Lattice Boltzmann Simulations of Breakup, Coalescence and Chemical Mixing

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Objectives

- Explore the possibility of using the lattice Boltzmann method to simulate drop breakup and coalescence.
- Compare the simulation results with existing experimental or theoretical results
- Gain a better understanding of the basic physics associated with changes in interface topology.

Dimensionless groups

$$Ca = \frac{\mu_c G d}{\sigma}$$ capillary number

$$Re = \frac{G d^2}{\mu}$$ Reynolds number

$$We = \frac{d u^2 \rho}{\sigma}$$ Weber number

Characteristics of system

- d — **equivalent spherical diameter**
- μ_c — **drop viscosity**
- ν — **continuous phase kinematic viscosity**
- σ — **interfacial tension**
- ρ_d — **density of drop**

Breakup in shear flows

In low Reynolds number laminar flows:

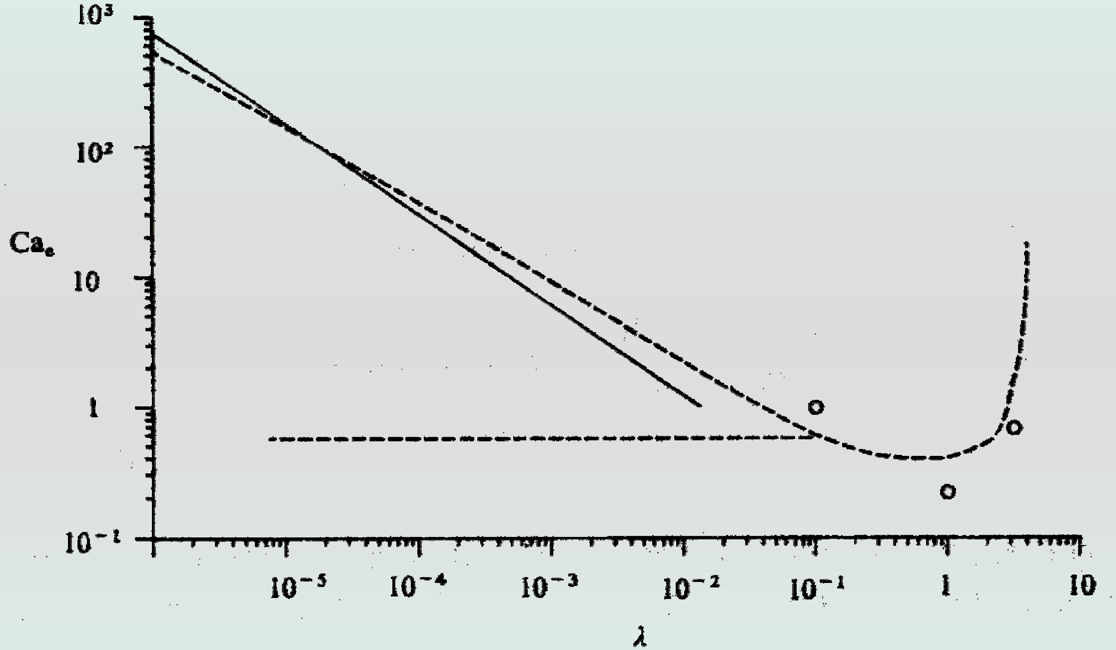
• Critical capillary number depends strongly on the viscosity ratio

• Different breakup modes for different viscosity ratios

• If the flow field was suddenly turned off, a highly deformed drop can break.

• Little experimental work available for large Reynolds number laminar shear flows.

Experiments on drop breakup



Variation of critical Ca with viscosity ratio for simple shear flow.

Rallison (1984)

Breakup in turbulent flows

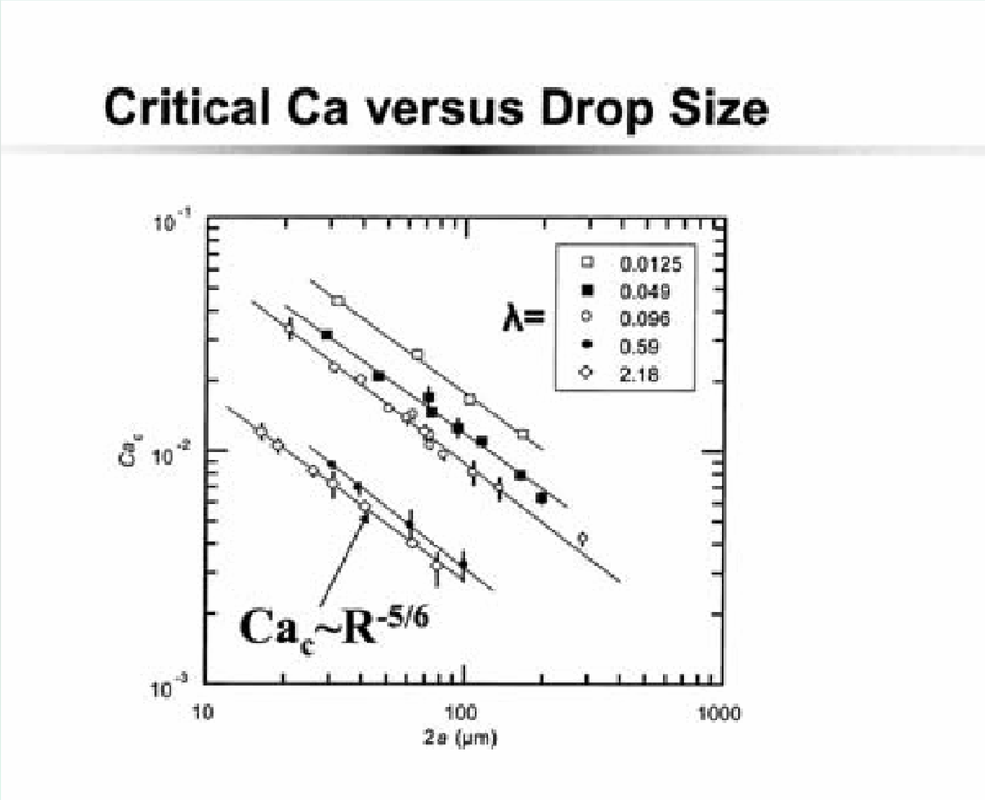
- Weber number should be based on the mean square velocity difference across the drop.
- The critical Weber number should be independent of Reynolds number

