TUTORIAL REVIEW

Theory and numerical simulation of droplet dynamics in complex flows—a review[†]

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Received 3rd March 2004, Accepted 12th May 2004 First published as an Advance Article on the web 1st July 2004

We review theoretical and numerical studies and methods for droplet deformation, breakup and coalescence in flows relevant to the design of micro channels for droplet generation and manipulation.

Introduction

Microscopic droplet formation and manipulation are key processes (e.g., see ref. 1) in DNA analysis,2-4 protein crystallization,5,6 analysis of human physiological fluids,7 and cell encapsulation.8 Droplets are often used to either meter or mix small volumes of fluids to improve significantly the mixing efficiency and allow more complexity in chemical processing. For example, nanoliters of reagents can be added (through droplet coalescence) and removed (breakup) from a droplet leading to desired chemical reaction rates and times. Droplet generation and manipulation using immiscible flows,⁹⁻¹⁸ has the advantage that generation is fast and provides flexibility for the amount of reagent in each droplet, and the cost of the micro channels is low, compared to electrowettingbased devices. In addition, repeated fission and fusion of a single stream of droplets at a bifurcating junction can be used to produce parallel streams of smaller droplets containing a fraction of the original chemical concentrations. Reactions of large volumes of solution can be rapidly analyzed by splitting the solution into tens or hundreds of smaller droplets.¹⁰ This method can be applied to studying protein conformations,19 determining reaction kinetics,20 and characterizing single molecule polymerase chain reactions.²¹

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dynamics, where he has published about twenty papers. For his important work on droplet breakup in laminar and turbulent flows, Dr Cristini was the first recipient of the "Andreas Acrivos Dissertation Award in Fluid Dynamics" from the American Physical Society-Division of Fluid Dynamics. Dr Cristini has also published several papers in the fields of crystal and tumor growth.

JOI: 10.1039/b403226h

† Lab on a Chip special issue: The Science and Application of Droplets in Microfluidic Devices. ‡ Also at the Department of Mathematics.

For droplet systems controlled by external flows, the design of the channel geometry is used to control the forces that create, transport, split and fuse droplets. To our knowledge, droplet generation in microfluidic circuits using flow was first demonstrated (Fig. 1) by Thorsen et al.¹⁴ Song et al.¹¹ were the first to demonstrate droplet fission in microfluidic channels, and to show that the channel walls, while significantly hindering droplet motion, can improve the chemical mixing efficiencies by rotating the droplets. Tan et al.¹⁰ first demonstrated sorting and separation of satellite droplets from droplets of larger sizes in microfluidics by controlling the shear gradient at the bifurcating junction (Fig. 2),



Fig. 1 Control of droplet sizes by the pressure of the water-in-oil flow (Fig. 4 from ref. 14 reproduced with permission from the American Physical Society).



Fig. 2 Creation, sorting and collection of satellite droplets. (a) Satellite droplets are created with larger primary droplets. (b) Primary droplets are sorted towards the lower daughter channel while satellite droplets move into the loop region of the sorter. (c) The channel collecting the satellite droplets is free of primary droplets (data from ref. 10).



and droplet fusion control using droplet focusing designs over a variety of droplet sizes, numbers and generation speeds (Fig. 3). Control of both the droplet generation speed⁹ and size^{9,16,18} has been achieved in novel microfluidic designs (Figs. 4, 5 and 6). Tan *et al.*⁹ were successful in generating monodispersed pico- to femtoliter sized droplets in a PDMS based microfluidic device by controlling both the magnitude and type of flow in the micro channels. Flow magnitude and type are controlled by varying the difference between oil flow rates⁹ and the difference between oil and water flow rates,^{9,16} in co-flowing streams at the droplet generation site, and by varying the geometry and thus the flow resistance of the channels at various junctions downstream.^{10,18} Both designs lead to effectively varying the amount of straining of the flow and thus provide finer control of the droplet sizes.

