interfaces exactly [35]. The method of Youngs computes the normal vector explicitly from the volume fractions and is first-order accurate, while the full least-squares minimization or Swartz' s method is second-order [42]. Other methods that achieve second-order accuracy on smooth interfaces are the minimization methods of LVIRA [37] and ELVIRA [36]. When the interface has sharp corners, second-order methods like ELVIRA reduce their accuracy to first order [55].

An important quantity that determines the accuracy of the solutions in multiphase flows involving surface-tension forces is the curvature. Among different techniques used to compute the curvature, the height function (HF) method offers second-order convergence on mesh refinement [12,14,30,48]. Despite the advances in the field with the HF method since the work of Helmsen et al. [19], hybrid methods, like the "best candidate" method of Liovic et al. [30] that selects the curvature from different stencils/methods, seem to be the solution to overcome the errors incurred when using the traditional HF methods. The largest error in curvature using the HF method occur in regions where the components of the normal vector at the interface are of similar magnitude and when the radius of curvature is comparable to or smaller than the grid size Cummins et al. [10]. By advecting the normal vector, Raessi et al. [39] introduces another approach that produces curvatures with second-order convergence. In comparison, traditional level-set methods show no convergence.

Here, VOF methods are compared using classical problems involving viscous flows. A simplified method to transport the volume fraction, denoted as BDR, is briefly compared with the DDR method. The semi-analytical DDR method here developed is tested for different problems in 3D. The nonlinear oscillation of an initially-deformed drop is studied to show the overall accuracy, robustness and long-term stability. Finally, the deformation and breakup of drops in a simple shear flows is considered for high confinement geometry.

2. Problem formulation

The problem of an isothermal immiscible viscous drop sheared by two closely located walls, as depicted in Fig. 1, is addressed numerically and the critical Capillary number for breakup is sought for different viscosity ratios between the drop and the medium. The classical two-fluid mixture model is considered, where the velocity field is given by a mixture-averaged velocity. The domain is filled with a dispersed phase "d" and a continuous phase or medium "m".