Hinze (1955)

Coalescence in laminar shear flows

- * *No drop inertia, all results for* $Re \ll 1$.
- * *Coalescence for* $Ca < Ca_c$.
- * *Typically* $Ca_c \ll 1$.
- * Ca_c *decreases with drop size.*
- * Ca_c *depends on viscosity ratio.*
- * Ca_c *decreases with impact parameter.*

Experimental results



Hu et al. (2000)

Speculation:

$$Ca_c = A / d^{5/6}$$

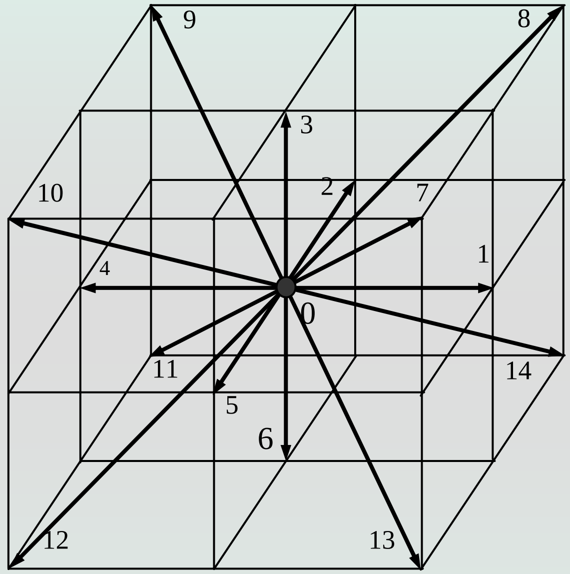
$$A = O(10^{-1})$$

$$Ca_c = O(1) \Rightarrow R \sim 10 - 100nm$$

Theory *Chesters (1991)*

$$Ca_c = C / d^{2/3}$$

Lattice Boltzmann Method



3D-15 velocity lattice

BGK Formulation

$$f_i(\mathbf{x}+\mathbf{e_i},t+1)=f_i(\mathbf{x},t)+\Omega_i(\mathbf{x},t)$$

Collision step: $f_i^c(\mathbf{x},t+1)=f_i(\mathbf{x},t)+\Omega_i(\mathbf{x},t)$

Streaming step: $f_i(\mathbf{x}+\mathbf{e_i},t+1)=f_i^c(\mathbf{x},t+1)$

$$\Omega_i=-\frac{f_i(\mathbf{x},t)-f_i^{eq}(\mathbf{x},t)}{\tau}$$

Oxford Method

$$f_{\sigma i}(\mathbf{x}+e_{\sigma i}\Delta x,t+\Delta t)-f_{\sigma i}(\mathbf{x},t)=-\frac{1}{\tau_f}[f_{\sigma i}(\mathbf{x},t)-f_{\sigma i}^{eq}(\mathbf{x},t)]$$

$$g_{\sigma i}(\mathbf{x}+e_{\sigma i}\Delta x,t+\Delta t)-g_{\sigma i}(\mathbf{x},t)=-\frac{1}{\tau_g}[g_{\sigma i}(\mathbf{x},t)-g_{\sigma i}^{eq}(\mathbf{x},t)]$$

$$f_{\sigma i}^{eq}=A_{1\sigma}+B_{1\sigma}e_{\sigma i\alpha}u_\alpha+C_{1\sigma}u^2+D_{1\sigma}e_{\sigma i\alpha}e_{\sigma i\beta}u_\alpha u_\beta+G_{\sigma\alpha\beta}e_{\sigma i\alpha}e_{\sigma i\beta}$$

$$g_{\sigma i}^{eq}=A_{2\sigma}+B_{2\sigma}e_{\sigma i\alpha}u_\alpha+C_{2\sigma}u^2+D_{2\sigma}e_{\sigma i\alpha}e_{\sigma i\beta}u_\alpha u_\beta$$

