

Role of inertia in two-dimensional deformation and breakdown of a droplet

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We investigate by lattice Boltzmann methods the effect of inertia on the deformation and breakdown of stability of a two-dimensional fluid droplet surrounded by fluid of equal viscosity (in a confined geometry) whose shear rate is increased very slowly. We give evidence that in two dimensions inertia is *necessary* for the loss of stability, so that at zero Reynolds number there is always a stable stationary droplet shape. We identify two different routes to breakdown, via two-lobed and three-lobed structures and give evidence for a sharp transition between these routes as parameters are varied.

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The role of inertia in the deformation and loss of stability of a droplet in a shear flow remains an open problem in fluid mechanics. In three dimensions (3D), a droplet in a steady shear field will cease to have a stable shape at a critical capillary number $Ca \approx 0.5$ even without inertia [1]. Crudely speaking, this happens when it is deformed enough to undergo the Rayleigh instability, which is the peristaltic instability of a long tube of one static fluid in another, driven by interfacial tension. In three dimensions this loss of stability of the steady-state droplet shape (which we call breakdown) leads in finite time to the hydrodynamic fission of the droplet (often called breakup). Ca measures the relative importance of viscous to interfacial forces; the effect of inertia, whose importance is quantified by the Reynolds number Re , is essentially perturbative. Thus, although situations arise where a droplet that would be stable at zero Re is unstable at a finite Re , this really amounts to an inertia-induced shift of the critical Ca . The contribution of inertia was studied in recent numerical work [2–5]. Much of this work uses a flow protocol based on sudden onset of shearing at different flow rates, rather than a gradual ramping up of the rate; this saves much time numerically but describes a distinct physical situation from the slow ramp studied here; both are of interest experimentally.

The situation is somewhat different in two dimensions. Although not realizable directly in laboratory experiments, this case is more accessible by simulation [6,7], and is interesting because the nonlinear physics involved may not be the same as in 3D. In 2D, the Rayleigh instability is effectively switched off, because periodic variations in the width of the droplet (at fixed volume) always increases the amount of interface. Also, in 2D breakdown (loss of steady-state stability) is distinct from breakup (droplet fission): breakdown leads to the formation of a long neck that might in principle elongate and thin indefinitely. In practice this will pinch off, albeit through a nonhydrodynamic mechanism, once the two interfaces get close enough. (When “breakup” is referred to below, this is what we mean.) In the present work we study numerically in 2D the breakdown of stability of a droplet, and find quite distinctive nonlinear physics, in which inertia

plays an essential part. The relatively moderate demands of two-dimensional simulations allows us to establish the scenario relatively clearly, even for the case of an “infinitesimal” ramp, which we here approach numerically by a recursive updating scheme for the flow rate.

Method. We use the lattice Boltzmann (LB) method to simulate a (symmetric) binary fluid deep within the two-phase region. The phase separation of the order parameter ϕ is induced by a chemical potential $\mu = A\phi + B\phi^3 - \kappa\nabla^2\phi$ derived from a ϕ^4 Landau free energy [8]. The evolution equation for the order parameter is

$$\partial_t\phi + \mathbf{u} \cdot \nabla\phi = M\nabla^2\mu \quad (1)$$

with M being a mobility; this is coupled with a Navier-Stokes equation

$$\rho(\partial_t\mathbf{u} + \mathbf{u} \cdot \nabla\mathbf{u}) = -\nabla p + \phi\nabla\mu + \eta\nabla^2\mathbf{u}, \quad (2)$$

where \mathbf{u} is the fluid velocity, ρ its density, and η is the viscosity. The interfacial tension is included in this model through the gradient terms in the chemical potential and it is given by $\sigma = (2A/3B)\sqrt{-2\kappa A}$. Note that topological reconstructions of the fluid-fluid interface are handled implicitly by the order parameter diffusion and no singularity is encountered at breakup. Care was taken with parameter selection to ensure that the droplet behavior is dominated by hydrodynamic and capillary forces, except very close to the breakup point, where both diffusion and an interaction arising from the finite breadth of the interfaces (a few lattice spacings) kick in.

