

LETTERS

The purpose of this Letters section is to provide rapid dissemination of important new results in the fields regularly covered by *Physics of Fluids*. Results of extended research should not be presented as a series of letters in place of comprehensive articles. Letters cannot exceed three printed pages in length, including space allowed for title, figures, tables, references and an abstract limited to about 100 words. There is a three-month time limit, from date of receipt to acceptance, for processing Letter manuscripts. Authors must also submit a brief statement justifying rapid publication in the Letters section.

Drop breakup in three-dimensional viscous flows

Vittorio Cristini, Jerzy Bławdziewicz,^{a)} and Michael Loewenberg

Department of Chemical Engineering, Yale University, New Haven, Connecticut 06520-8286

(Received 12 March 1998; accepted 21 April 1998)

A new three-dimensional boundary integral algorithm is presented that is capable of simulating the process of drop breakup in viscous flows. The surface discretization is fully adaptive, thus providing accurate resolution of the highly deformed drop shapes that are characteristic of breakup events. Our algorithm is used to study drop breakup in shear flow and in buoyancy; the predictions are compared with experimental observations. © 1998 American Institute of Physics. [S1070-6631(98)01508-6]

Drop breakup in viscous flows has been the subject of several experimental investigations.¹ However, comprehensive numerical simulations of this phenomenon are present in the literature only for axisymmetric flows.¹

Three-dimensional boundary integral algorithms have been developed for predicting critical conditions for breakup of an isolated drop in steady shear flow.²⁻⁴ Breakup was inferred by the nonexistence of a steady three-dimensional shape. More recent simulations suggest that drop breakup may occur as the result of pair interactions in buoyancy.⁵ However, detailed three-dimensional simulations of drop breakup have been hampered by the difficulties of accurately resolving highly deformed drop interfaces.

The algorithm presented herein overcomes this obstacle and provides the capability for detailed simulations of three-dimensional drop breakup. Such simulations are needed for reliable determination of: (1) breakup criteria in steady and time-dependent flows, (2) breakup times for calculating breakup rates,⁶ and (3) drop fragments for predicting drop size distributions.

Here we use our new algorithm to study the detailed process of drop breakup in shear flow and in buoyancy motion.

Under Stokes flow conditions, drop dynamics are characterized by the capillary number, the Bond number, and the viscosity ratio:

$$\text{Ca} = \frac{\mu \dot{\gamma} a}{\sigma}, \quad \text{Bo} = \frac{\Delta \rho g a^2}{\sigma}, \quad \lambda = \frac{\hat{\mu}}{\mu}, \quad (1)$$

where μ and $\hat{\mu}$ are the viscosities of the continuous and dispersed phases, σ is the interfacial tension, $\Delta \rho$ is the density contrast between the two phases, g is the acceleration of gravity, $\dot{\gamma}$ is the imposed shear rate, and a is the undeformed drop radius. Surface tension gradients associated with adsorbed surfactant are omitted.

The evolution of a deformable drop is described by time integrating the fluid velocity on a set of N interfacial marker

points. Marker point velocities are obtained by solving a second-kind boundary-integral equation over the drop surfaces.⁷ The equation is recast into a singularity-subtracted form for efficient numerical integration,⁸ and solved by simple iterations after purging the eigensolutions.⁷ The normal vector and curvature on the drop interfaces are calculated by a local surface-fitting algorithm.⁵ Our numerical calculations are $O(1/N)$ accurate.

Previous three-dimensional boundary-integral algorithms rely on surface discretization with fixed topology, where the number of marker points and their connections are kept constant during a simulation. However, the number of marker points and the optimal connections needed to accurately resolve the interface depend strongly on the instantaneous drop shape. At only modest deformations, a fixed computational grid becomes highly strained,⁸ highly deformed shapes cannot be described. The adaptive surface discretization that we have developed removes these difficulties. (An alternative grid-restructuring algorithm has been recently proposed by Yon and Pozrikidis.⁹)

