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Interfacial Fluid Dynamics
and Transport Process

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Preface

Springer Verlag has been pleased to bring out this special volume on interfacial fluid dynamics and transport processes. There are seventeen articles and each article is written in a pedagogical manner dealing with relevant research issues and questions. The intended audience is post-doctoral scientists, academicians and graduate students intending to pursue research and it is our hope that this volume will have lasting value.

Several issues arise within the general field of interfacial transport such as the instability of interfacial processes and driven flows. Instabilities occur when there is a sudden change in the structure of a solution as a control parameter is smoothly varied. They are usually accompanied by a change in the patterns in fluid flow or temperature and concentration fields. Transport phenomena related instability at the interface has much of its origin in the seminal works of Rayleigh who in the later part of the 19th century worked on jets, gravitationally unstably stratified fluid layers, and on the first ideas on convection. Some of these ideas were subsequently modified by the work of Marangoni, Block and Pearson on surface tension driven instabilities. Over the years similar concepts have found place in solidification and melting, electrodeposition, and other phase change problems.

Renewed interest in this subject has occurred because of its applications to materials science, biomedical engineering and space processing. Understanding instabilities is very important as this is related to pattern formation during the processing of materials on earth, in space and related to information technology and the bio-sciences. The first five papers of this volume are related to instabilities at the interface. Four papers are presented on topics of interfacial instabilities due to Marangoni flows in multiple layers or with multiple effects such as double diffusion. A fifth paper gives a tutorial presentation on the instability of spreading films. All of these papers discuss several research issues that have gained importance in recent years.

The next eight papers are concerned with flows that are driven by thermocapillary means. Many of these papers are concerned with the technologically important configuration of the liquid bridge, the numerical calculation of the flows in the bridge and the onset of instabilities from a basic flow state. The eighth paper in this part is concerned with the controlled migration of a droplet on account of thermocapillary effects. All of the articles discuss the physics and provide several helpful references for newcomers to the field.
The last four papers of the volume deal with a variety of very interesting problems that are tied to the general theme of this volume and offer an assortment of topics. A paper on electrocapillary flows acquaints the reader with electric fields that are applied tangentially to surfaces and provides experimental evidence of the phenomena that arise. There is a detailed paper on the numerical simulation of a drop undergoing fragmentation, a problem that is of technological importance in emulsification. This is followed by an article on the stability of emulsions under thermocapillary effects. The volume then concludes with a very helpful article that discusses the energetics of phase change between two fluids.

This volume was motivated by the first International Marangoni Association workshop held on September 12 2001 in the Castle Rauischholzhausen near Marburg in Germany. Despite the unfortunate fateful events that took place the day before, the conference saw the presentation of over 40 papers and posters. A follow-up meeting in Gainesville, FL was held in March 2002 as many U.S. scientists were unable to attend the first meeting. Authors were selected, based on their research interests and presentations to write the articles that are presented in this volume. In short, the reader will get a very good idea of the various facets of interfacial fluid flow and transport from several scholars who have devoted several years of research to this important field.

No meeting can be run successfully without a nominal amount of funding. We are indeed fortunate to have received support from a number of agencies and institutions. We acknowledge with gratitude support from the U.S. National Science Foundation’s Chemical and Thermal Systems Directorate via grant number CTS 0109096, NASA’s Office of Biological and Physical Research, Physical Sciences Division, Code UG via grant number W-24346, The European Space Agency (ESA), WE-Heraeus-Stiftung through Deutsche Physikalische Gesellschaft (DPG) and the Justus-Liebig-Universität Giessen as well as the University of Florida’s Research Foundation and College of Engineering.

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Direct simulation of drop fragmentation under simple shear

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Abstract. The numerical investigation of drop deformation and breakup under simple shear is a basis for theoretical studies of emulsification and mixing. A three-dimensional Couette flow without gravity is considered; the matrix liquid is bounded at the top and bottom by two parallel horizontal plates and the liquid drop is suspended there. The boundaries move horizontally, and generate a simple shear flow. The fluid and flow properties, such as viscosities, Reynolds number and plate separation, influence the subsequent evolution. The pinching off of daughter drops is investigated with the use of volume-of-fluid methods. The convergence of such methods, particularly with respect to drop size distributions, is evaluated, and a novel parabolic reconstruction of the interfacial tension force for the VOF method (PROST) is introduced.