In our simulations, we first set up a droplet of fluid in a surrounding immiscible phase of the same viscosity. To impose a shear flow with strain rate $\dot{\gamma}$, we introduce moving walls at the top and bottom edges of the simulation cell with opposite velocities $\pm L\dot{\gamma}/2$ where L is the cell width. A droplet in such a shear profile will deform with the flow until and unless the viscous stress is balanced by interfacial tension. The ratio of these forces is expressed in the capillary number

$$Ca = \frac{\eta\dot{\gamma}R_0}{\sigma}, \quad (3)$$

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where R_0 is the radius of the undeformed droplet; the Reynolds number measures the ratio of inertial and viscous forces:

$$\text{Re} = \frac{\rho \dot{\gamma} R_0^2}{\eta}. \quad (4)$$

We quantify the deformation of a droplet by calculating the following moments of the order parameter field

$$b = \sum_{\mathbf{x}} \theta(\phi) \phi, \quad (5)$$

$$c_\alpha = \sum_{\mathbf{x}} \theta(\phi) x_\alpha, \quad (6)$$

$$d_{\alpha\beta} = \sum_{\mathbf{x}} \theta(\phi) \phi (x_\alpha - c_\alpha)(x_\beta - c_\beta). \quad (7)$$

Here b gives the two-dimensional droplet's area and \mathbf{c}/b the position vector of its center. The eigenvalues of $d_{\alpha\beta}/b$ give us two length scales $l_1 \geq l_2$ corresponding to the two axes of the droplet. The Taylor deformation is defined as

$$D = \frac{l_1 - l_2}{l_1 + l_2}. \quad (8)$$

Note that very deformed droplets have D close to (but still less than) unity.

To study the breakdown of stability of droplets and find the critical capillary number (beyond which no steady state for a single droplet stably exists) we need to find the stationary shapes of droplets at various Ca and Re . We ramp up the shear rate in a way that finds all stable droplet shapes before the breakdown. To do this efficiently we use an algorithm that increases the shear rate $\dot{\gamma}$ stepwise and then waits for the droplet shape to reach steady state before calculating Ca and Re . If droplet fission occurs, or if the resulting deformation increment is too large (exceeding a threshold $\Delta D_c \approx 0.05$) a smaller increase $\Delta \dot{\gamma}$ in the shear rate is tried. This process is iterated until either equilibrium is achieved, or $\Delta \dot{\gamma}$ falls below a pre-set limit chosen very close to zero ($\Delta \dot{\gamma}_c \approx 10^{-7}$). In the latter case, the last value of $\dot{\gamma}$ for which equilibrium was reached is identified as the final stable shear rate; this fixes the value of Ca and Re at breakdown of stability for the chosen run. By varying simulation parameters (such as viscosity) an ensemble of curves of Re versus Ca was generated. Each terminated in a breakdown point.

The simulations reported below have lattices bounded by moving walls separated by 120 lattice sites, with periodic boundary conditions along the flow direction (in which the lattice length is 400). Other parameters common to all runs were, in lattice units [9], $-A=B=0.06$; $\kappa=0.039$, from which the interfacial tension is derived as 0.046; and $M=3.0$. Ten viscosity values were selected in the range 0.23–0.88, again in lattice units [9]. These parameter values were chosen to minimize lattice anisotropy, spurious diffusive currents, and other well-documented but fairly controllable arte-



FIG. 1. For zero Reynolds number a two-dimensional droplet remains hydrodynamically stable at all Ca studied. It extends until the width of the droplet is of the order of the interface width. The picture shows a droplet with $\text{Ca} = 1.1$; the upper wall is moving rightward, the lower, leftward.

facts of the LB method [9,10]. The initial droplet radius in each run was 21 lattice units. However, it was found that the increased curvature of a sheared droplet could lead to slight changes in its size as a result of increased Laplace pressure causing a shift in solubility. This effect was minimized by using the true size of the droplet when calculating R_0 for the purposes of Re and Ca (see below).

