Numerical Simulation of Drop Coalescence in the Presence of Inter-Phase Mass Transfer

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Contents

Introduction: Drop coalescence and applications; Effect of inter-phase mass transfer.

Mathematical model:

- Simplifications;
- Hydrodynamic model - Stokes equations, lubrication approximation;
- Inter-phase transport of solutes - convection-diffusion equations in the phases.

Numerical method:

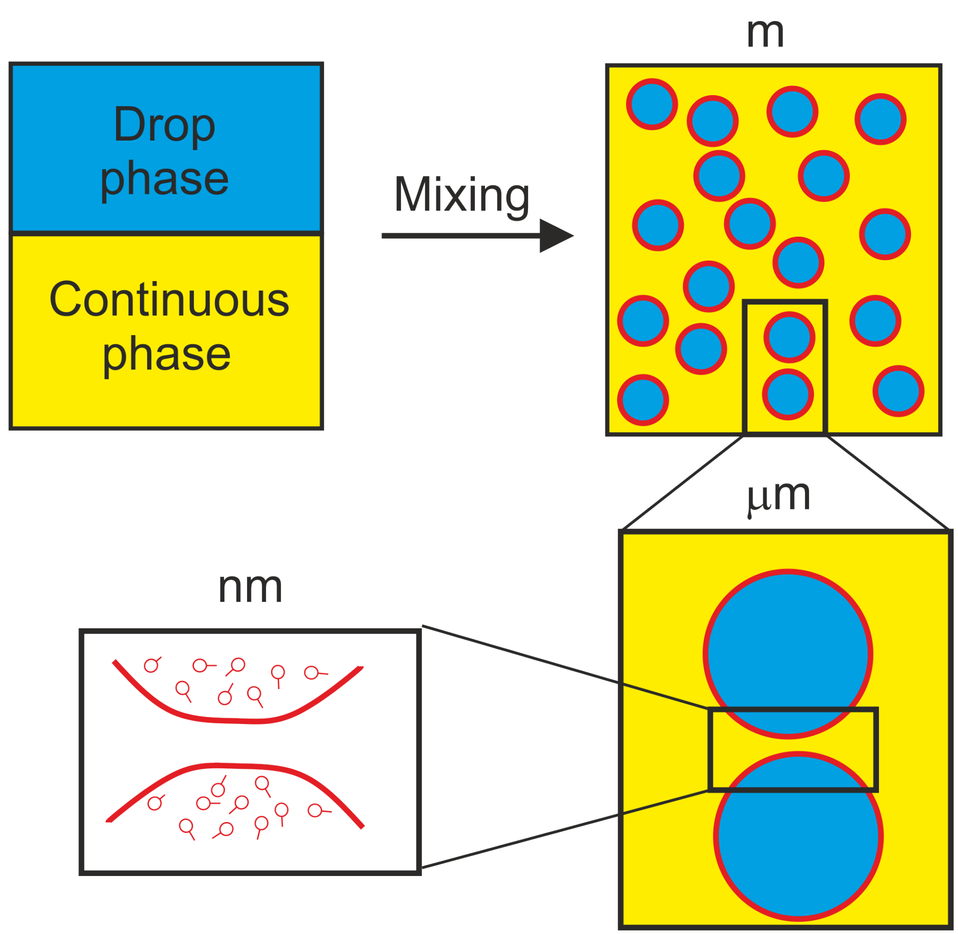
- Boundary Integral Method for the Stokes equations in the drops;
- Finite Difference Method for the flow in the film and the convection-diffusion equations.