In our algorithm, the resolution of solid angle is kept uniform over the drop surface, and is maintained constant during the simulation. For this purpose a marker-point density function

$$n(\kappa) = C_0 \kappa^2 \quad (2)$$

is introduced, where κ is the local curvature and C_0 is a constant that determines the resolution of the interface. We model the grid as a dynamical system of damped massless springs connecting the marker points: each spring has a tension $l - l_0$, where l is the instantaneous edge length and $l_0 \sim n^{-1/2}$ is the equilibrium length. Equilibration velocities of the marker points are determined as the resultant of local spring tensions projected onto the drop interface. The system of springs has well-defined minimum-energy equilibrium states corresponding to zero equilibration velocities of all

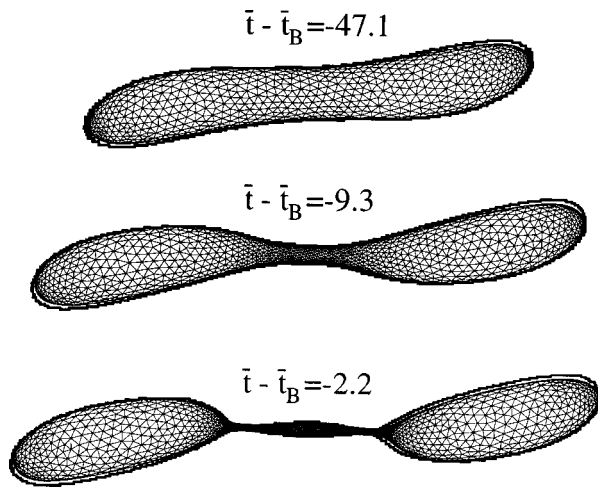


FIG. 1. Drop breakup in steady shear, $Ca=0.48$, $\bar{t}_B=180.2$; length at breakup $\approx 9a$. Simulation ($\lambda=1.38$); experiments of Dr. Guido (heavy curve, $\lambda=1.42$).

marker points. An equilibrium configuration is attained in several iterations after every fluid-dynamic displacement of the marker points.

Optimal marker-point connectivity is maintained by local reconnection. Accordingly, the edge between adjacent triangular elements is switched to connect the two opposite vertices if their distance is shorter. The procedure is similar to a recent grid-restructuring algorithm for finite-element calculations.¹⁰

The desired local density of marker points (2) is maintained by addition and subtraction of points in the regions of the drop surface where tensions $|l-l_0|$ are large. This provides access to the global minimum-energy equilibrium state, corresponding to $l-l_0 \approx 0$ everywhere on the interface.

Our interface discretization is independent of fluid velocity and history of deformation. It maintains nearly equilateral triangulation and optimal marker-point density needed to resolve the interface and accurately calculate the fluid velocity for highly deformed drop shapes characteristic of breakup events.

Grid equilibration is a robust $O(N)$ calculation; the $O(N^2)$ fluid-velocity calculation is time controlling. Thus, by keeping nearly equilateral triangles and minimizing the number of marker points, the efficiency of the simulations is greatly increased.

Previous three-dimensional boundary integral calculations that rely on fixed-grid algorithms with uniform marker-point density cannot resolve the extreme changes in interface geometry that occur during breakup. If N_0 marker points accurately describe a spherical drop, then—with a fixed grid— $N \approx 10^4 N_0$ points are required to describe a breaking drop with a 1% neck width. Detailed drop breakup calculations would therefore be impossible because the CPU time scales¹¹ as $N^{5/2}$.

The examples shown in Figs. 1 and 2 demonstrate that the new algorithm is capable of detailed three-dimensional simulations of drop breakup. The simulations presented require a few days of CPU time on a workstation.