1 Introduction

The study of dynamics of a drop in shear flow is of fundamental importance in dispersion science, and has evoked great interest, most notably since the experiments of G. I. Taylor [21,29]. These processes, which yield daughter drops, are paradigms of theoretical investigations into emulsification and mixing [19]. Emulsions arise in a wide range of industrial applications: in materials processing, waste treatment, and pharmaceuticals [3,16]. There has been considerable interest in incompatible polymer blends because of the need for recycling plastics [9,20]. In order to apply the emulsion technology, we need to control and manipulate its microstructure. A starting point is to consider the deformation and breakup behavior of single droplets in a well-defined flow field [7]. There are several broad categories for making emulsions; one category is shear mixing while adding one fluid to another [19]. The reader is referred to review articles [21,29] on drop breakup under a variety of flow conditions, and to recent experimental studies on breakup under simple shear [8,10,18,33].

In this paper, we focus on the numerical investigation of fragmentation with particular interest on the volumes of the daughter drops. Figure 1 shows a schematic of the initial condition for a numerical simulation. A drop of viscosity $\mu_d$ and density $\rho_d$ is suspended in another liquid of viscosity $\mu_m$ and density $\rho_m$. In this article, we keep the densities the same ($\rho_d = \rho_m$) to simplify the investigation. There is an imposed constant shear rate $\dot{\gamma}$ (the top wall moves in the $x$-direction, and the bottom wall in the opposite direction). The undeformed radius is $a$, the plate separation is $L_z$, and the computational box has periodic
boundary conditions in the $x$ and $y$ directions. There are seven dimensionless parameters: the viscosity ratio of the drop to matrix liquids

$$\lambda = \frac{\mu_d}{\mu_m},$$  \hspace{0.5cm} (1)

the capillary number,

$$Ca = \frac{\mu_m \dot{\gamma} a}{\sigma},$$  \hspace{0.5cm} (2)

the Reynolds number

$$Re = \frac{\rho_m \dot{\gamma} a^2}{\mu_m},$$  \hspace{0.5cm} (3)

the dimensionless plate separation $L_z/a$, and dimensionless spatial periodicities, $L_x$ in the $x$ and $L_y$ in the $y$ directions. We take the densities of the drop and matrix liquids to be the same and focus on the competition between viscous force, capillary force and inertia. The effect of changing other parameters, such as the viscosity ratio, is also interesting but is not touched in this article.

Fig. 1. Sketch of initial condition in our numerical simulation for three-dimensional drop deformation. A drop is suspended in a matrix liquid, and subjected to simple shear generated by the motion of the top and bottom walls.

Taylor [30] gives a detailed description about his experiments with very viscous drops in Stokes flow. This is delved further in section 5 of [5]. We summarize the main features here. Initially, the most noticeable motion is the elongation of the drop, stretched by viscous shear stress in the external flow. The matrix fluid undergoes a flow in the $x$-$z$ plane with velocity

$$\dot{x} = \dot{\gamma} z, \quad \dot{z} = 0,$$  \hspace{0.5cm} (4)

where $\dot{\gamma}$ is a constant shear rate. We decompose this velocity field:

$$\begin{pmatrix} \dot{x} \\ \dot{z} \end{pmatrix} = \frac{\dot{\gamma}}{2} (S + A) \begin{pmatrix} x \\ z \end{pmatrix}, \quad S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.  \hspace{0.5cm} (5)$$
We denote $\mathbf{x} = \begin{pmatrix} x \\ z \end{pmatrix}$. The motion generated by the symmetric matrix $\mathbf{S}$ satisfies

$$\frac{d\mathbf{x}}{dt} = \mathbf{Sx} = \begin{pmatrix} z \\ x \end{pmatrix}. \tag{6}$$

The solution of this system is

$$c_1 e^t \begin{pmatrix} 1 \\ 1 \end{pmatrix} + c_2 e^{-t} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{7}$$

(a) (b)

![Figure 2](image)

**Fig. 2.** In (5), the motion driven by (a) $\mathbf{S}$, (b) $\mathbf{A}$.

Figure 2(a) shows the motion of the fluid, which is pure elongation (stretch), with the axis of elongation along $x = z$. The motion generated by the antisymmetric matrix $\mathbf{A}$ satisfies

$$\frac{d\mathbf{x}}{dt} = \mathbf{Ax} = \begin{pmatrix} z \\ -x \end{pmatrix}. \tag{8}$$

This is a conservative system with the solution

$$x^2 + z^2 = c, \tag{9}$$

where $c$ is an integration constant. Figure 2(b) shows the motion which is pure rotation.