$$\sum_{\sigma i}f_{\sigma i}^{\ eq}=\rho$$

$$\sum_{\sigma i}f_{\sigma i}^{\ eq}e_{\sigma i\alpha}=\rho u_\alpha$$

$$\sum_{\sigma i}f_{\sigma i}^{\ eq}e_{\sigma i\alpha}e_{\sigma i\beta}=P_{\alpha\beta}+\rho u_\alpha u_\beta$$

$$\sum_{\sigma i}g_{\sigma i}^{\ eq}=\varphi$$

$$\sum_{\sigma i}g_{\sigma i}^{\ eq}e_{\sigma i\alpha}=\varphi u_\alpha$$

$$\sum_{\sigma i}g_{\sigma i}^{\ eq}e_{\sigma i\alpha}e_{\sigma i\beta}=\Gamma\mu\delta_{\alpha\beta}+\varphi u_\alpha u_\beta$$

Binary model

$$F = \int [\frac{A}{2}\varphi^2 + \frac{B}{4}\varphi^4 + \frac{\kappa}{2}(\nabla\varphi)^2 + nT\ln n]dV$$

$$\mu = A\varphi + B\varphi^3 - \kappa\nabla^2\varphi$$

$$P_{\alpha\beta} = \left[\rho T + \frac{A}{2}\varphi^2 + \frac{3B}{4}\varphi^4 - \kappa\varphi\nabla^2\varphi - \frac{\kappa}{2}(\nabla\varphi)^2\right]\delta_{\alpha\beta} + \kappa(\partial_\alpha\varphi)(\partial_\beta\varphi)$$

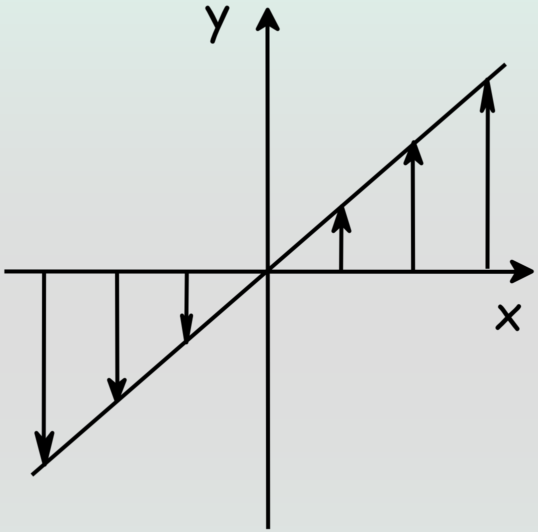
If we choose A=-B,the bulk equilibrium solutions are:

$$\rho_c = \rho_d = 1 \qquad \varphi = \pm 1$$

Interfacial thickness $\xi = \sqrt{\frac{\kappa}{B}}$

Surface tension $\sigma = \kappa \int_{-\infty}^{+\infty} \left(\frac{\partial\varphi}{\partial\xi}\right)^2 d\xi = \left[\frac{8\kappa B}{9}\right]^{1/2}$

