Numerical simulation of drop coalescence in the presence of drop soluble surfactant

I. Bazhlekov and D. Vasileva

Section Computational Mathematics
Institute of Mathematics and Informatics
Bulgarian Academy of Science

The second author is partially supported by the Bulgarian National Science Foundation under Grant DDVU02/71
Contents

Introduction: Drop coalescence and applications; Effect of surfactants.

Mathematical model:

• Simplifications;

• Hydrodynamic model - Stokes equations, lubrication approximation;

• Surfactant transport - convection-diffusion equations.

Numerical method:

• Boundary Integral Method for the Stokes equations in the drops;

• Finite Difference Method for the flow in the film and the convection-diffusion equations.

Results

Conclusions
Introduction: Drop coalescence and applications

Applications of multiphase systems: Emulsions - Food; drugs; cosmetics; composite materials; chemicals; petroleum; etc.
Drop-to-drop interaction in simple shear flow at $Ca = 0.25$
Schematic sketch of the problem

- viscosity $\mu/\lambda$
- surface tension $\sigma(\Gamma)$
- bulk concentration $c(r,z,t)$
- surface concentration $\Gamma(r,t)$

Equation:
\[
\Gamma(r,t) = K \cdot C(r,z = h(r,t)/2, t)
\]
Head-on collision in axisymmetric compressional flow, insoluble surfactant.
Mathematical model: Hydrodynamic part.

In the drops:

\[ \nabla \cdot v = 0; \quad -\nabla p_d + \mu \nabla^2 v = 0; \quad \text{Stokes equations in the drops} \quad (1) \]

In the film:

\[ \frac{\partial h}{\partial t} = -\frac{1}{r} \frac{\partial (rh u^{av})}{\partial r}; \quad \tau = -\frac{h \partial p}{2 \partial r} + \frac{\partial \sigma (\Gamma)}{\partial r}; \quad \text{Lubrication eq. in the film} \quad (2) \]

\[ p = \frac{2\sigma_{\text{pure}}}{R_{eq}} - \frac{\sigma (\Gamma)}{2} \left( \frac{\partial^2 h}{\partial r^2} + \frac{1}{r} \frac{\partial h}{\partial r} \right) + \frac{A}{6\pi h^3}; \quad \int_0^{r_\infty} \left( p - \frac{A}{6\pi h^3} \right) r dr = F(t) \quad (3) \]

\[ u = u_{int} + \frac{\lambda}{2\mu} \frac{\partial p}{\partial r} \left( z^2 - \left( \frac{h}{2} \right)^2 \right); \quad u^{av} = u_{int} - \frac{\lambda}{12\mu} h^2 \frac{\partial p}{\partial r} \quad (4) \]

\[ \tau = \mu \frac{\partial v_1}{\partial z}; \quad u_{int} = v_1; \quad \text{BC at the interface} \quad (5) \]
Mathematical model: Surfactant transport.

On the interface $z = h/2$:

$$\frac{\partial \Gamma}{\partial t} + \frac{1}{r} \frac{\partial (r \Gamma u_{int})}{\partial r} - \frac{D_{int}}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \Gamma}{\partial r} \right) = -D (n \cdot \nabla C)_{int}$$  \hspace{1cm} (6)

$$\left( \frac{\partial \Gamma}{\partial r} \right)_{r=0} = 0; \quad \left( \frac{\partial \Gamma}{\partial r} \right)_{r=\infty} = 0$$  \hspace{1cm} (7)

In the drops:

$$\frac{\partial C}{\partial t} + \frac{1}{r} \frac{\partial (r Cv_1)}{\partial r} + v_3 \frac{\partial C}{\partial z} = D \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C'}{\partial r} \right) + \frac{\partial^2 C}{\partial z^2} \right)$$  \hspace{1cm} (8)

$$\left( \frac{\partial C'}{\partial r} \right)_{r=0} = \left( \frac{\partial C'}{\partial z} \right)_{z=\infty} = \left( \frac{\partial C'}{\partial r} \right)_{r=\infty} = 0 \quad C(r, z = 0) = \Gamma(r)/K.$$  \hspace{1cm} (9)

$$\sigma(r) = \sigma_{pure} - \Gamma(r) R_G T; \quad R_G \text{ gas constant; } T \text{ absolute temperature.}$$  \hspace{1cm} (10)
Mathematical model: Initial conditions.