An order-of-magnitude estimate for drop stabilization vs breakup is as follows.
• First, shear stress is continuous across the drop/matrix interface, and this is the order of magnitude of viscous stress. Thus,

\[ \mu_d \cdot \text{rate of elongation in the drop} \]
\[ \sim \mu_m \cdot \text{rate of elongation in the matrix liquid}, \]

which yields that \( \lambda \times (\text{rate of elongation in the drop}) \) is on the order of the rate of elongation in the matrix liquid.

• Secondly, the decomposition (5) shows that in the matrix liquid, the rate of rotation and rate of stretching have similar orders of magnitude:

\[ \text{rate of rotation in matrix} \sim \text{rate of elongation in matrix}. \]

The velocity is continuous across the fluid interface so that

\[ \text{rate of rotation in matrix} \sim \text{rate of rotation in drop}. \]

• From (11)-(13), it follows that \( \lambda \times (\text{rate of stretch in the drop}) \) is of the order of the rate of rotation in the drop. Thus, when the drop is very viscous \( \lambda >> 1 \), the rate of stretch in the drop is small compared to the rate of rotation in the drop; i.e., before the drop can stretch, it has rotated and is pulled in a new direction. The stretching averages out, and the drop attains a steady shape with rotational motion inside the drop. When the drop is infinitely viscous, it cannot elongate and the motion is that of rotation.

• Surface tension \( \sigma \) makes a deformed drop relax back to spherical. There is a competition between the deforming forces and the restoring force, parametrized by \( Ca \). A stationary shape occurs when the deforming viscous force \( \sim \mu \dot{\gamma} \) is much less than the restoring surface-tension force \( \sim \sigma/a \) (\( Ca << 1 \)). When \( Ca >> 1 \), the drop elongates with the flow. As \( Ca \) increases, the drop approaches the critical condition for breakup (\( \lambda = 1 \), Stokes flow):

\[ Ca \sim 1. \]

Figure 3 shows a steady state shape for Stokes flow, with swirling motion inside the drop.

• The critical capillary number is denoted \( Ca_{c} \), above which a steady-state shape ceases to exist.
Fig. 3. Numerical simulation of drop evolution to steady drop shape, with velocity vector plot in the $x – z$ plane through the center of the drop. Stokes flow, $Ca = 0.35$, $\lambda = 1$ [23]. The algorithm is described in section 3.2. This evolution has been checked to be within 1% of the results from the boundary integral code of [6].
The sequence of events for fragmentation in laboratory experiments is described at length in [18]. Figures 4-5 show the main features.

- The drop evolves to an ellipsoidal shape, then to a *dumbbell* shape.
- The necks between the bulbs and the central portion of the drop continue to stretch and thin. There is vortical motion inside the bulbs.
- Next, the bulbs detach. These daughter drops reach steady state because their capillary numbers are a fraction of the critical value. This sequence is known as end-pinching. The first end-pinching results in the largest daughter drops.
- Experimental observations [18] of breakup all begin with a breakup of the elongative end pinching type. If the mother drop is large enough, the ends of the remaining portion will retract slightly due to surface tension, then *bulb up* and end-pinching repeats. If the capillary number is sufficiently high, end-pinching leaves behind a long cylindrical thread, where capillary wave breakups are observed. This results in a distribution of large satellite droplets, interspersed with small droplets.
Fig. 4. Numerical simulation of fragmentation. $Re = 12, Ca = 0.175 = 1.14Ca_c, \lambda = 1, t = 0, 1, 9, 19, 21, 22, 24.4\gamma^{-1}$. The VOF-PROST algorithm described in section 3.2 is used.
In Stokes flow at $\lambda = 1$, the critical capillary number is approximately 0.43. Below this, the stationary shape is found. On the other hand, if we introduce inertia, then a drop can break up for $Ca < 0.43$ [15,22]. At each capillary number, an increase in the Reynolds number elongates the drop. There are three trends for the overall effect of inertia. These are illustrated in Figure 6: velocity vector fields are shown in the $x - z$ cross-section for $Re = 1, 10, 60$.