Results

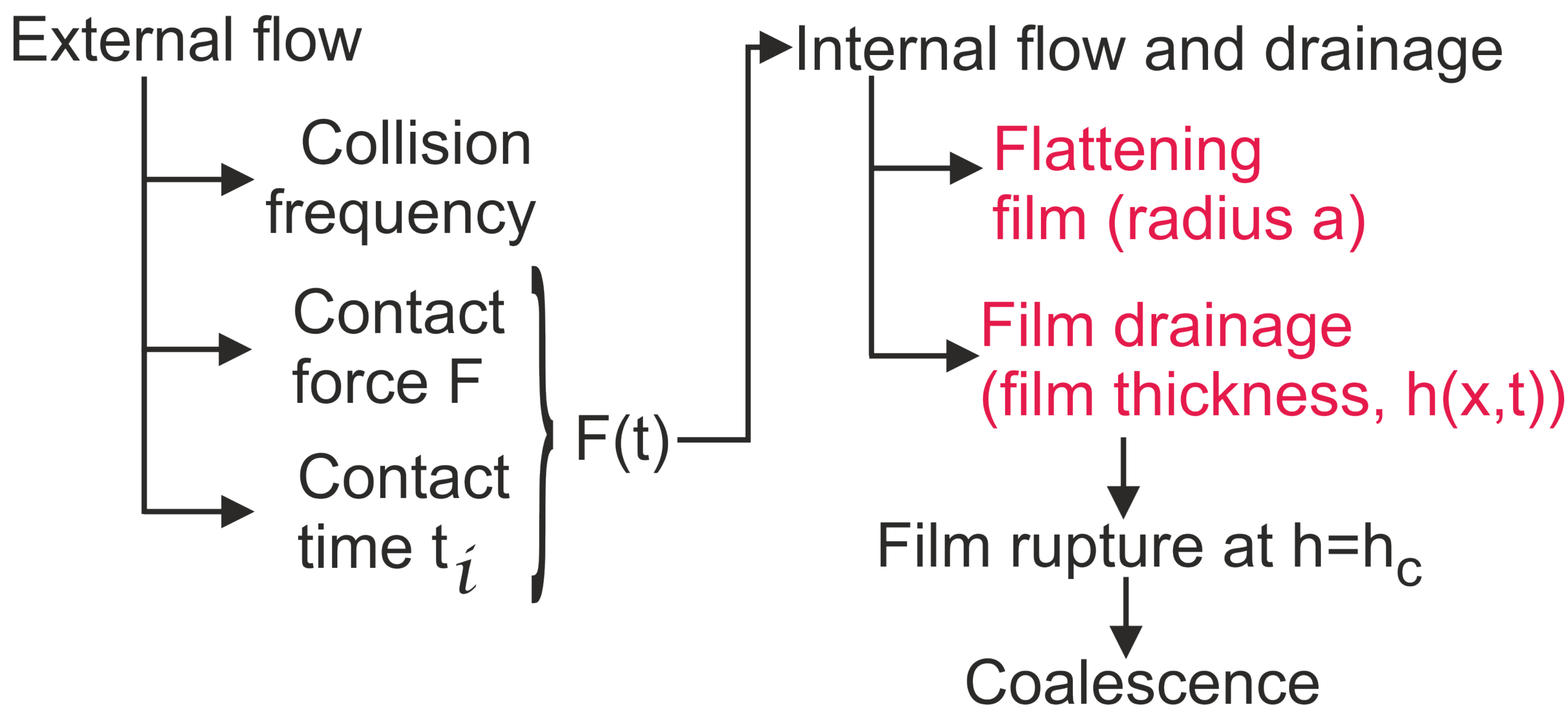
Conclusions

Introduction: Drop coalescence and applications

Applications of multiphase systems: Emulsions - Food; drugs; cosmetics; composite materials; chemicals; petroleum; etc.