To control and optimize the creation, mixing, sorting, fusion and splitting of droplets, droplet dynamics, and droplet breakup and coalescence criteria and rates in 3-D flow and channel geometry (*e.g.*, in channel junctions and in non symmetric flow-focusing streams) must be understood and controlled. The relative fluid motions induced by the droplets, the detailed characteristics of the droplet–solid contact angles, the interfacial tension at the droplet–liquid interface, the flow induced by the carrier flow around the droplets affect the design. The current design is often empirical and not founded on a rigorous study of the flow characteristics. Thus, there is room for considerable improvements by using theory and direct flow calculation.



Fig. 3 Fusion of large droplet slugs and free flowing droplets is controlled by the external flow, which changes depending on the geometry and surface properties of the walls (data from ref. 10). Flow rates are in μ l min⁻¹.



Fig. 4 Two different scalings are shown for droplet generation (from data in ref. 9). D/Di is the ratio of droplet diameter to the width of the orifice. *Qo* with units of μ l min⁻¹, is the flow rate of the oil phase. The flow rate of the water phase is 0.5 μ l min⁻¹.

Breakup and coalescence transitions are the result of the complex interplay of viscous, inertial, capillary, Marangoni, electrostatic and van der Waals forces over a wide variety of spatial and timescales. Asymptotic (e.g. lubrication) theories describe the limiting behaviors (e.g. pinching or film-drainage rates) of the geometrical and field variables at the onset of these transitions based on simplified assumptions on geometry (e.g. one-dimensionality), fluid and flow conditions. Numerical methods are capable of describing transitions accurately and efficiently in simulations of a variety of flow geometries (2-D and 3-D) and conditions where interfaces deform significantly in principle without relying on simplifying assumptions. A weakness of numerical simulations is computational expense because the transition regions characterized by small length- (and time-) scales need to be resolved by the numerical discretization requiring a very large number of computational elements. Thus it is often practice to incorporate asymptotic theories in numerical simulations, limiting direct numerical solution to the larger scales.



Fig. 5 Phase diagram for drop formation in flow focusing design (Fig. 3 from ref. 16 reproduced with permission from the American Institute of Physics). For increasing oil flow rates (top-to-bottom) and increasing oil flow rates relative to the water flow rate (left-to-right), water droplet sizes decrease.



Fig. 6 Passive breakup at T-junctions (from Figs. 1 and 2 from ref. 18 reproduced with permission from the American Physical Society): by varying the relative resistance (length) of the two side arms, the split droplet volumes also vary. Bottom: the line dividing breaking and non-breaking droplets is given by eqn. (2).

In this article, we review recent theoretical and numerical investigations of droplet dynamics in flow and we provide an overview of numerical methods that can be applied to describe breakup and coalescence phenomena in microfluidic design. Computational accuracy and efficiency and the potential impact of mesh adaptivity will also be discussed.

Theoretical and numerical investigations of droplet breakup and coalescence

Drop breakup

Droplet generation in flow-focusing design, and breakup in flow, are the result of the competition of viscous stresses associated with the imposed flow field, and capillary stresses due to surface tension between the two phases. In the flow-focusing design of water-in-oil emulsions (*e.g.* see refs. 9 and 16), the shearing comes from the relative magnitude of the co-flowing streams of oil and water. At a channel T-junction,¹⁸ droplets are sheared and extended as they travel through the junction and can be split. It is necessary to know under which conditions for the microphysical parameters and flow type breakup occurs and at what rates, or droplets are stable (non breaking), and the extent of droplet deformation.