- First, inertia rotates the drop, so that at higher Reynolds numbers, the steady states are more aligned toward the vertical than in Stokes flow and therefore the drop experiences greater shear.
- Secondly, in Stokes flow, the flow inside the drop consists of a single vortical swirl. When the Reynolds number increases, the velocity field bifurcates, with additional swirls.
- Thirdly, the length of the drop in steady states just below breakup shortens as inertia increases.
- The symmetry across the mid-plane of the steady state, evident in Stokes flow, is lost.
Fig. 6. Velocity vector plot for the cross-section through the center of the drop in the x-z plane, just below criticality. (a) $Re = 1, Ca = 0.27, L/a = 1.8, \theta = 25 \text{ deg}$. (b) $Re = 10, Ca = 0.15, L/a = 1.9, \theta = 23 \text{ deg}$. (c) $Re = 60, Ca = 0.053, L/a = 1.52, \theta = 53 \text{ deg}$.

What is the mechanism for inertia-induced breakup? For large Reynolds numbers, the Reynolds stress is of order $\rho |v|^2 \sim \rho \dot{\gamma}^2 a^2$. This is balanced by capillary stresses of order $\sigma/a$. The critical condition is, upon division by the viscous stress $\mu \dot{\gamma}$,

$$Re \sim 1/Ca. \quad (15)$$
In fact, the ratio of inertial to capillary forces is the Weber number

\[ We = ReCa. \]  

The inviscid limit law is that the critical Weber number \( We_c \sim \text{constant} \) [24].

2 The volume-of-fluid method: try it and you’ll savor the (finite) difference

In the numerical treatment, we must answer three questions: (1) how do we represent the interface on a mesh? (2) how will the interface evolve in time? and (3) how should we apply the boundary conditions on the interface? The VOF method \([1,2,11,14,28,32]\), provides a simple way of treating the topological changes of the interface. The algorithm is a finite-difference code on a Cartesian grid; figure 7 shows the cells. The MAC grid is used. This is a staggered grid for the unknowns; the pressure and the VOF function \( C \) are given at nodes in the center of each cell, and the velocities are given at the centers of the faces.

![Fig. 7. Three dimensional Cartesian mesh with variable cell sizes](image)

There are three components to the overall algorithm: a VOF method to track the interface, a projection method to solve the Navier-Stokes equations on the MAC grid, and a continuum method for modeling the interfacial tension force. We describe these components below.
2.1 The Equations of Motion

The flow is incompressible:
\[ \nabla \cdot \mathbf{u} = 0, \tag{17} \]
and governed by the Navier-Stokes equation:
\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \mathbf{S} + \mathbf{F}, \tag{18} \]
where \( \mathbf{S} \) is the viscous stress tensor:
\[ S_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right). \tag{19} \]

At the fluid interface, velocity is continuous, shear stress is continuous, and the jump in the normal stress is balanced by interfacial tension force. These conditions appear in the VOF method as a body force over the cells which contain the interface. In the Continuous Surface Force (CSF) algorithm, [2,4,27], the body force \( \mathbf{F} \) includes the interfacial tension force \( \mathbf{F}_s \),
\[ \mathbf{F}_s = \sigma \kappa \mathbf{n} \delta_S, \tag{20} \]
where \( \sigma \) denotes the coefficient of surface tension, \( \kappa \) the mean curvature, \( \mathbf{n} \) the normal to the surface, and \( \delta_S \) is a delta function concentrated on the interface.

Fluid interfaces are reconstructed from the values of a color (or VOF) function which represents the volume fraction of one of the fluids in each grid cell:
\[ C(x) = \begin{cases} 1 & \text{fluid 1}, \\ 0 & \text{fluid 2}. \end{cases} \tag{21} \]
This is transported by the velocity field \( \mathbf{u} \). The density and the viscosity in each discretized cell are given by
\[ \rho = C \rho_1 + (1-C) \rho_2, \quad \mu = C \mu_1 + (1-C) \mu_2, \tag{22} \]
for fluids 1 and 2. In equation (20),
\[ \mathbf{n} \delta_S = -\nabla C. \tag{23} \]

When the equations are discretized, the VOF function \( C_{ijk} \) in each \((ijk)\)th cell is equal to the volume fraction of fluid 1. Any cell that is cut by an interface will have \( 0 < C_{ijk} < 1 \). A cell that contains only fluid 1 will have \( C_{ijk} = 1 \) and a cell with only fluid 2 will have \( C_{ijk} = 0 \). This approximates the function which is discontinuous across the interface. Finite differences of \( C \) give derivative values which are used, for example, for the normal, and second derivatives are used for the mean curvature. There are problems with this, because at the continuum level \( C \) is discontinuous. See the discussion below in Section 3.1.
2.2 Temporal Discretization and Projection Method

