Two-Dimensional Navier-Stokes Simulation of Deformation and Breakup of Liquid Patches

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(Received 21 February 1995)

The large deformations and breakup of circular 2D liquid patches in a high Reynolds number (Re = 1000) gas flow are investigated numerically. The 2D, plane flow Navier-Stokes equations are directly solved with explicit tracking of the interface between the two phases and a new algorithm for surface tension. The numerical method is able to pursue the simulation beyond the breaking or coalescence of droplets. The simulations are able to unveil the intriguing details of the nonlinear interplay between the deforming droplets and the vortical structures in the droplet's wake.

PACS numbers: 47.55.Dz, 02.60.Cb

The dynamical processes leading to the breakup of a single lump of fluid into several pieces and, conversely, the coalescence of several pieces into a single one have captured considerable attention from both the theoretical [1–3] and experimental side [4–6]. From the theoretical point of view, much of the interest stems from the fact that breakup and coalescence provide eminent examples of topological singularity formation in hydrodynamic systems. Practical interest is even more evident if one thinks of the enormous wealth of physicochemical phenomena in which drop formation and breakup play a crucial role. The merging of galaxies, spray vaporization combustion in diesel engines, and deformation of biological cells are just but a few representative examples. In many instances the primary question is just to assess under which conditions do breakup and coalescence occur. However, it is clear that the exploration of what happens after breakup or coalescence is of paramount importance to deepen our understanding. The latter question is even more formidable, but the numerical simulations presented in this Letter should offer a preliminary answer.

The physics of drop deformation and breakup is governed by the competition between hydrodynamic stresses, viscous or inertial, which act to deform the droplet, and surface tension, which opposes an increase of the surface area, and thus tends to restore weakly deformed objects to a spherical shape.

In this Letter we present simulations of droplets of liquid moving about in a gas environment. The mathematical idealization of this problem is that of a 2D, incompressible Newtonian flow with surface tension on the interface and viscous dissipation in the bulk. The momentum balance equations are the Navier-Stokes equations for an incompressible fluid of variable viscosity

$$\rho(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \nabla\cdot(\mu\mathbf{E}) + \nabla\cdot[\sigma(\mathbf{I}-\mathbf{n}\otimes\mathbf{n})\delta_S], \quad (1)$$

where $E_{ij} = \partial_i u_j + \partial_j u_i$ is the strain tensor rate, $I_{ij} = \delta_{ij}$ the unit tensor, δ_S a distribution concentrated on the interface, $\mathbf{n}$ the normal to the interface, and σ the surface tension coefficient. The fluid density ρ and the viscosity μ are constant in each phase but vary from phase to phase. The specific form of the surface tension term used is equivalent to the more classical Laplace law [7,8]. We consider incompressible flow with $\nabla\cdot\mathbf{u} = 0$, and the interface moves at a normal velocity $U_I = \mathbf{u}\cdot\mathbf{n}$. In addition to these equations, a condition is needed for the reconnection of interfaces. In a real flow, this reconnection is a complex process, involving long range molecular interactions between interfaces. It is impossible with current computing capabilities to simulate both the large scale, high Reynolds flow around a droplet and the molecular interactions. The pragmatic alternative is to introduce a cutoff scale δ_C below which one will not attempt to model the interface physics. Such a cutoff is consistent with the spontaneous behavior of the volume of fluid methods described below, in which liquid sheets of thickness smaller than the mesh size h tend to break.

Taking as a length scale the diameter D of the droplet and a characteristic speed U of the flow, the problem has four dimensionless numbers, the gas and liquid Reynolds numbers $\mathrm{Re}_i = \rho_i UD/\mu_i$, $i = L, G$, the gas Weber number $\mathrm{We}_G = \rho_G U^2 D/\sigma$, and the density ratio ρ_L/ρ_G. Experiments show that droplets suddenly placed in a high speed flow break when We_G is between 10 and 20 [9,10]. Several droplet breakup regimes have been identified [11,12], and the basic theory involves various instability mechanisms for the liquid gas surface [13,14], following the pioneering work of Taylor [15]. We are not aware, at this date, of numerical simulations of this problem beyond relatively small droplet deformations. However, it must be noted that simulations exist in the limit of vanishing Re_i [4].

We used the method described in [8,16]. A first order in time explicit integration of Eqs. (1) was performed using the MAC staggered finite difference grid for the momentum balance equation. The 2D version of the method was used in order to achieve calculations on larger grids. The incompressibility condition is accurately met by a projection method [17] with the help of a

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multigrid algorithm [18]. Surface tension is implemented in a momentum conserving way, via the introduction of a nonisotropic stress tensor concentrated near the interface [8]. This representation of surface tension stresses is especially interesting for the simulation of breakup, since it avoids the singularity which would occur in the continuum limit when interfaces change topology and the curvature becomes locally infinite.