Simple shear flow



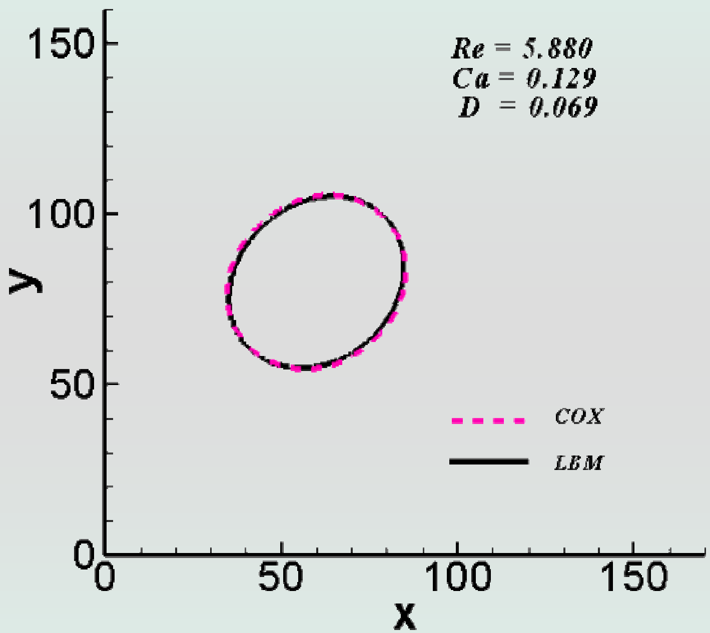
$$u = 0$$

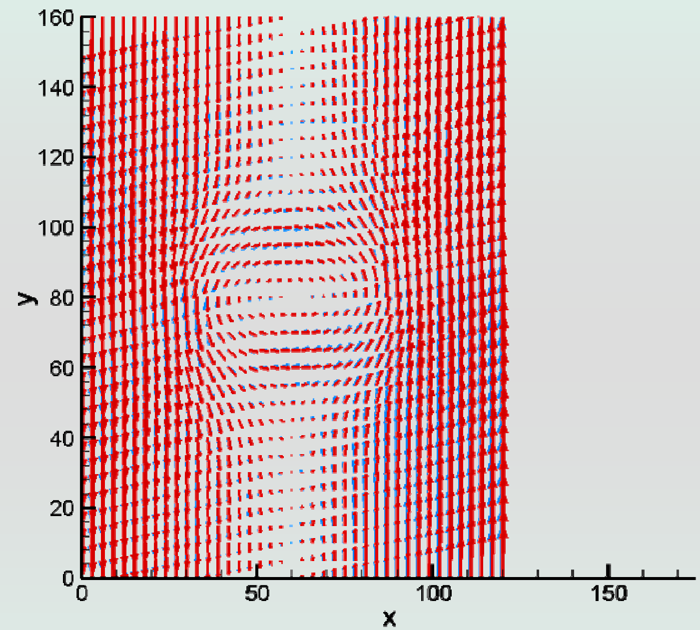
$$v = Gx$$

- The criterion for breakup is generally expressed in terms of a critical capillary number