The ratio $L/R_0 \approx 5.7$ is not so large as to approach the behavior of a droplet being sheared in an infinite medium. Wall proximity effects are present in our results (as they are in many experiments), but we do not study these systematically here. In addition, the slight change in R_0 with shear rate mentioned above means that the wall effects vary slightly during each run. By varying lattice size and shape we checked that there was no undue influence on the results. The same applies to the effect caused by proximity of a droplet to its periodic image along the flow direction.

Although it is hard to quantify precisely all systematic errors in LB [9] we believe the quantitative results reported below are generally good to within 10% and mostly rather better. Our main conclusions, however, are qualitative in nature.

Zero Reynolds number results. First we report a simulation for $\text{Re}=0$. While LB fully treats inertial effects, a stationary zero Reynolds number flow can also be simulated (essentially by switching off the term in the algorithm that handles fluid convection). In contrast to previous suggestions [6,11], we found that a two-dimensional droplet in a shear flow at zero Re does not break down by any fluid-mechanical process. Instead it continues to deform (Fig. 1) until the width of the droplet is comparable to the interface width, at which point dissolution-assisted breakup occurs. This corresponds to a molecular rather than a hydrodynamic breakup mechanism. A similarly elongated droplet in 3D would certainly not survive, due to the Rayleigh instability.

Finite Reynolds number results. Both Re and Ca depend linearly on the shear rate. We can, however, form the dimensionless number $I = \text{Re}/\text{Ca}$ which will be almost constant for each run (deviations arising only from the small changes in droplet size R_0 ; see above). The nominal I values for the nine different runs simulated are identified in the caption to Fig. 2, where we show deformation curves in each case. At modest Ca values the curves with a higher I (more inertia) show a larger deformation. A likely explanation for this is the Bernoulli effect. This will create regions of lower pressure at the edges of the droplet, tending to stretch it into the flow so

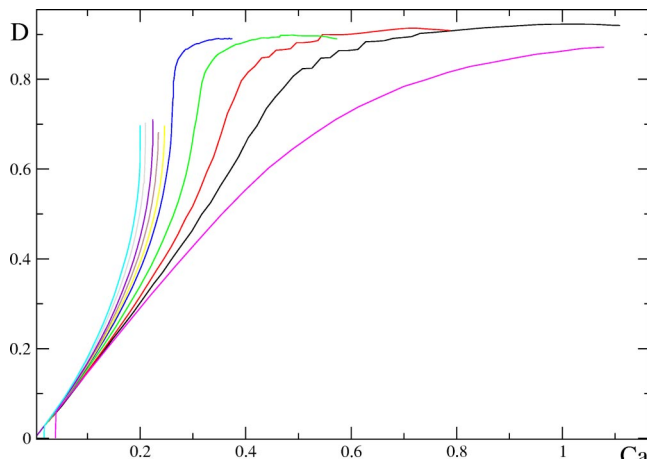


FIG. 2. Taylor deformation against capillary number under slow ramping of shear rates for (top to bottom) nine runs of viscosities in the range 0.181–0.877 (lattice units) and the zero Re limit. Values of the parameter $I = \text{Re}/\text{Ca}$ are $I = 18, 13, 11, 9.1, 7.3, 6.3, 3.7, 2.2, 1.3, 0$ (top to bottom).

that it experiences a stronger flow than applies for a droplet at zero Re.

The simulation corresponding to the lowest curve is the zero Reynolds number case, and here breakdown does not occur, as previously discussed. All other curves end at the last stable configuration for the droplet that could be found using our ramp method. It can be difficult to establish the stability of the very slowly evolving, near-critical droplets that arise close to this last stable configuration (particularly if they are very deformed) so we have taken care to run the simulations for tens of thousands of time steps per iteration in these parts of the curves.