In shear flow, breakup occurs when $Ca=O(1)$. Figure 1

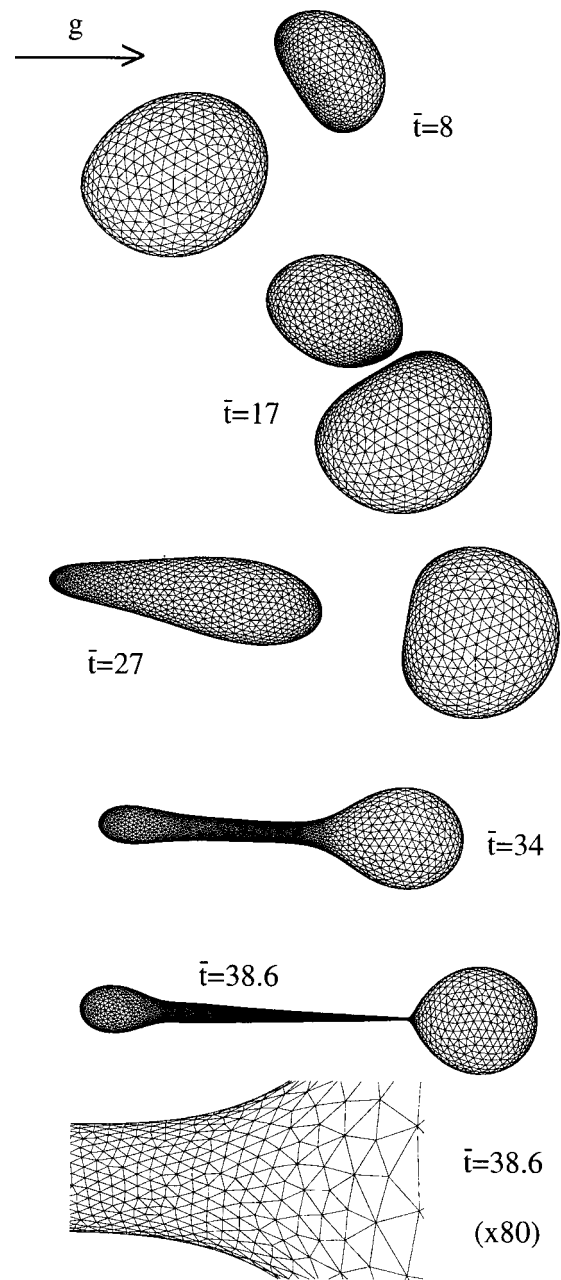


FIG. 2. Drop breakup in buoyancy; $Bo=5$, $\lambda=1$, radius of small drop $0.7a$. Inset shows 80 \times magnification of the neck.

shows a neutrally buoyant drop deforming and breaking in steady shear flow. The predictions of our calculations and digitized experimental observations^{12,13} (Guido, personal communication¹⁴) are compared. Here, time is normalized by the drop-relaxation time $\mu a/\sigma$. The conditions are slightly supercritical thus the drop length increases slowly during much of the evolution and the breakup time is long ($\bar{t}_B=180.2$). As shown in the first two frames in Fig. 1, the neck forms gradually; in the last frame pinch-off is imminent.

Under near-critical conditions, drop dynamics is sensitive to numerical errors, experimental uncertainties in σ , μ , and $\hat{\mu}$ ($\approx 5\%$), and wall effects which are not included in our calculations. Uncertainties in the physical properties were accommodated by setting $\lambda=1.38$ (experimental value: 1.42)

and by increasing the drop-relaxation time by 6%. The predictions closely match the experimental results shown in Fig. 1.

In buoyancy-driven motion an isolated spherical drop remains spherical. However, finite surface tension is required for a deformed drop to regain its spherical shape. Thus for $Bo = O(1)$ interaction-induced breakup can occur.

During pair interactions, the smaller drop deforms more and is thus more likely to burst. Drop (1) imparts a viscous stress $\tau_{1 \rightarrow 2} \sim \Delta \rho g a_1^3 / r^2$ on drop (2) at distance r . The restoring stress on drop (2) is σ / a_2 . The induced deformation of drop (2) is $D_2 \sim \tau_{1 \rightarrow 2} / (\sigma / a_2)$. Similarly, $D_1 \sim \tau_{2 \rightarrow 1} / (\sigma / a_1)$. Thus, we find $D_2 / D_1 = (a_1 / a_2)^2$.

Figure 2 depicts a drop breaking as a result of pair interaction in buoyancy-driven motion. As shown in the first two frames, lubrication stresses between the deformed drops prevent coalescence; the smaller drop slides past the larger one. The third frame shows the smaller drop highly stretched in the straining flow behind the larger one. Surface tension is too weak for the drop to recover: it continues to stretch under the action of buoyancy. As illustrated in the last two frames, a neck forms and pinches off under the action of surface tension. The sequence shown in Fig. 2 is consistent with our observations of centimeter-size silicon-oil drops breaking in corn syrup.