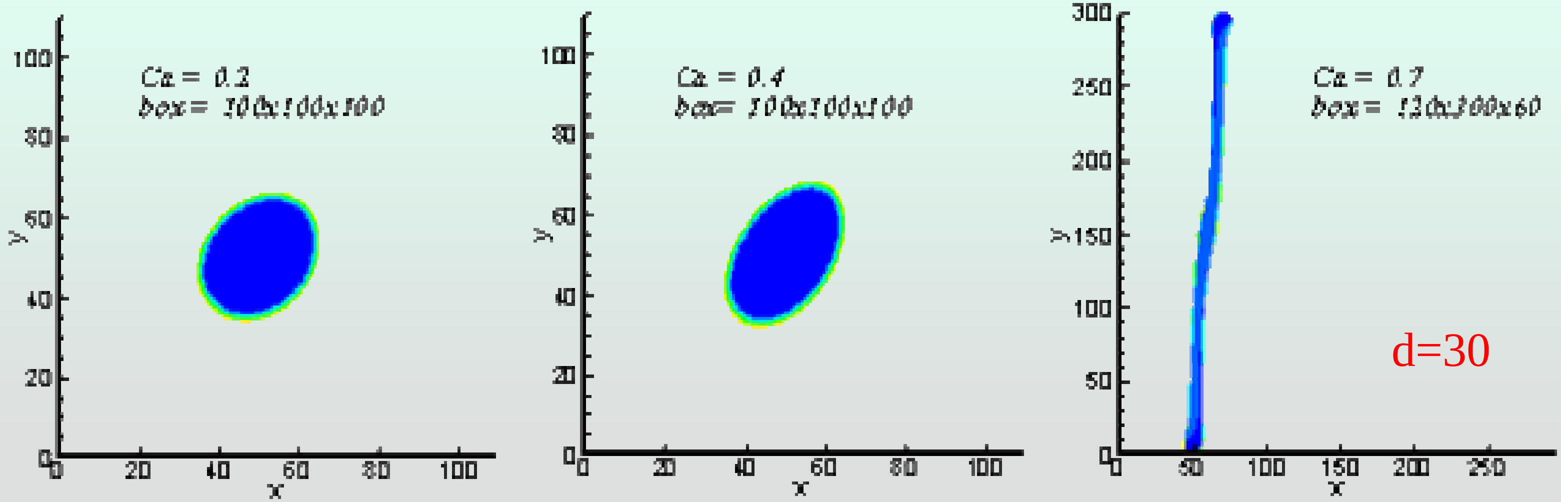
$$Ca_c = \frac{\mu_c G d}{\sigma}$$

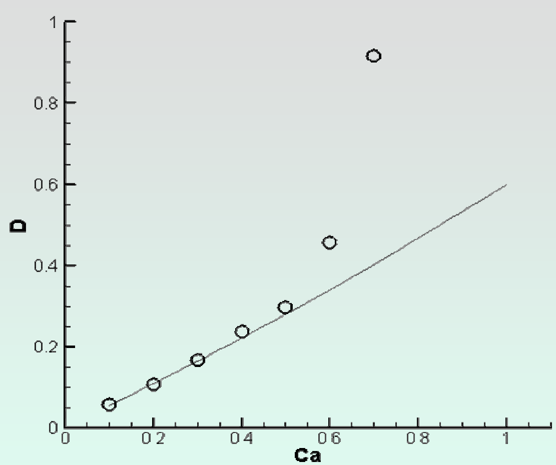
Drop deformation

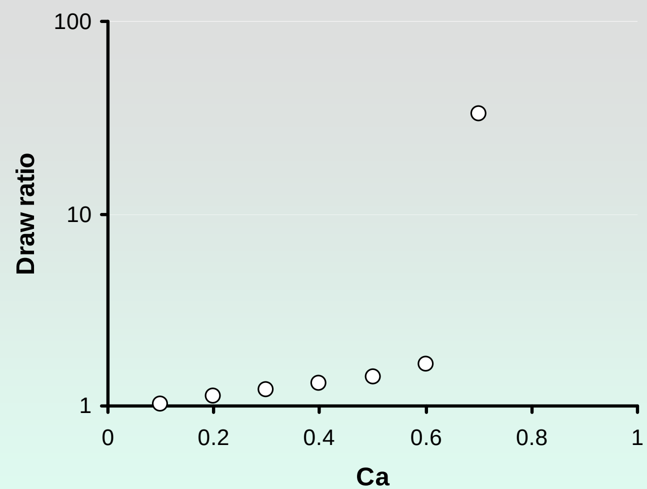


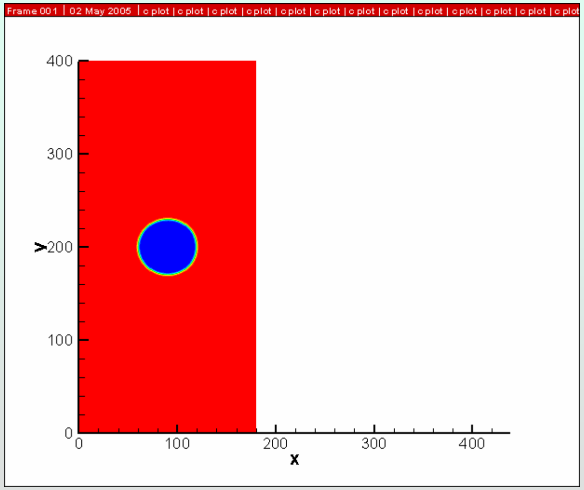


Cox, (1969)

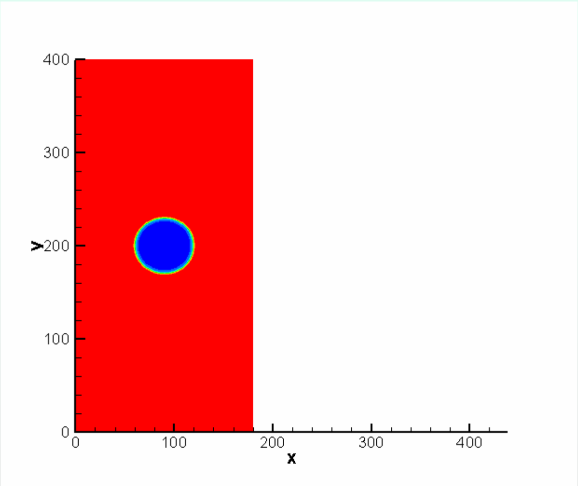

Ca = 0.2
box= 100x100x100
Ca = 0.4
box= 100x100x100
Ca = 0.7
box= 120x300x60
d=30
x
y


D
Ca

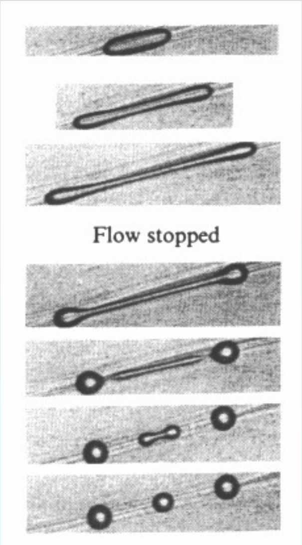

Draw ratio
Ca



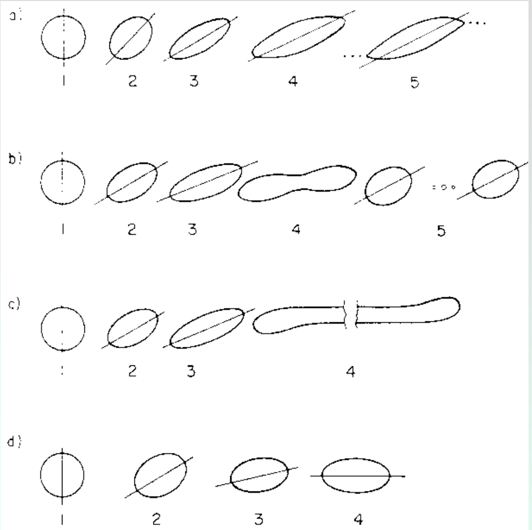
d=60, Ca=1.0
box=180*400*120



d=60, Ca=0.7
box=180*400*120



Stone et al. (1986)