With increasing I we find that there is a trend towards steeper deformation curves, and at a critical I_c between 6.3 and 7.3 we observe a singularity in which the deformation curve appears to develop an infinite slope at its end point. Further all deformation curves with larger I end similarly at a deformation of about 0.7. We performed simulations for a number of different lattice sizes and the exact value of I_c depends on the cell dimensions, with increasing wall separation causing a shift to smaller I_c [12].

As explained earlier, our ramp algorithm is designed to allow only a certain amount of deformation for each new stationary state. So, before the algorithm reaches a region of infinite slope it will force ever smaller shear-rate increments; when these fall below the pre-set threshold the algorithm will save the last configuration and exit. To check the fate of these droplets we reloaded the last configurations manually and again increased the shear rate by a very small amount. All these droplets were unstable to extension and eventually broke up into two droplets (not three) as the necks became too thin.

We show the dependence of the last stable capillary number on Re in Fig. 3. Each of the runs appears a (almost) straight line on the plot, ending at the breakdown point. Two different critical capillary number regimes are clearly separated in the Re/Ca plane. Figure 3 gives examples of the last stable droplet shapes for both $I < I_c$ and $I > I_c$. For $I < I_c$ we

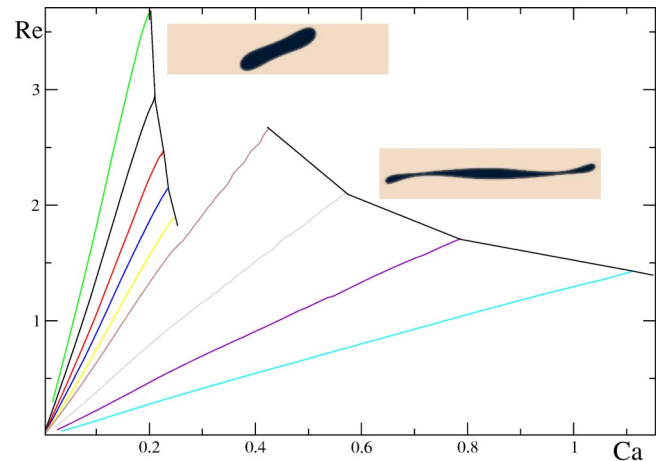


FIG. 3. Deformation curves plotted in the (Re, Ca) plane. Note that the zero Re curve coincides with the x axis and does not end in breakdown. The envelope of breakdown points is shown to guide the eye: this has two disconnected parts, corresponding to two-lobe and three-lobe droplets at the last stable configuration. Typical shapes are as indicated.

find that the droplets develop a double dimple; beyond the critical capillary number $\text{Ca}_c(I)$ these elongate and break up into three. For $I > I_c$ the last stable droplet shows one dimple; beyond Ca_c these elongate and break up into only two droplets.

Note that in these simulations we only observed breakdown of stability for $\text{Re} < 1.2$. The shape of the breakdown envelope in Fig. 3, together with the knowledge that the zero Reynolds number case remains stable, suggests that the envelope could have a horizontal asymptote at some nonzero value of Re (perhaps close to unity). This would imply a finite critical Re below which no breakdown could occur, however large Ca. However, more detailed work would be needed to reach a firm conclusion on this point.

We also performed simulations with a less sophisticated ramp algorithm in which the shear rate was increased as before, but without restriction on the deformation increment. In this case, different behavior was seen around I_c . Droplets which, when ramped more carefully, would show the two-lobed breakdown mode (with a vertical tangent to the deformation curve at its end point; Fig. 2) could now jump past this onto the upper branch of the deformation curve, developing instead a stable three-lobed shape, finally breaking up at higher Ca into three droplets. The deformation curve for one such case is compared to the more careful ramp for the same I in Fig. 4. This proves that the details of the flow history can strongly affect the breakdown mode and also the shear rate at which breakdown occurs.