Consider a drop of size (e.g. undeformed diameter) D, in a matrix fluid of viscosity μ undergoing flow with characteristic magnitude G of the local velocity gradient, and with surface tension σ . Viscous stresses scale as μG , and extend a drop on a timescale²² $(1 + \lambda)/G$, where λ is the ratio of drop-to-matrix viscosities, taking equally into account the contributions to friction coming from the fluid viscosities. Surface tension σ tends to relax a deformed drop back to spherical. From a dimensional analysis, the capillary relaxation velocity scales as σ/μ , thus the drop relaxation timescale is $(1 + \lambda)$ $\mu D/\sigma$, and capillary stresses scale as σ/D . The relevant dimensionless number is the capillary number Ca = $\mu GD/\sigma$ (assuming that inertia is negligible), the ratio of viscous-to-capillary stresses, or equivalently, the inverse ratio of the two corresponding timescales. When Ca = O(1), viscous stresses deform the droplet significantly and breakup may occur. The velocity gradient in a micro channel of hydraulic diameter $\sim D_i$ and flow rate Q_0 can be estimated as $G \sim$ Q_0/D_i^3 and, under conditions of Ca = O(1), this gives a simple relationship between generated droplet size and imposed flow rate:

$$D \sim \sigma D_i^3 / \mu Q_o \tag{1}$$

Thus, the larger the flow rate, the smaller the droplet size. Using9 $\sigma \simeq 10^{-3} \,\mathrm{N}\,\mathrm{m}^{-1}, D_{\mathrm{i}} = 40 \,\mathrm{\mu}\mathrm{m}, \mu \simeq 30 \times 10^{-3} \,\mathrm{kg}\,\mathrm{ms}^{-1}$ and Q_{o} = $12 \,\mu l \,\min^{-1}$, formula (1) gives a droplet size of $D \simeq 10 \mu m$ (and Re ≈ 0.01) and is in agreement with the data in Fig. 4. These and similar scalings have been employed to generate monodispersed emulsions of controlled droplet sizes by Thorsen et al.,14 Anna et al.¹⁶ and by Tan et al.⁹ as illustrated in Figs. 4 and 5. Fig. 4 reveals that droplet sizes fall in the theoretical scaling (1) when $D < D_i$, that is, droplets are small enough that the hydrodynamic forces exerted by the channel walls are not important and breakup fully relies on the straining of the imposed flow. When drops are large, wall effects are dominant over the stresses directly imposed by the flow, and the dependence of droplet sizes on flow rate is weaker. These considerations are corroborated by the trend observed in Fig. 5. Similar scalings for breakup criteria have also been successfully applied (Fig. 6) to the design of channel T-junction geometry and inlet and outlet flow rates.¹⁸ Interestingly, they found that the capillary number above which droplets passively break at a Tjunction scales as

$$Ca \sim \varepsilon_0 (1/\varepsilon_0^{2/3} - 1)^2 \tag{2}$$

where $\mathcal{E}_0 \sim l_0/w_0$, the ratio of length-to-width of the droplets in the mother channel are upstream of the junction. Downstream of the junction, split droplet volumes scale inversely with the lengths of the side arms.

Experimental, theoretical and numerical studies of drop breakup in imposed flows have been reviewed by Rallison²³, Stone²⁴ and Guido and Greco²⁵ (see also the review by Basaran²⁶ for jets). Criteria for breakup were investigated experimentally (e.g. by Bentley and Leal²⁷) and analytically (e.g. by Navot²⁸ and Blawzdziewicz et al.^{29,30}). The distribution of drop fragments resulting from breakup in shear flow was studied (e.g. see refs. 22 and 31). Numerical simulations have been developed (e.g. see refs. 22,32–34). Emulsification is typically promoted using surfactants that decrease surface tension on the droplet interfaces thus favouring drop and jet breakup (see refs. 35-42 and the review by Maldarelli and Huang⁴³). Methods for producing controlled micro sized droplets were developed for shear flow, 22,31,44-47 using coflowing streams (see ref. 48 and the recent microfluidics literature listed above) and extrusion flow.49 Monodispersed emulsions of large numbers of droplets with controlled sizes were generated in flow using the tip-streaming phenomenon due to redistribution of surfactants to localized end caps on the drop interface.^{50,51} Cristini et al.22 reported a study on the deformation and breakup of drops in shear flow demonstrating that nearly bi-disperse emulsions of large numbers of microscopic droplets of controlled sizes and generation times can be achieved even without surfactants (Fig. 7). Interestingly, the two sizes alternate (as also found by Tan et al.9). The reason for this lies perhaps in the asymmetrical evolution of the drop interface near the pinch-off region into cones with different angles during the latest stages of pinch-off (Fig. 8, top), as described by the theories of Blawzdziewicz et al.52 and Lister and Stone.53 It was also found²² that the breakup times have a nonmonotonic dependence on the capillary number, and have a (broad) minimum corresponding to moderately supercritical shear rates. This information can be used to optimize emulsification times.