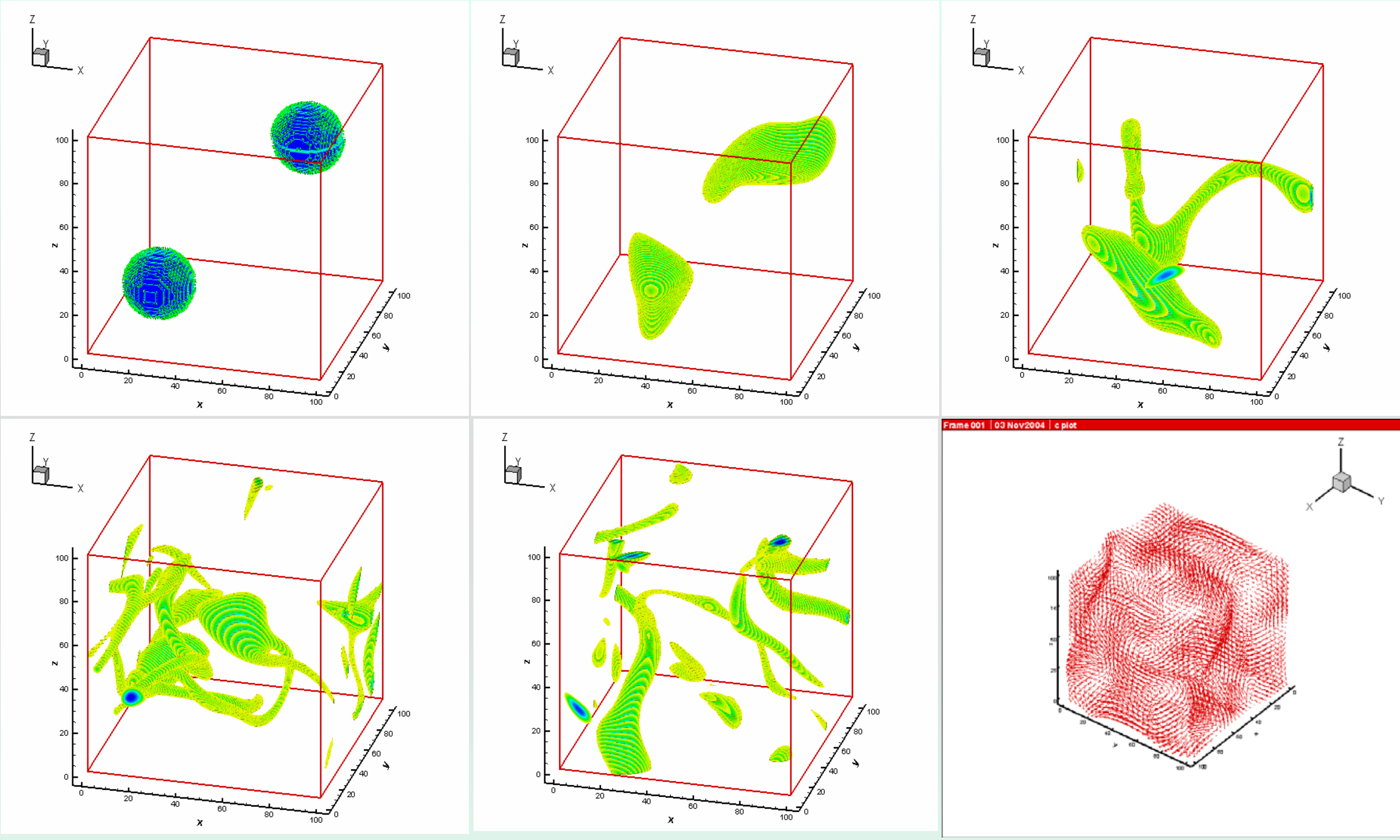


Rumscheidt and Mason (1961)

Turbulent Flow

- Weber number should be based on the mean square velocity difference across the bubble for homogeneous turbulence; the critical Weber numbers for breakup should be independent of Reynolds number.

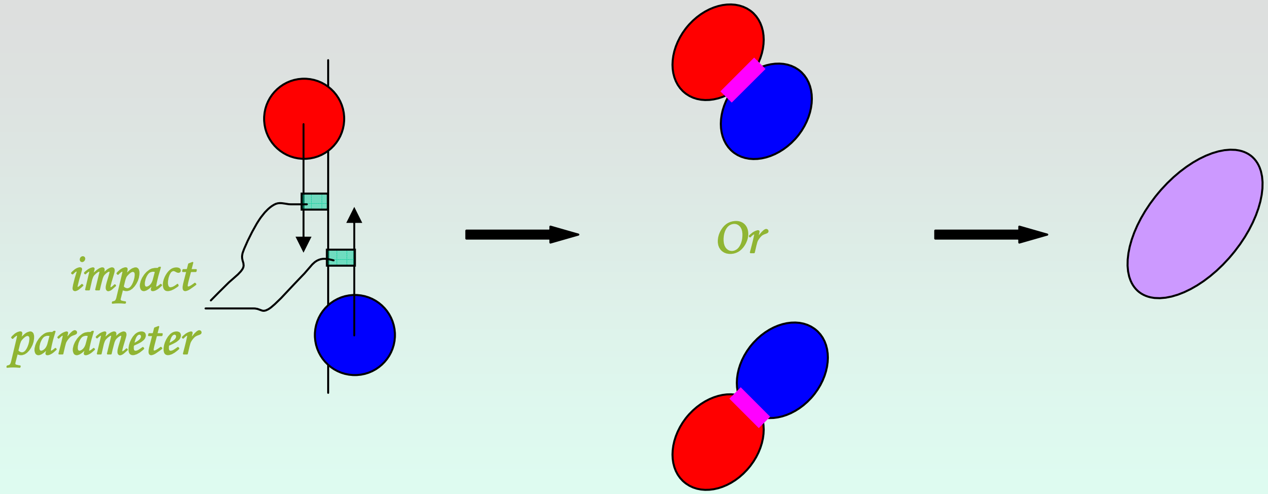
$$We = \frac{\rho < \Delta u^2 > d_e}{\sigma} \approx \frac{2\rho d_e u'^2}{\sigma}$$



$$We \sim 20 \qquad Re_{box} \sim 60$$

Shear-induced coalescence

- Because of shear, drops have different velocities and collide.
- Surface tension causes coalescence.
- Shear causes the drop to reorient.