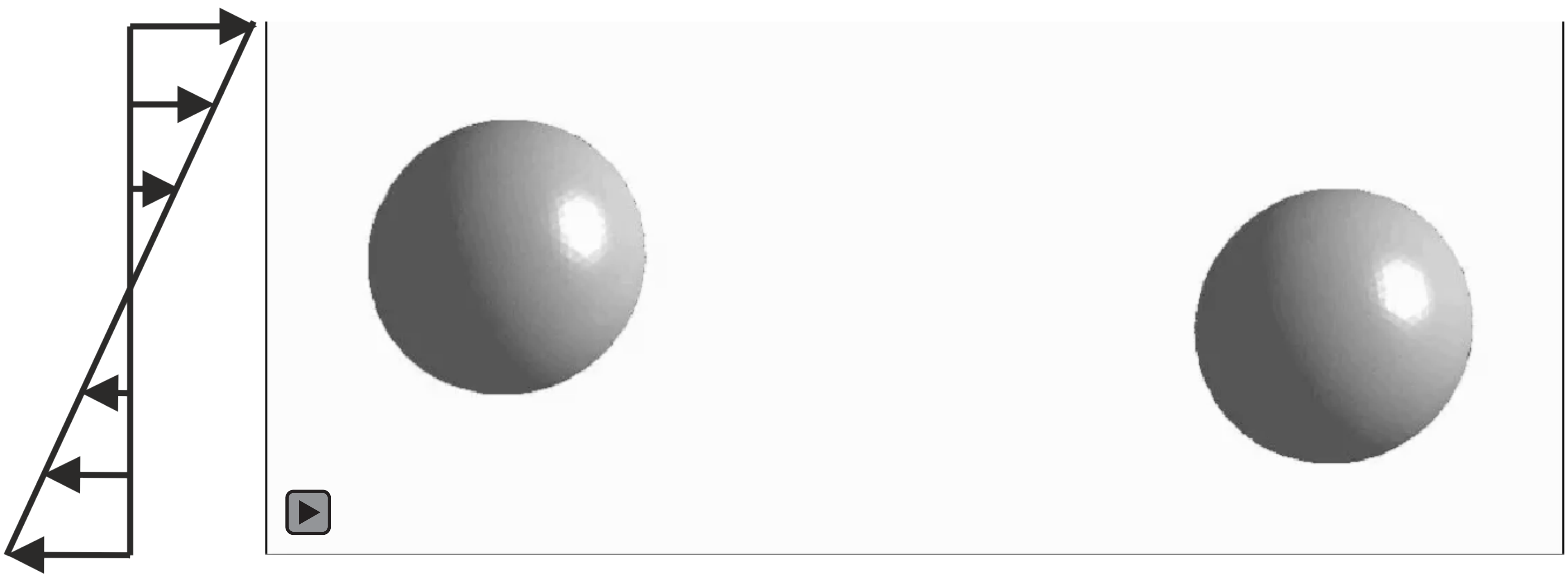


Introduction: Conceptual framework for coalescence modelling.