It has been shown,^{52,53} that during pinch-off of a thin liquid thread under zero-Reynolds-number conditions (Fig. 8), the thinning rate becomes asymptotically constant in time. Thus pinchoff occurs in a finite time. As the thread thickness h_{\min} decreases, viscous stresses $\mu u/h_{\min}$ ($u = -dh_{\min}/dt$ is the thinning rate) balance the capillary pressure : σ/h_{\min} : $\mu u/h_{\min} \sim \sigma/h_{\min}$. Thus the neck pinching velocity $u \sim \sigma/\mu$ and is (asymptotically) constant. This is illustrated in Fig. 8 (bottom).⁵³ The axial curvature H' of the thread (rescaled with $h_{\min}(t)$) at the minimum $h_{\min}(t)$ is also found to be asymptotically constant as $h_{\min} \rightarrow 0$, thus revealing self-similarity of the shape in the transition region. These scalings for the capillary-driven pinch-off can be used when estimating drop formation times in a micro channel. In a flow-focusing design9,16 for water-in-oil emulsions, the time for accumulation of enough water for one droplet is given by D^3/Q_w (the volume of the droplet divided by the water flow rate). Capillary driven pinch-off time can



Fig. 7 Generation of a nearly bi-dispersed emulsion (From Figs. 11 and 12 from ref. 22 reproduced with permission from the American Institute of Physics). The cumulative distribution of droplets of alternating sizes (inset) formed from breakup of a mother drop in shear flow is shown. The droplet sizes \bar{a} are rescaled with the maximum stable size in the flow.

be estimated as $(1 + \lambda) \mu D/\sigma$. Droplet generation time will be determined by the larger of these two times. For droplets that are smaller than the channel width $(D < D_i)$, the droplet size *D* is given by the scaling (1), and thus the ratio of the two times is $O(D/D_i)^3$ indicating that droplet generation time is dominated by the capillary time for small droplets.

Drop coalescence

Coalescence rates and efficiencies between droplets depend on the local dynamics of the fluid drainage in the near contact region between the two approaching fluid interfaces. Asymptotic theories and numerical simulations of film drainage between coalescing fluid–fluid interfaces,^{54–63} including surfactant effects,^{64–70} provide useful information such as the rates of drop–drop approach.

Two drops approaching each other trap a thin film of the continuous phase between their interfaces. At small enough gaps the hydrodynamic forces overcome capillarity and the drop interfaces deform and often acquire a dimpled shape that traps more fluid thus opposing coalescence.55,62,69 In flow-driven drop interactions, coalescence occurs for capillary numbers smaller than a critical value such that the drop interaction time is larger than the drainage time for the fluid trapped in the gap.57 For sub-critical capillary numbers, at sub-micron separations, van der Waals forces become dominant leading to rapid coalescence (film rupture). Surfactants (through Marangoni stresses, surface viscosity, Gibbs elasticity, surface and/or bulk diffusivity and intermolecular forces) can have a significant effect and stabilize emulsions by increasing deformation and causing surface tension gradients (Marangoni stresses, see the book by Edwards et al.71) that resist radial flow in the gap and interface-interface approach thus preventing coalescence.^{68–70,72,73} Chesters and Bazhlekov⁶⁹ studied numerically the axi-symmetric film drainage and rupture between two drops