The momentum equations are first solved for an approximate $u^*$ without the pressure gradient, assuming that $u^n$ is known:

$$\frac{(u^* - u^n)}{\Delta t} = -u^n \cdot \nabla u^n + \left(\frac{1}{\rho}\right)(\nabla \cdot (\mu S) + F)^n. \quad (24)$$

In general, the intermediate flow field $u^*$ does not satisfy the incompressibility equation. It is corrected by the pressure

$$\frac{(u^{n+1} - u^*)}{\Delta t} = -\left(\frac{\nabla p}{\rho}\right), \quad (25)$$

in order to yield a divergence free velocity $u^{n+1}$ at the next time step. The pressure field is not known in this equation, but by taking the divergence of this equation, it is found to satisfy a Poisson equation,

$$\nabla \cdot \left(\frac{\nabla p}{\rho}\right) = \nabla \cdot u^* \Delta t. \quad (26)$$

In the problems we address below, the boundary conditions for the velocity are periodicity and the Dirichlet condition.

For this explicit method, the time step should be less than the viscous time scale, $\rho h^2/\mu$, where $h$ denotes the mesh size, $\rho$ the density, $\mu$ the viscosity. Therefore, simulations of low Reynolds number flows typical of very viscous liquids, are subject to strict stability limitations and are expensive. In order to overcome this difficulty, an unconditionally stable semi-implicit scheme [13–15] has been incorporated. In comparison with the explicit scheme, the speed-up is twenty-fold or more in the simulations shown in this paper.

2.3 Advection of the Interface

Since we lose interface information when we represent the interface by a volume fraction field, the interface needs to be reconstructed approximately in each cell. To do this, the Piecewise Linear Interface Construction (PLIC) method is used. For a review of interface representation methods see [12].

The normal $n$ to the interface is calculated in each cell, since this determines one unique linear interface with the volume fraction of the cell. The discrete gradient of $C$ yields:

$$n = \frac{\nabla h C}{|\nabla h C|}. \quad (27)$$

The second step of the VOF method is to evolve the volume fraction field $C$. The Lagrangian method is the natural choice for interface evolution. In this scheme (figure 8), once the interface is reconstructed, the velocity at the interface is interpolated linearly and then the new interface position is calculated via

$$x^{n+1} = x^n + u(\Delta t). \quad (28)$$
Fig. 8. The Lagrangian method illustrated for a 2D mesh. The shaded polygon represents the portion of the central cell occupied by the fluid. The broken line shows the polygon position after advection in the local velocity field (represented by arrows). The fluid is redistributed between neighboring cells, which are partially overlapped by the new polygon.

Fig. 9. Evolution of length and breadth of a drop undergoing oscillatory shear. Circles represent experimental data [17] and the line is the numerical simulation.

2.4 Results

Numerical simulations for drop deformation under oscillatory shear is shown in figure 9. The figure gives a good comparison with experimental data. Here, the top and bottom walls oscillate with speeds \( u = U \cos(\omega t) \) and \( u = -U \cos(\omega t) \), respectively. The experimental data were taken by S. Wannaborworn [17] with certain polymeric fluids: PDMS as the drop and PIB as the matrix phase. The frequency is 0.3Hz (\( \omega = 2\pi(0.3) = 1.88 \) per second), and the percentage strain
(i.e. the maximum relative displacement of the boundaries divided by their distance) is 250%. The initial drop diameter is 30.175 mm. The data are taken from a top view: The plots show the major and minor axes of the deformed ellipsoid, respectively. The interfacial tension between these two polymers reported in the literature is 2.3-4 mN/m. The numerical simulations are performed for 4 mN/m, because the effect of varying surface tension over the interval of values is found to be small. The viscosity ratio is approximately 1 and the viscosity is 80 Pas.