The velocity field **u** obtained at each time step is used to propagate the interface using the volume of fluid method: the location of the interface is represented by the volume fraction C_{ij} of fluid 1 in the computational cell i, j [16,19–21]. We have $0 < C_{ij} < 1$ in cells cut by the interface and $C_{ij} = 0$ or 1 away from it. The propagation of the interface at velocity U is performed in several steps. In a first step, the interface is reconstructed in each cell independently. Linear segments of the slope approaching that of the interface are constructed, in the so-called piecewise linear interface construction (PLIC). The construction uses a local interface normal **n** estimated using an 8 point (in 2D) centered finite difference of C_{ij}. In a second step, the interface motion is calculated in a Lagrangian manner with velocities obtained by linear interpolation. Finally the volume fractions are recalculated. With the PLIC method [16,19–21], the position of the interface is reconstructed with errors of order $\mathcal{O}(\kappa h^2)$, where κ is the local curvature, for the position of the interfaces, and thus more accurately than in most volume fraction methods, including that of Ref. [8]. During the simulations, we observe that only a very small fraction of the mass is lost. In the complex case of Fig. 3 this fraction is less than 2×10^{-3} over the entire simulation.

We performed our simulations in a square periodic box of size $5D \times 5D$. The simulation was initialized with a uniform velocity U in the gas and the liquid droplet at rest. In all simulations reported here we kept $\mathrm{Re}_L = 2000$, the liquid to gas density ratio $\rho_L/\rho_G = 10$, and $\mathrm{Re}_G = 1000$. Several droplet deformation and breakup scenarios have been unveiled for varying We_G. The first scenario is shown in Fig. 1. As a result of the presence of two rear vortices engendered by the droplet motion, a concavity develops in the droplet surface which takes a typical "banana-shaped" configuration, with its concave side facing downstream [Figs. 1(b) and 2]. These vortices further stretch the droplet until rupture occurs near the tips. The coherent structures in the wake of the droplet are characteristic of 2D turbulence. A boundary layer develops on the front of the droplet as predicted by Taylor [15]. However, at this We_G the boundary layer is stable.

The "mother" droplet may again break in a similar fashion thus generating additional children droplets. Alternatively, if We_G is sufficiently high then second-generation droplets may also breakup, producing third-generation droplets in a kind of bifurcation cascade. Moderate resolution (256^2) and high resolution (512^2) simulations exhibited similar results.

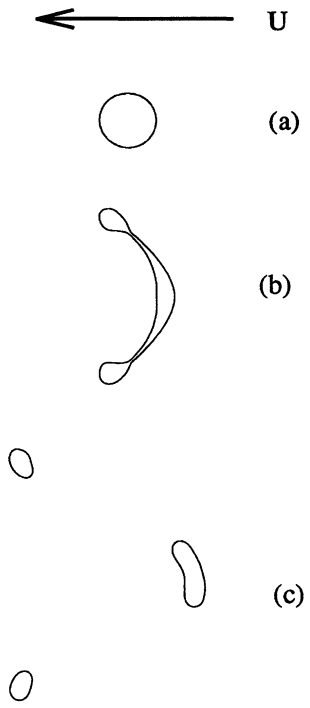

FIG. 1. Simulations of droplet breakup for $\mathrm{We}_G = 10$. 512^2 grid points in a periodic box are used.

Simulations at larger Weber numbers such as the $\mathrm{We}_G = 100$ simulation of Fig. 3 show the formation of much smaller scale structures. The droplet forms elongated filaments. The boundary layer on the front side of the droplet is now unstable, and hornlike structures typical of the Kelvin-Helmholtz instability are seen to grow while they are transported downstream [see Fig. 3(b)].

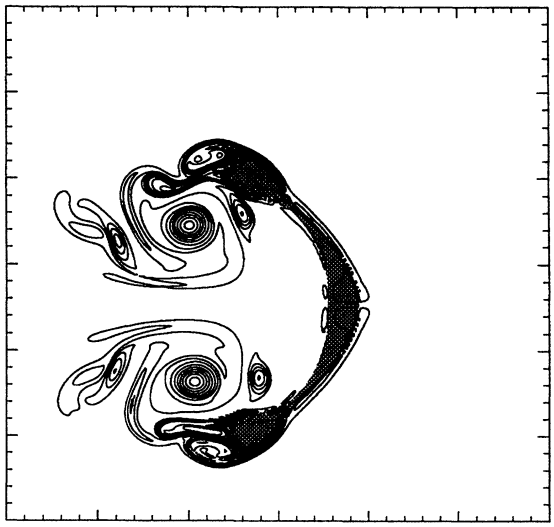

FIG. 2. Same as Fig. 1(b), but with vorticity contours shown.