approaching each other under a constant force in the presence of an insoluble surfactant. For drops in the millimeter size range the influence of surfactant diffusion is typically negligible. Drainage is virtually unaffected by the presence of surfactants down to a film thickness at which high Marangoni stresses and a transition to immobile interfaces set in, leading to drainage orders of a slower magnitude. These phenomena are illustrated in Fig. 969 for the minimum film thickness h_{\min} . Analytical approximations for the drainage time were derived.⁶⁹ For smaller drops the influence of diffusion alleviates gradients in surfactant concentration reducing the effect of surfactants. Yeo et al.⁷⁰ (see also ref. 73) using theory and numerical simulations focused on constant approach velocity collisions and highlighted the differences in dynamics that arise. They showed that adding even a slight amount of insoluble surfactant results in the immobilization of the interface. Three regimes of drainage and possible rupture exist depending on the relative magnitudes of the drop approach velocity and the van der Waals interaction force: nose rupture, rim rupture, and film immobilization and flattening. The possibility of forming secondary droplets by encapsulating the continuous phase film into the

coalesced drop at rupture was also quantified. Recent experimental^{74,75} and numerical investigations⁷⁶ of flow driven drop–drop coalescence with surfactants revealed that there is a non-monotonic dependence of the critical capillary number for coalescence on the surfactant coverage (Fig. 10). The critical capillary number has a minimum for intermediate coverage due to Marangoni stresses, and increases at high coverage (close to the maximum packing of molecules on the interface) perhaps as a consequence of interface immobilization and reduced deformation.



Fig. 8 Top: initial (dashed) and final (solid) shapes during pinch-off (Fig. 2 from ref. 53). Liquid threads separate large daughter drops and have nearly conical shapes near the locations of minimum thickness. Bottom (Fig. 6 from ref. 53): constant thread-thinning velocity and shape self-similarity as $h_{\min} \rightarrow 0$. Reproduced with permission from the American Institute of Physics.



Fig. 9 Schematic illustrating the effects of surfactants and transition to immobilized interfaces and slow drainage (Fig. 13,⁶⁹ reproduced with permission from Elsevier).



Fig. 10 Coalescence occurs for capillary numbers below the critical curve. Curves are shown (data from ref. 76) as a function of surfactant coverage c of the interface for insoluble surfactants and for a surfactant that is soluble in the bulk fluids, for different values of a dimensionless van der Waals force, indicating non-monotonic dependence on the surfactant coverage.

These findings demonstrate that while much progress has been made in the theoretical understanding of film drainage, there are still open questions.

Numerical methods

The two main approaches to simulating multiphase and multicomponent flows are interface tracking and interface capturing.

Interface tracking methods

In interface tracking methods (or sharp-interface methods) the computational mesh elements lay in part or fully on the fluid–fluid interfaces. Such methods, including boundary-integral methods,^{32,33,34,70,77–80} finite-element methods^{81–83} and immersed-boundary methods,^{84,85} are very accurate for simulating the onset of breakup and coalescence transitions but have difficulties in simulating through and past the transitions.

In boundary-integral methods, the flow equations are mapped from the immiscible fluid domains to the sharp interfaces separating them thus reducing the dimensionality of the problem (the computational mesh discretizes only the interface). In finiteelement methods, the fluid domains are discretized by a volume mesh and thus the dimensionality is not reduced. Both these approaches lead to accurate and efficient solution of the flow equations because the interface is part of the computational mesh and the equations and interface boundary conditions are posed exactly. In immersed-boundary methods, the interfacial forces are calculated on a surface mesh distinct from the computational volume mesh where the flow equations are solved and thus in addition, interpolation onto the volume mesh is needed. A threedimensional boundary integral simulation of the onset of drop breakup in simple shear flow is shown in Fig. 11 (top).³³ In the three frames, the evolution of a drop towards breakup and the formation of a thinning liquid thread separating two large daughter drops are



Fig. 11 Top: adaptive 3-D boundary-integral simulation of the onset of drop breakup in shear flow (Fig. 1 from ref. 33 reproduced with permission from the American Institute of Physics). Bottom: the simulation is continued past the transition by reconnecting the computational mesh (Fig. 6 from ref. 34 reproduced with permission from Elsevier).