The first daughters detach in a flow where the horizontal velocity is significant, as well as capillary effects which come into play to detach them. Simulations with mesh refinement on the volumes of the first daughters agree well. Next, we enter a regime where the capillary effects becomes more and more significant compared to the magnitudes of the velocity field. After the first daughter drops detach, the neck undergoes its fragmentation. Figure 10 shows the final states after fragmentation of the neck, which occurs after the first daughter drops have pinched off and moved out of the picture. These are snapshots taken from the top of the computational domain for a variety of mesh refinements. The small satellites which come off of the first neck just after the first daughters pinch off are the ones farthest from the center; these are on the scale of the mesh every time, so that the spatial resolution is not enough to get them correctly. This influences what happens to the rest of the neck because the evolution is sensitive to the volume that is left. Typically, breakup results in small moons between larger drops. It is clear that the high curvature that results at the first pinch-off degrades the subsequent numerical simulation.

3 That’s incurable! (unless you devise a sharp-interface VOF algorithm)

3.1 Calculation of surface tension force from finite differences of the VOF function

One weakness of the VOF-CSF algorithm is that when the capillary force is the dominant physical mechanism, there is lack of convergence with spatial refinement, or convergence to a solution that is slightly different from the exact solution [23]. There are a number of examples in the literature; one is the simulation of breakup of the neck of the drop after the first daughters pinch off. The creation of the first daughters is in a shear-dominated regime, after which the neck retracts slightly, and then more fragments are created in a flow field with less shear [26].

At the continuum level, the VOF function $C$ satisfies equation (21), and the surface tension force satisfies equations (20)-(23). $C$ is discontinuous across the interface.

The approximation of derivatives of a discontinous function by finite differences converges only weakly. The expression for the surface tension force, however, is nonlinear, and weak limits cannot be interchanged with nonlinear
Fig. 10. \( Re = 12, Ca = 0.175 = 1.14Ca_c \), top view. Fragmentation of the neck after the first daughter drops have detached and moved out of the picture. Mesh refinement from top down: \( \Delta x = \Delta y = \Delta z = a/8 \), \( a/12 \) \((t = 26\gamma^{-1})\), \( a/16 \) \((t = 27\gamma^{-1})\), \( a/20 \) \((t = 27\gamma^{-1})\), \( a/24 \) \((t = 29\gamma^{-1})\). VOF-CSS is used. Timesteps \( \Delta t = 10^{-3} \).
functions. One attempt to get around the dilemma of having to take finite differences of a discontinuous function is to change the discontinuous function to a smooth one [2,31], and mollify the VOF function in equation (20)

$$\tilde{C}(x) = \int_{\Omega} C(x')\phi(x' - x, \epsilon)dx',$$

where $\phi(x, \epsilon)$ is a kernel. This kernel is smooth and is zero outside of $\Omega$, which denotes a region local to the interface. This region must include many cells surrounding the interface, and the mollification must take place on a length scale that is much smaller than physical length scales in the problem. This requires a very fine mesh, not feasible in three dimension. In addition, mollification introduces new complications, diffusing the surface tension force; a weakness that affects regions of high curvature, e.g., when the neck of the drop thins out just before pinch-off of fragments. If there are regions of high curvature in the flow, those are usually the places where interesting things happen and accuracy is important. Moreover, if we include new physics into the code, such as surfactants [25], any inaccuracy in the surface tension force will produce unphysical solutions.

The moral of this is that we cannot win the game if we rely on finite differences of the VOF function to give curvature.

**Spurious currents** A well-known example of inaccuracy in VOF schemes that rely on finite-differencing the VOF function is shown in this section. A spherical drop with non-zero interfacial tension is suspended in a second liquid of the same density and viscosity. The boundary conditions on the computational box are zero velocity. The initial velocity is zero. The exact solution for this problem is that the drop stay the same with zero velocity for all time.

The equations which matter in the numerical simulation are:

$$\mathbf{F}_s = \sigma \kappa \mathbf{n} \delta_S,$$

where $\mathbf{n} \delta_S = -\nabla C$, which is balanced by the pressure field:

$$\mathbf{F}_s = -\sigma \kappa \nabla C, \ \nabla p = -\mathbf{F}_s. \quad (30)$$

Therefore, $\mathbf{F}_s$ is a gradient when the interface is the exact solution, a sphere (constant $\kappa$). The surface tension force is cancelled by the pressure gradient; at the discrete level, this holds if the same finite difference approximation is used for $\nabla C$ and $\nabla p$. This is the case, and also in commercial codes. Where is the inaccuracy? Equation (30) shows that the crucial ingredient for avoiding spurious currents is an accurate approximation of the curvature (among other things).