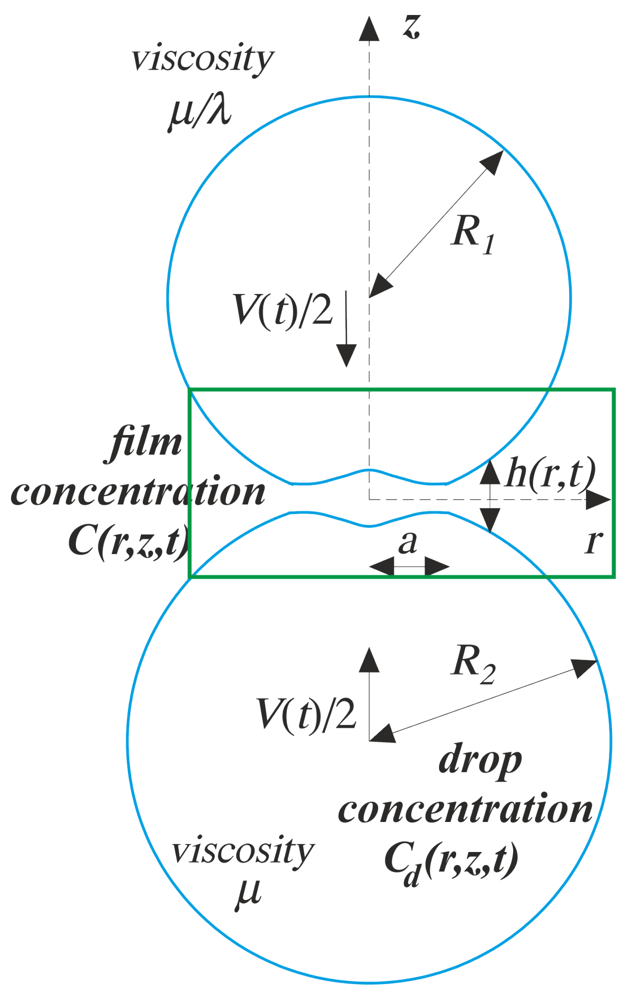


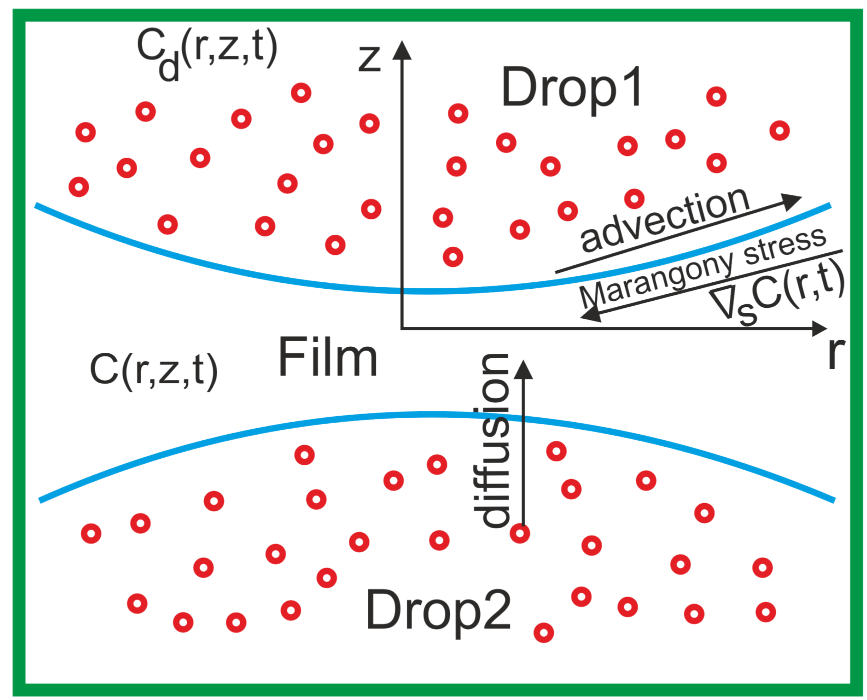
coalescence if $t(h_c) < t_i$

Drop-to-drop interaction in simple shear flow at $Ca = 0.25$



Schematic sketch of the problem





Mathematical model: Hydrodynamic part.

In the drops:

$$\nabla \cdot v = 0; \qquad -\nabla p_d + \nabla^2 v = 0; \qquad \text{Stokes equations in the drops} \qquad (1)$$

In the film:

$$\frac{\partial h}{\partial t} = -\frac{1}{r}\frac{\partial (rhu_u)}{\partial r} + \frac{1}{r}\frac{\lambda}{12}\frac{\partial}{\partial r}\left(h^3 r \frac{\partial p}{\partial r}\right); \qquad \text{Lubrication eq. in the film} \qquad (2)$$

$$u_r = u_u + \frac{\lambda}{2}\frac{\partial p}{\partial r}\left(z^2 - \left(\frac{h}{2}\right)^2\right); \qquad (3)$$

$$p = 2 - \frac{1}{2}\left(\frac{\partial^2 h}{\partial r^2} + \frac{1}{r}\frac{\partial h}{\partial r}\right); \qquad \int_0^{r_\infty} p \; r dr = F(t) \qquad (4)$$

$$\tau_d = -\frac{h}{2}\frac{\partial p}{\partial r} - Ma\frac{\partial C}{\partial r} = \mu\frac{\partial v_r}{\partial z}; \qquad u_u = v_r; \qquad \text{BC at the interface} \qquad (5)$$

Mathematical model: Surfactant transport.