shown. The labels report the dimensionless time from breakup. The calculated drop shapes (computational mesh) are compared to an experiment (solid contour) by Dr Guido and coworkers (University of Naples, Italy, personal communication), demonstrating the high accuracy of the numerical method. These simulations used an adaptive triangulated mesh.34 In Fig. 12 a boundary-integral simulation of the flow of deformable droplets through a channel is shown.86 In Fig. 13 an application of the finite-element method to high-Reynolds-number satellite production from a jet is illustrated.⁸³ Cross sections of the computed evolution in time (top) compare well with the experiments (bottom) (corresponding to different initial conditions). The computational accuracy allowed the authors to recover features of the evolutions such as capillary waves (a)-(c), overturning of the top and bottom of the satellite in (f), spade-shaped profiles, (g) and (h), and spawning of a subsatellite. In Fig. 14, immersed-boundary simulations of bubbles interacting and coalescing are shown.84,87

Near breakup and coalescence transitions, sharp interface models break down because of the formation of singularities in flow variables⁸⁸ and complex *ad hoc* cut-and-connect algorithms have been employed^{34,84,89} to change the topology of the meshes and continue simulating through a transition. (A method to automatically reconnect sharp interfaces has been recently developed by Shin and Juric⁸⁵). In the simulation in Fig. 14 (bottom), Nobari et al.87 reconnected the interfaces as their separation fell under a prescribed value but noticed that the flow can depend sensitively on the time at which the interface reconnections are performed. Reconnection conditions based on asymptotic theories describing liquid thread pinch-off and film drainage52,53,90-92 are also used to extrapolate to the instant of breakup or coalescence, as illustrated in Fig. 11 (bottom), where Cristini et al.³⁴ simulated the evolution of the drop in shear after the pinch-off transition by employing a cutand-connect mesh algorithm after the asymptotically linear thinning of the liquid thread^{52,53} had been established. This allows simulations to be continued past the transition while preserving



Fig. 12 Boundary-integral simulation of 3-D droplet motion through a channel (Fig. 8 from ref. 86 reproduced with permission from Cambridge University Press).



Fig. 13 Finite-element simulation (top) of satellite formation and dynamics from a jet compared to an experiment (bottom) (Figs. 2 and 3 from ref. 83 reproduced with permission from the American Institute of Physics).

accurate information on breakup time (Fig. 11, top) and fragment sizes.

Interface-capturing methods

Simulations through breakup and coalescence transitions using interface capturing methods, i.e. lattice-Boltzmann and latticegas,93-98 constrained-interpolation-profile,99 level-set,100 volumeof-fluid,101 coupled level-set and volume-of-fluid102 and partialmiscibility-model and phase-field methods,99,103-114 do not require mesh cut-and-connect operations because the mesh elements do not lay on the interface, but rather the interface evolves through the mesh. The fluid discontinuities (e.g. density, viscosity) are smoothed and the surface tension force is distributed over a thin layer near the interface to become a volume force (surface tension being the limit as the layer approaches zero thickness). Interfacecapturing methods are then ideal for simulating breakup and coalescence in immiscible two-fluid systems (and the effect of surfactants) and for three or more liquid components, and can be especially powerful for micro channel design. Lattice-Boltzmann methods are based on a particle distribution function and on averaging to capture the macroscopic behavior. The constrainedinterpolation-profile, level-set and volume-of-fluid methods describe the macro scale directly and use auxiliary functions advected by the flow (e.g. level-set, volume fraction, and color functions) to mark the different fluid domains. In Fig. 15, we reproduce a simulation of drop breakup in shear flow using a volume-of-fluid method;¹¹⁵ (see also refs. 116–118). The drop is strongly stretched in the supercritical flow leading to rupture into numerous fragments of alternating sizes (see for comparison refs. 9 and 22). The diffuseinterface (phase-field) approach is based on free-energy functionals and uses chemical diffusion in narrow transition layers between the different fluid components as a physical mechanism to smooth flow discontinuities and to yield smooth evolution through breakup and coalescence. Through the energy formulation, van der Waals interactions, electrostatic forces and components with varying miscibilities can be described. An example of simulation of jet pinch-off using the partial-miscibility model is shown in Fig. 16 (J. Lowengrub, U. C Irvine E. Longmire and U. Minnesota, personal communications, see also refs. 111 and 112). The liquid-liquid