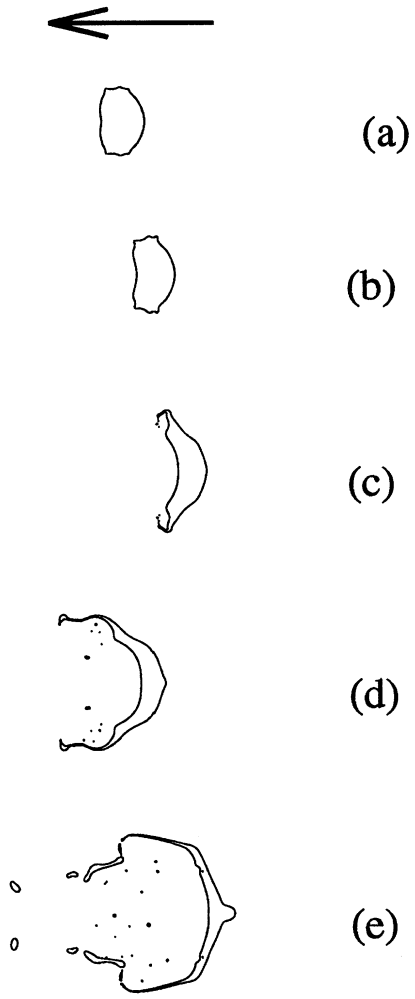

FIG. 3. Simulations of droplet breakup for $We_G = 100$.

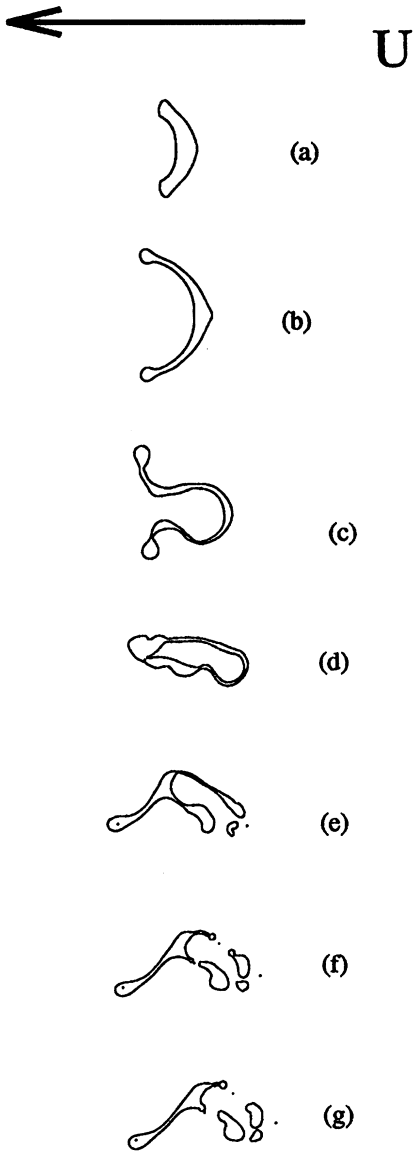

FIG. 4. Simulations of droplet breakup for $We_G = 20$.

Yet another mechanism is shown in Fig. 4. There the droplet elongates, then makes a bag with its concave side facing downstream. The bag closes, then breaks on the upstream side before yielding several separated droplets.

The simulation, although 2D, may be qualitatively compared to the experimental results. There are qualitative similarities, such as the breaking near the tips in Fig. 1(b) or the bag formation. The $We_G = 100$ simulation shows the sheet stripping mode mechanism reported by [12] for $100 < We_G < 350$. The most important difference occurs at $We_G = 10$ where in experiments the concave side faces mostly upstream. We believe that this difference arises because of the initial conditions we use, which result in a jump of the velocity—a vortex sheet—at the interface. This vortex sheet rolls up behind the droplet and creates structure seen in Fig. 2. Work is in progress to investigate the influence of initial conditions.

In conclusion, the results highlight the power of advanced numerical techniques to unveil the fascinating complexity resulting from the nonlinear interplay between gas-liquid interface and gas vortex motion. In particular, the crucial role played by coherent vortical structures suggests that the inclusion of the Re_G dependence is key to the formulation of more advanced and realistic breakup criteria. On the other hand, these results also indicate that caution is needed before the results provided by the numerical tool can be effectively converted into quantitative information of engineering interest, such as phase diagrams and similar data.

One difficulty rests with the slow convergence of such calculations with the number of grid points. In some regimes, the lower resolution experiments produce a similar picture as provided by higher resolution ones, the main

difference being that transitions in phase diagrams occur at different We_G. In some instances, however, genuinely new mechanisms arise: The bag mechanism of Fig. 4 was observed only in 512^2 simulations. A second difficulty is the two-dimensional nature of these calculations. As is well known, coherent vortical structures behave quite differently in two with respect to three dimensions, and so should breakup mechanisms. The Rayleigh instability, which plays such an important role in the final stages of capillary driven breakup [5], is absent in 2D. (However, this may affect only the smallest scales of a large We breakup.) Despite these difficulties, we regard two-dimensional simulations as a very useful warmup for more realistic three-dimensional investigations. While the former are already rather computationally expensive (about 3 CPU seconds per time step for a 512^2 resolution on a IBM RS/6000 mod. 590 workstation), the latter set a pressing demand for high-resolution computations requiring the use of the most powerful present-day supercomputers.

DRET, CNES, and SEP are gratefully acknowledged for their funding. The authors wish to thank Daniel Lhuillier for illuminating discussions. S. S. wishes to thank LMM for their kind hospitality and financial support.

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