In the film:

$$\frac{\partial C}{\partial t} + u_r \frac{\partial (C)}{\partial r} + u_z \frac{\partial C}{\partial z} = \frac{1}{Pe} \left(\frac{\partial^2 C}{\partial z^2} \right) \tag{6}$$

$$\left(\frac{\partial C}{\partial r} \right)_{r=0} = 0; \qquad \left(\frac{\partial C}{\partial r} \right)_{r=\infty} = 0 \tag{7}$$

In the drops:

$$\frac{\partial C_d}{\partial t} + (u_r)_d \frac{\partial (C_d)}{\partial r} + (u_z)_d \frac{\partial C_d}{\partial z_d} = \frac{1}{Pe_d} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_d}{\partial r} \right) + \frac{\partial^2 C_d}{\partial z_d^2} \right) \tag{8}$$

$$\left(\frac{\partial C_d}{\partial r} \right)_{r=0} = \left(\frac{\partial C_d}{\partial z_d} \right)_{z_d=\infty} = \left(\frac{\partial C_d}{\partial r} \right)_{r=\infty} = 0 \tag{9}$$

At the interface:

$$C_d = C; \qquad \frac{\partial C_d}{\partial z_d} = \frac{1}{P} \sqrt{\frac{Pe_d}{Pe}} \; \frac{\partial C}{\partial z} \tag{10}$$

Mathematical model: Initial conditions.

For the film thickness:

$$h(r, t = 0)) = h_{ini} + r^2, \tag{11}$$

For the solute distribution:

- initially uniform concentration only in the drops:

$$C_d(r, z_d, t = 0) = 1; \qquad C(r, z, t = 0) = 0. \tag{12}$$

- initially uniform concentration only in the film:

$$C_d(r, z_d, t = 0) = 0; \qquad C(r, z, t = 0) = 1. \tag{13}$$

Transformation and Parameters:

$$\lambda; \qquad P; \qquad Pe; \qquad Pe_d; \qquad Ma$$

Numerical method: Hydrodynamic part in the drops.

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

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

where $\mathbf{n}$ is the inward normal to the boundary ∂V of V and

$$\mathbf{J} = (1/8\pi)(\mathbf{I}/|\mathbf{x}-\mathbf{y}| + (\mathbf{x}-\mathbf{y})(\mathbf{x}-\mathbf{y})/|\mathbf{x}-\mathbf{y}|^3).$$

Let

$$\mathbf{x} = (r^*, 0, z), \quad \mathbf{y} = (r' \cos\theta, r' \sin\theta, 0), \quad \mathbf{T}(\mathbf{y}) = (\mathbf{T_1}, \mathbf{T_2}, \mathbf{T_3}),$$

then

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

$$\mathbf{T}(\mathbf{y}) \cdot \mathbf{n} = \mathbf{T_3}(\mathbf{y}) = (|\mathbf{T_3}|\cos\theta, |\mathbf{T_3}|\sin\theta, 0), \quad |\mathbf{T_3}| = \tau_d(r'),$$

Thus the two components of the velocity in the drop is given by:

$$(u_r)_d(r, z_d) = \int_0^{r_l^*} \phi_1(r^*, r')\tau_d(r')\, dr', \quad (u_z)_d(r, z_d) = \int_0^{r_l^*} \phi_3(r^*, r')\tau_d(r')\, dr',$$

where

$$\begin{aligned} \phi_1(r^*, r') &= \frac{r'}{4\pi} \int_0^{2\pi} \Bigg(\frac{2\cos\theta}{(r^{*2} + r'^2 - 2r^* r' \cos\theta + z^2)^{1/2}} \\ &- \frac{z^2 \cos\theta + r^* r' \sin^2\theta}{(r^{*2} + r'^2 - 2r^* r' \cos\theta + z^2)^{3/2}} \Bigg)\, d\theta \end{aligned}$$

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

Numerical method: Hydrodynamic part in the film. Convection diffusion in the drops and on the interface

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.