As illustrated in Figs. 1 and 2, the grid remains well-structured during the entire simulation. Nearly equilateral triangles are maintained by edge reconnection and local equilibration. As drop deformation increases, marker points are continuously added (and subtracted) to guarantee constant interface resolution according to the density function (2). For the simulation depicted in Fig. 1, only 162 marker points are used for the initial discretization of the spherical drop ($\bar{r} = 0$); in the last frame of Fig. 1, where pinch-off is imminent, $N \approx 3500$.

The success of the new algorithm is most clearly illustrated by the inset in the last frame of Fig. 2, which reveals the neck of the breaking drop. The neck width is approximately 1% of the initial drop size and yet the local surface resolution is the same as for the modestly deformed drops shown in the first frame. In principle, our new algorithm can describe any drop shape, the only limitation being computational expense.

We developed a new boundary-integral algorithm that involves adaptive grid restructuring which allows detailed numerical simulations of drop breakup in viscous flows. Here the algorithm has been used to study drop breakup in shear flow and in buoyancy. The numerical predictions have been compared with experimental measurements of drop breakup in shear flow.

Our algorithm can be generalized. For example, the marker-point density function (2) can be modified to resolve the lubrication flow between closely spaced drops in concentrated emulsions.⁸

Drop pinch-off occurs with nearly constant neck-thinning velocity¹⁵ $\sim \sigma / \mu$. Thus, the algorithm presented in this letter can be used to predict breakup rates using breakup times obtained by extrapolation. The results of such calculations have application to systems such as sub-Kolmogorov drops in turbulent liquid-liquid dispersions,⁶ where the Reynolds number based on drop size is small.

It should be possible to continue numerical simulations beyond the breakup event to describe the evolving drop size distribution in viscous multiphase flows.

ACKNOWLEDGMENTS

We gratefully acknowledge the experimental data provided by Dr. Stefano Guido. This work was supported by NSF Grant No. CTS-9624615 and NASA Grant No. NAG3-1935.

^{a)}Permanent address: IPPT PAN, Świątokrzyska 21, 00-049 Warsaw, Poland.

¹H. A. Stone, "Dynamics of drop deformation and breakup in viscous fluids," *Annu. Rev. Fluid Mech.* **26**, 65 (1994).

²J. M. Rallison, "A numerical study of the deformation and burst of a viscous drop in general linear shear flows," *J. Fluid Mech.* **109**, 465 (1981).

³R. A. de Bruijn, "Deformation and Breakup of drops in simple shear flows," Ph.D. thesis, Technical University at Eindhoven, 1989.

⁴M. R. Kennedy, C. Pozrikidis, and R. Skalak, "Motion and deformation of liquid drops and the rheology of dilute emulsions in simple shear flow," *Comput. Fluids* **23**, 251 (1994).

⁵A. Z. Zinchenko, M. A. Rother, and R. H. Davis, "A novel boundary-integral algorithm for viscous interaction of deformable drops," *Phys. Fluids* **9**, 1493 (1997).

⁶L. Collins, J. Bławdziewicz, V. Cristini, and M. Loewenberg, "Drop deformation and breakup in isotropic turbulence, 121e," AICHE Annual Meeting, Los Angeles, 1997 (unpublished).

⁷C. Pozrikidis, *Boundary Integral and Singularity Methods for Linearized Viscous Flow* (Cambridge University Press, Cambridge, 1992).

⁸M. Loewenberg and E. J. Hinch, "Numerical simulation of a concentrated emulsion in shear flows," *J. Fluid Mech.* **321**, 395 (1996).

⁹C. Pozrikidis (personal communication).

¹⁰S. O. Unverdi and G. Tryggvason, "A front-tracking method for viscous, incompressible, multi-fluid flows," *J. Comput. Phys.* **100**, 25 (1992).

¹¹M. Loewenberg and E. J. Hinch, "Collision of deformable drops in shear flow," *J. Fluid Mech.* **338**, 299 (1997).

¹²S. Guido and M. Simeone, "Binary collision of drops in simple shear flow by computer-assisted video optical microscopy," *J. Fluid Mech.* **357**, 1 (1998).

¹³S. Guido and M. Villone, "Three dimensional shape of a drop under simple shear flow," *J. Rheol.* **42**, 395 (1998).

¹⁴S. Guido (personal communication).

¹⁵J. Bławdziewicz, V. Cristini, and M. Loewenberg, "Analysis of drop breakup in creeping flows," *Bull. Am. Phys. Soc.* **42**, 2125 (1997).