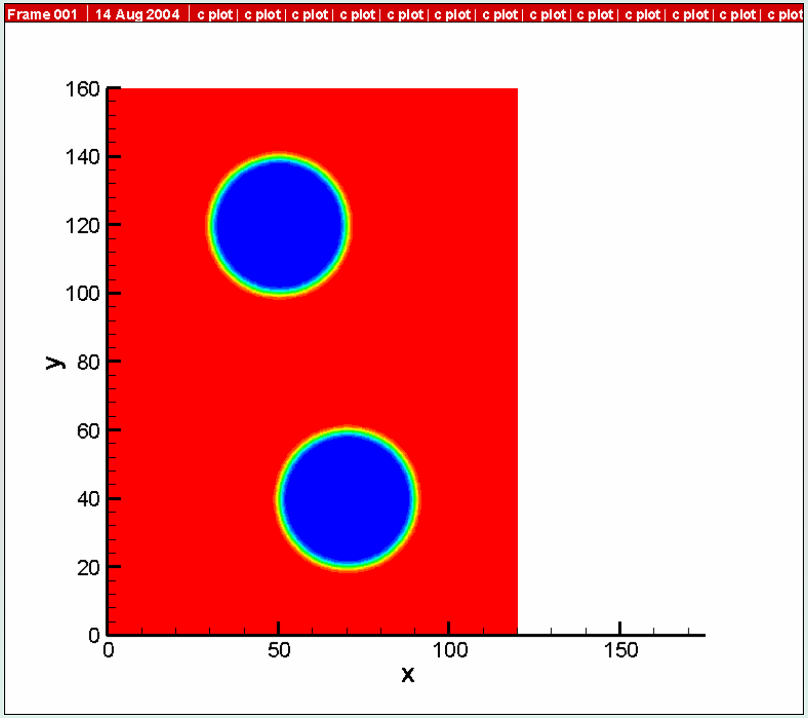


LBM simulation

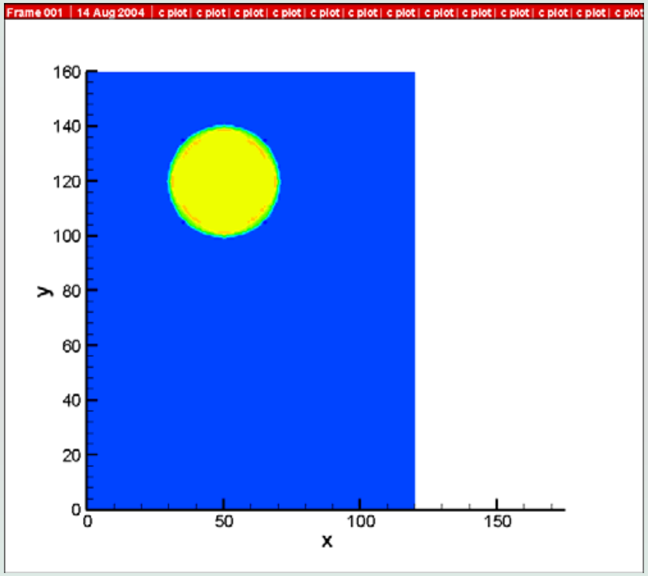
Drop coalescence

$$Ca = 0.113$$

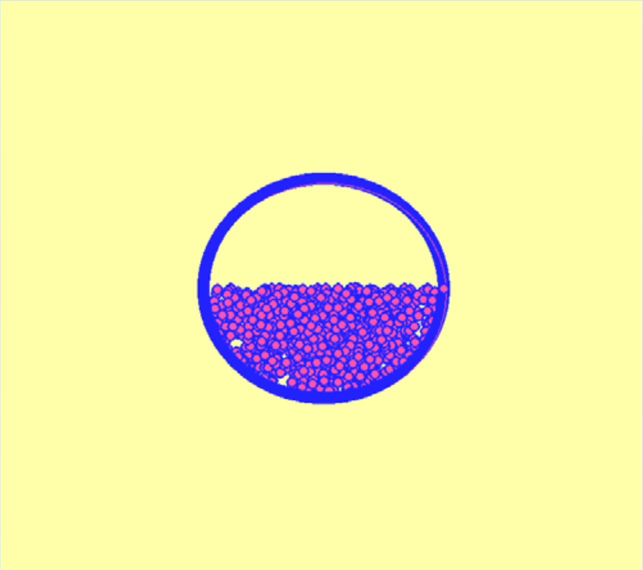
$$Re = 2.115$$



Mixing Result



Sc=100



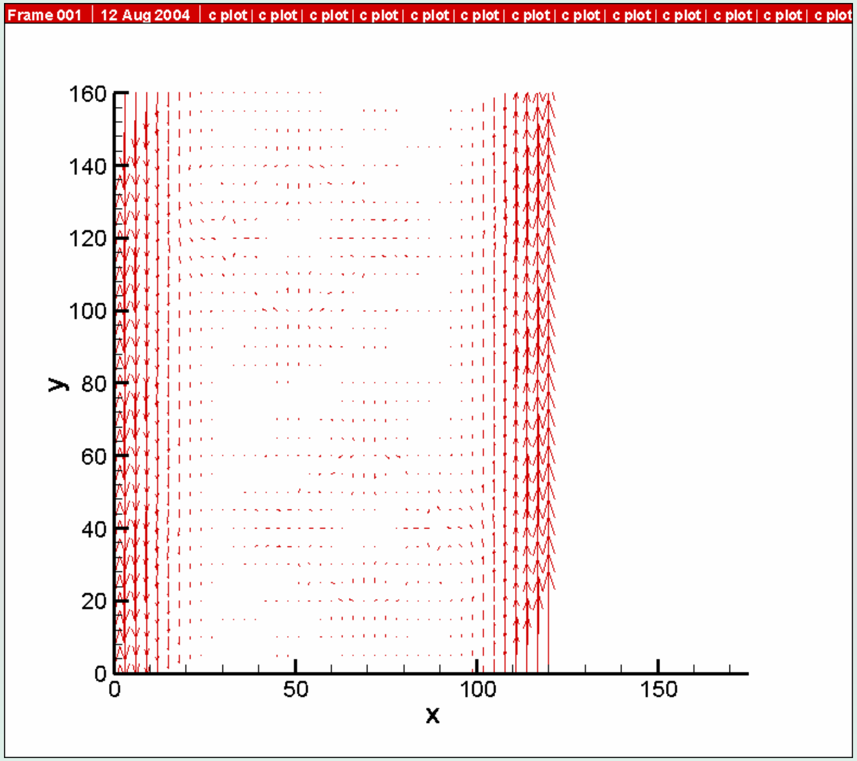
LBM

Re=2.1, t=28,000

Cox (1969) solution

Re=0, t=40,000

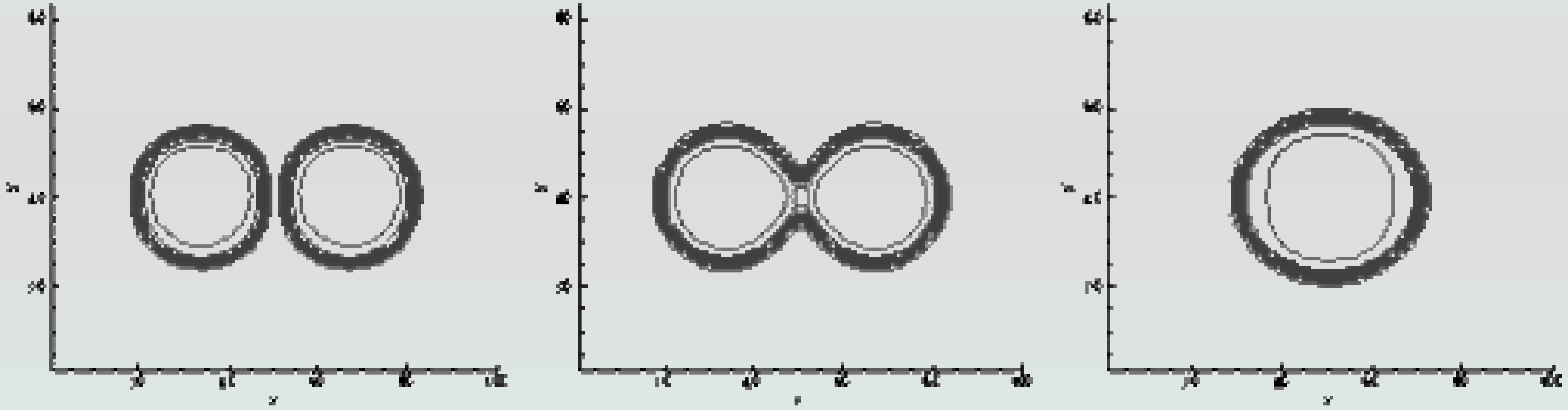
Velocity field



LBM

Re=2.1, t=28,000

Self coalescence of diffusive interfaces



The drops coalesce because their interfaces overlap.

Conclusions

- The Oxford method is capable of simulating drop breakup and coalescence in laminar and turbulent flows.
- The results for drop deformation in laminar shear flow agree well with published results for small and moderate deformations. For breakup, it is important that bulbs form at the ends of a drop; this is true only for sufficiently large drops The result for breakup after zeroing the velocity field is consistent with experiments.
- In turbulent flow, drops with large Weber numbers broke down into smaller and smaller drops. This is consistent with Hinze's theory.
- During coalescence, two impinging jets prevent mixing of a dissolved chemical. The subsequent mixing agreed with particle tracking simulations using an exact solution for the flow field in a spherical drop.

Acknowledgments

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