For the film thickness:

\[ h(r, t = 0)) = h_{ini} + \frac{r^2}{R_{eq}}, \quad R_{eq}^{-1} = \frac{1}{2} \left( R_1^{-1} + R_2^{-1} \right) \]  \(11\)

For the surfactant distribution:

- initially clean interfaces:

\[ \Gamma(r, t = 0) = 0; \quad C(r, z, t = 0) = C_{ini} \]  \(12\)

- equilibrium surfactant distribution in the film and on the interfaces:

\[ \Gamma(r, t = 0) = KC_{ini}; \quad C(r, z, t = 0) = C_{ini} \]  \(13\)

Transformation and Parameters:

\[ r^* = \frac{r}{R_{eq}a'}; \quad h^* = \frac{h}{R_{eq}a'r^2}; \quad z^* = \frac{z}{R_{eq}a'}; \quad a' = \frac{a}{R_{eq}} \quad \lambda^*; \quad K^*; \quad Pe_{intf}^*; \quad Pe^*; \quad C_{ini}^* \]
Numerical method: Hydrodynamic part in the drops.

BIM for the flow in the drops: The velocity in the drops is given by

\[ v(x) = \int_{\partial V} 2J(r) \cdot T(y) \cdot n \, dS, \]

where \( n \) is the inward normal to \( V \) with boundary \( \partial V \) and

\[ J = \left( \frac{1}{8\pi} \right) \left( \frac{I}{|x - y|} + \frac{(x - y)(x - y)}{|x - y|^3} \right). \]

Let

\[ x = (r^*, 0, z), \quad y = (r' \cos \theta, r' \sin \theta, 0), \quad T(y) = (T_1, T_2, T_3), \]

then

\[ x - y = (r^* - r' \cos \theta, -r' \sin \theta, z), \quad |x - y| = \sqrt{r^2 + r'^2 - 2r^*r' \cos \theta + z^2}, \]

\[ T(y) \cdot n = T_3(y) = (|T_3| \cos \theta, |T_3| \sin \theta, 0), \quad |T_3| = \tau_d(r'). \]
Thus

\[ v_1 = \int_0^{r_l^*} \phi_1(r^*, r') \tau_d(r') \, dr', \quad v_3 = \int_0^{r_l^*} \phi_3(r^*, r') \tau_d(r') \, dr', \]

where

\[
\phi_1(r^*, r') = \frac{r'}{4\pi} \int_0^{2\pi} \left( \frac{2 \cos \theta}{(r^{*2} + r'^2 - 2r^*r' \cos \theta + z^2)^{1/2}} \right. \\
- \left. \frac{z^2 \cos \theta + r^*r' \sin^2 \theta}{(r^{*2} + r'^2 - 2r^*r' \cos \theta + z^2)^{3/2}} \right) d\theta
\]

\[
\phi_3(r^*, r') = \frac{r'}{4\pi} \int_0^{2\pi} \frac{(r^* \cos \theta - r') z r' \, d\theta}{(r^{*2} + r'^2 - 2r^*r' \cos \theta + z^2)^{3/2}}.
\]

Forth-order, hyperbolic-type equation for \( h(r,t) \) is solved by an Euler explicit scheme in time and a second order FD scheme on non-uniform mesh in space.

Requirements for numerical stability:

\[
(\Delta t)_I \leq const \cdot \min_j \left( \frac{\Delta r_j^3}{h_j^2} \right); \quad (\Delta t)_{II} \leq \frac{24}{\lambda} \cdot \min_j \left( \frac{\Delta r_j^4}{h_j^5} \right)
\]

Adaptive mesh/step are used both for the time as well as space discretization: \( \Delta t \) of order \( 10^{-4} \) – \( 10^{-9} \) and in the film region \( \Delta r \) in the range \( 0.1 \) – \( 0.01 \).

The convection-diffusion equation for the surfactant concentration on the interface, \( \Gamma(r,t) \) is solved in similar manner as that for \( h(r,t) \).

The convection-diffusion equation for the surfactant concentration in the drops, \( C(r,z,t) \) is solved by Euler implicit or Crank-Nicolson scheme with respect \( z \) and Euler explicit with respect \( r \).
Numerical tests. Evolution of the minimal film thickness, $h_{\text{min}}$

\[ \lambda = 1; \quad K = 0.2; \quad Pe = 1000; \quad Pe_{\text{int}} = \infty \]
Numerical results. Flow in the drops, $\lambda = 1; \ K = 0.2; \ Pe = 1000; \ Pe_{int} = \infty$
Film profile and the concentration on the interface.
The evolution of the film thickness at different $Pe$
Future work:

- Investigation of the effect of the parameters
- Both phases soluble surfactant
Thank you for your patience and attention!