Figure 11 shows the spurious currents from a VOF-CSF simulation, and these currents arise in all VOF methods prior to VOF-PROST. The magnitude and location of the currents remain the same when the mesh is refined. If the user is naive, then these simulations give the appearance of a spatially converged solution. The Ohnesorge number

$$Oh = (Ca/Re)^{1/2} = \frac{\mu^2}{\sigma \rho a} \quad (31)$$
expresses the ratio of viscous effect to capillary and inertial effects. For instance, when the matrix liquid is a gas, and when surface tension is high, the Oh for the gas is small; spurious currents would be noticeable. Spurious currents are small when Oh is sufficiently large.

Fig. 11. CSF, velocity vector plot across centerline in the x-z plane at 200th timestep, $\Delta t = 10^{-5}$. These show the locations of the spurious currents with mesh refinement, $\Delta x = 1/96$ (a), 1/128 (b), 1/160 (c). The simulation does not converge to the exact solution (zero velocity) with spatial refinement.
3.2 Calculation of surface tension force with a sharp-interface algorithm

To our knowledge, VOF-PROST (Proper Representation Of Surface Tension) is the first sharp-interface VOF code for 3D simulations. PROST is detailed in [23] and we summarize the main features here. If a cell is intersected by the interface, we call it an interface-cell.

PROST

- reconstructs the interface in each interface-cell from a least square fit of a paraboloid to the values of the color function in the given cell and its neighbors. There are 27 neighboring cells per interface-cell in 3D. This is the most time-consuming part of the code.
- calculates the curvature directly from this quadratic surface;
- avoids any numerical differentiation of the discontinuous VOF function;
- implements a more accurate interface advection scheme than the one used before (Lagrangian, PLIC).

Results on the spurious currents of section 3.1 Table 1 shows the $L_{\infty}$, $L_{2}$ and $L_{1}$ norms of the velocity field for the spurious currents discussed in section 3.1. While the $L_{\infty}$ norm gives the maximum speed, the $L_{2}$ and $L_{1}$ norms indicate a measure in an average sense for the PROST. The entries in the table are converged with respect to temporal discretization.

For the CSF method, mesh refinement does not decrease the spurious currents in any of the norms. In fact, they increase slightly in $L_{\infty}$ and $L_{2}$ and stay about the same in $L_{1}$. To understand this, figure 11 shows the two-dimensional cross-section of the drop in the x-z plane. The spurious vortices are present at the same positions and spread over the same amount of the domain for all the meshes.

For the PROST method, spurious currents are so small that they are effectively not present. This is no surprise. As we pointed out earlier, there would be NO spurious currents if curvature were constant, and our initial interface were a sphere. The only reason the curvature is not exactly constant is because the least square fit approximates the sphere as piecewise paraboloids. The magnitude for the $\Delta x = 1/96$ mesh is $1/100$th that of CSF, and thereafter decreases with mesh refinement with $O(h)$, $h = \text{Max} \{ \Delta x, \Delta y, \Delta z \}$, to the exact solution.

Results on stationary drop evolution Figure 3 shows the stationary configuration for Stokes flow at $Ca = 0.35$, $\lambda = 1$. Figure 12 compares the temporal evolution of its length/radius to steady state, for VOF-CSF, VOF-PROST and the boundary integral code of [5]. The CSF output remains 3% away from the solution of the boundary integral method, whereas the PROST output converges to it.

Results on fragmentation Figure 13 shows a simulation for fragmentation for different mesh sizes (and different computational domain sizes). The flow
Table 1. Norms of velocity at 200th timestep, $\Delta t = 10^{-5}$.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>$L_\infty$</th>
<th>$L_2$</th>
<th>$L_1$</th>
<th>method</th>
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Fig. 12. Evolution of (half-length/initial-radius) for boundary integral method for $Ca = 0.35$, Stokes flow. Boundary integral method (line); VOF-PROST and VOF-CSF. [23]

parameters correspond to that of figure 10, but here there is convergence on the volumes of the fragments.
Fig. 13. Re = 12, Ca = 0.175 = 1.14Ca_c, top view. Fragmentation, including the first daughters. Mesh refinement $\Delta x = \Delta y = \Delta z = a/12$ (top), $t = 22.5\dot{\gamma}^{-1}$, computational box $2.5 \times 0.5 \times 1$. Lower: $a/16$, $t = 24\dot{\gamma}^{-1}$. Computational box $3 \times 1 \times 1$. VOF-PROST. $\Delta t = 10^{-3}$.

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