Fig. 14 Top: 3-D front-tracking simulation of rising bubbles (Fig. 13 from ref. 84 reproduced with permission from Elsevier). Bottom: axi-symmetric front-tracking simulation of droplet coalescence (Fig. 13 from ref. 87 reproduced with permission from the American Institute of Physics).

interface and the axial velocity profiles during jet pinch-off from the diffuse-interface simulation and from an experiment show good agreement.

Mesh adaptivity

Accurate numerical simulations of multiphase flow and topology transitions require the computational mesh to resolve both the macro (e.g. droplet size, channel geometry) and micro scale where pinch-off or coalescence occur, and to capture local interface curvature, interface-interface separation, van der Waals forces, surfactant distributions and Marangoni stresses. Adaptive mesh algorithms greatly increase accuracy and computational efficiency in boundary-integral,³⁴ finite element,^{81,82} immersed boundary,⁸⁴ and interface capturing119-127 methods. In Fig. 17 level-set simulations of drop coalescence in 2-D (top) and drop breakup in 3-D (bottom) under Stokes flow conditions are reported using novel unstructured adaptive meshes.^{34,127} The adaptive mesh algorithm automatically imposes a mesh element size proportional to the distance from the interface. As the interfaces deform, approach or pinch-off, the mesh dynamically maintains accurate resolution of the flow near the interface. This allows a simulation to recover the



Fig. 15 3-D volume-of-fluid simulation (Fig. 16 from ref. 115 reproduced with permission from the American Institute of Physics) of drop breakup in shear flow (view along the velocity gradient).



Fig. 16 Comparison between a diffuse-interface simulation (right) (J. Lowengrub, U. C Irvine) and an experiment (left) (E. Longmire, U. Minnesota, personal communications) of a liquid–liquid jet pinch-off.



Fig. 17 Adaptive unstructured meshes of triangles (top) and tetrahedra (bottom) maintain computational accuracy during simulations (data from ref. 127). Some tetrahedra may appear skewed (bottom) as a result of projecting the 3-D mesh onto the plane of the figure.

lubrication forces that resist drop approach and delay coalescence (top). The log-linear plot in the inset reports gap thickness history for increasing mesh resolution (left to right) and is compared with lubrication theory (straight line), that in 2-D predicts exponential gap thinning and thus an infinite coalescence time when only hydrodynamics are considered.¹²⁷ The simulation results converge to the lubrication theory. Below a gap thickness that decreases with increased resolution, numerical coalescence occurs. A 3-D simulation (bottom) accurately describes drop breakup during retraction of a previously elongated drop.

Conclusions

Theoretical considerations relevant to controlled droplet generation, breakup and coalescence in micro channels were discussed. Theoretical and numerical investigations of droplet breakup and coalescence in imposed flows were reviewed. Numerical methods were reviewed that can be applied for directly simulating droplet generation, dynamics, breakup and coalescence in micro channels. The magnitude and type of flow are both important in determining generation, breakup and coalescence times and droplet sizes. The local velocity gradient imposed on a droplet is a function of position in the micro channel, and depends strongly on the channel geometry. In microfluidics design, channel geometry and flow conditions can be optimised using (adaptive) simulations. Important issues are still open in the literature. In particular, one topic where theoretical and numerical work has been limited and further investigation is highly desirable in the near future is drop-wall interactions. For droplets of size comparable to the channel width, the hydrodynamic forces exerted by the wall on the drop may exceed those exerted by the imposed channel flow. Under these conditions, droplet deformation and droplet breakup and coalescence criteria and rates may be strongly affected.

V. C. is grateful to John Lowengrub for the many enjoyable and useful discussions on numerical methods, and acknowledges support from the National Science Foundation.

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