Comparing this result with the general trend shown for larger I in Fig. 2 suggests a conjecture: that the behavior is governed by an underlying, continuous deformation curve that has, for $I > I_c$, folded over into an S shape. With such a curve, one might naturally expect a discontinuous jump in deformation on ramping up to the point of vertical tangency. However, it appears that droplets cannot survive the jump

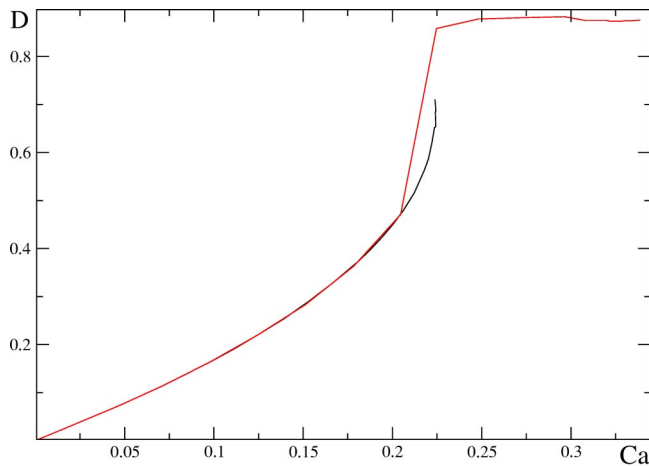


FIG. 4. Two deformation curves for $I=11$. For one run with the deformation restriction was removed. The droplet overshoots the underlying breakdown point and jumps into a three lobe structure, which survives to larger capillary numbers until eventually losing stability.

(but instead show a two-lobed breakdown of stability) if brought very close to this point before the jump is made. With a faster ramp, the jump occurs sooner; the droplet then can survive the jump and continue onto the upper branch of the deformation curve. The mechanism seems to involve transient stretching just after the shear rate is incremented; this allows the droplet to find the upper branch of the deformation curve, but only if the shear rate-increment is sufficient. Note that such an S-shaped deformation curve would also admit hysteresis, in which two states of deformation were both possible at exactly the same Ca . However, we

never got clear evidence of this in our simulations, so any hysteresis loop appears to be relatively small.

Conclusions. In this article we have provided evidence that the breakdown of droplet stability in two dimensions requires a nonzero Reynolds number. The dependence of the critical capillary number Ca_c on the dimensionless number $I=Re/Ca$ for two-dimensional droplet breakdown shows an unexpected transition at $I=I_c$. (The precise value of I_c depends on the wall separation.) This transition is consistent with an evolution of the underlying deformation curve $D(Ca)$ into an S shape. (However, we did not observe hysteresis around this transition.) A slow enough ramp leads to a two-lobed instability mode at Ca_c for $I>I_c$ whereas under different ramp conditions a droplet can, before reaching Ca_c , jump from a two-lobed structure to a three-lobed one, which is then stable to much higher Ca . For $I<I_c$ the droplet evolves to a three-lobed structure before losing stability, no matter how slow the ramp rate. From extrapolation of the critical capillary number we proposed that, even at very large Ca , a threshold in Re of order unity may need to be exceeded; but an alternative is that the Ca_c diverges only as $Re \rightarrow 0$.

Because of the care required in achieving equilibration close to Ca_c it would be difficult to perform similar numerical studies in three dimensions without very substantial resources. Nonetheless, an important open question is whether, on increasing the relative importance of inertia, the breakup mode in three dimensions also undergoes a sudden transition as we discovered here. We are unaware of experiments addressing this, and note that in such experiments (as well as in simulations) very careful control of the shear history might be needed to identify any transitions that may be present.

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could arise near the tips of sheared droplets if the diffusivity was too *small*; by increasing it, the currents were confined to a very thin region near the interface.

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