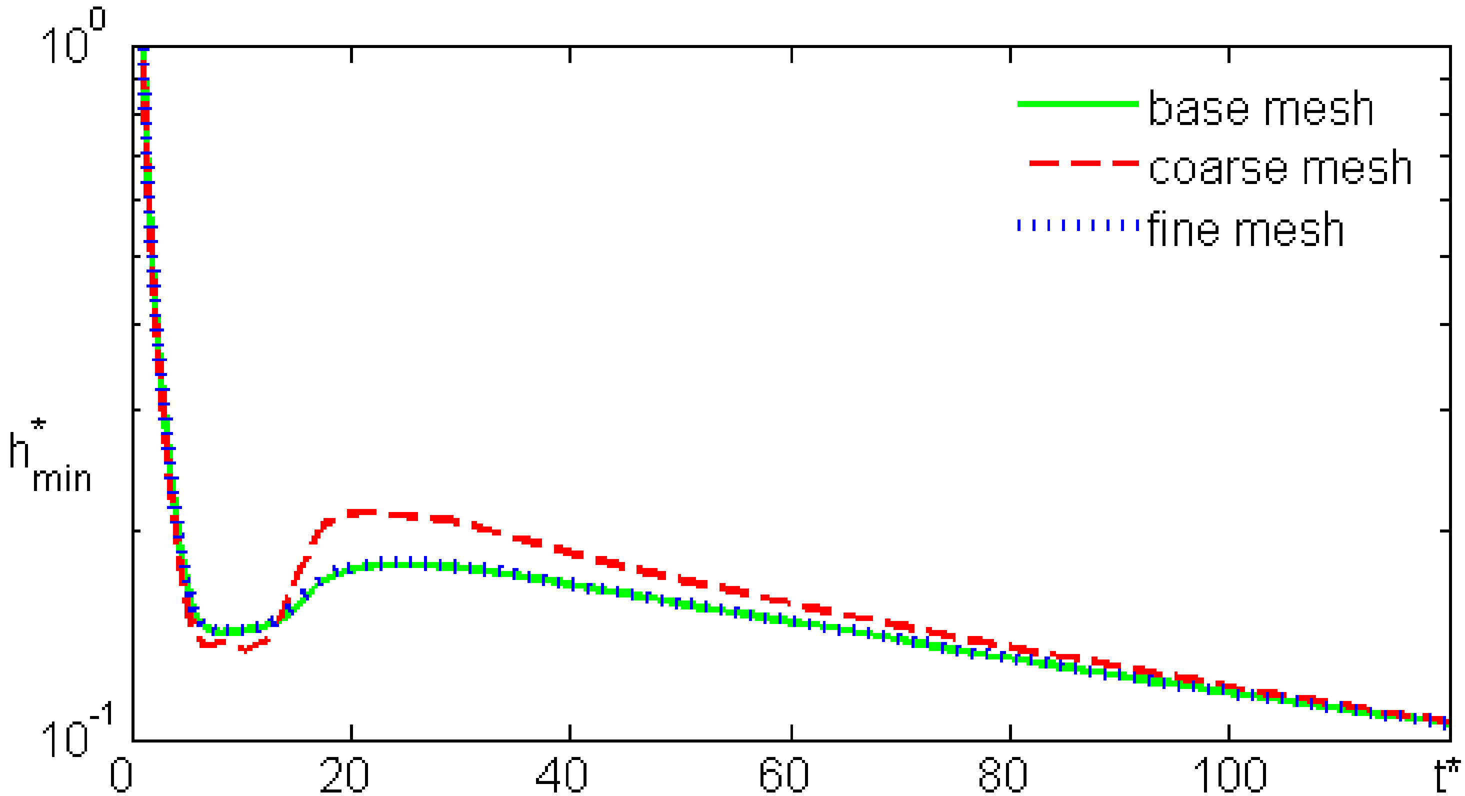
Requirements for numerical stability:

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

Adaptive mesh/step are used both for the time as well as space discretization: Δt of order $10^{-4} - 10^{-9}$; in the film region Δr and Δz of order 0.01

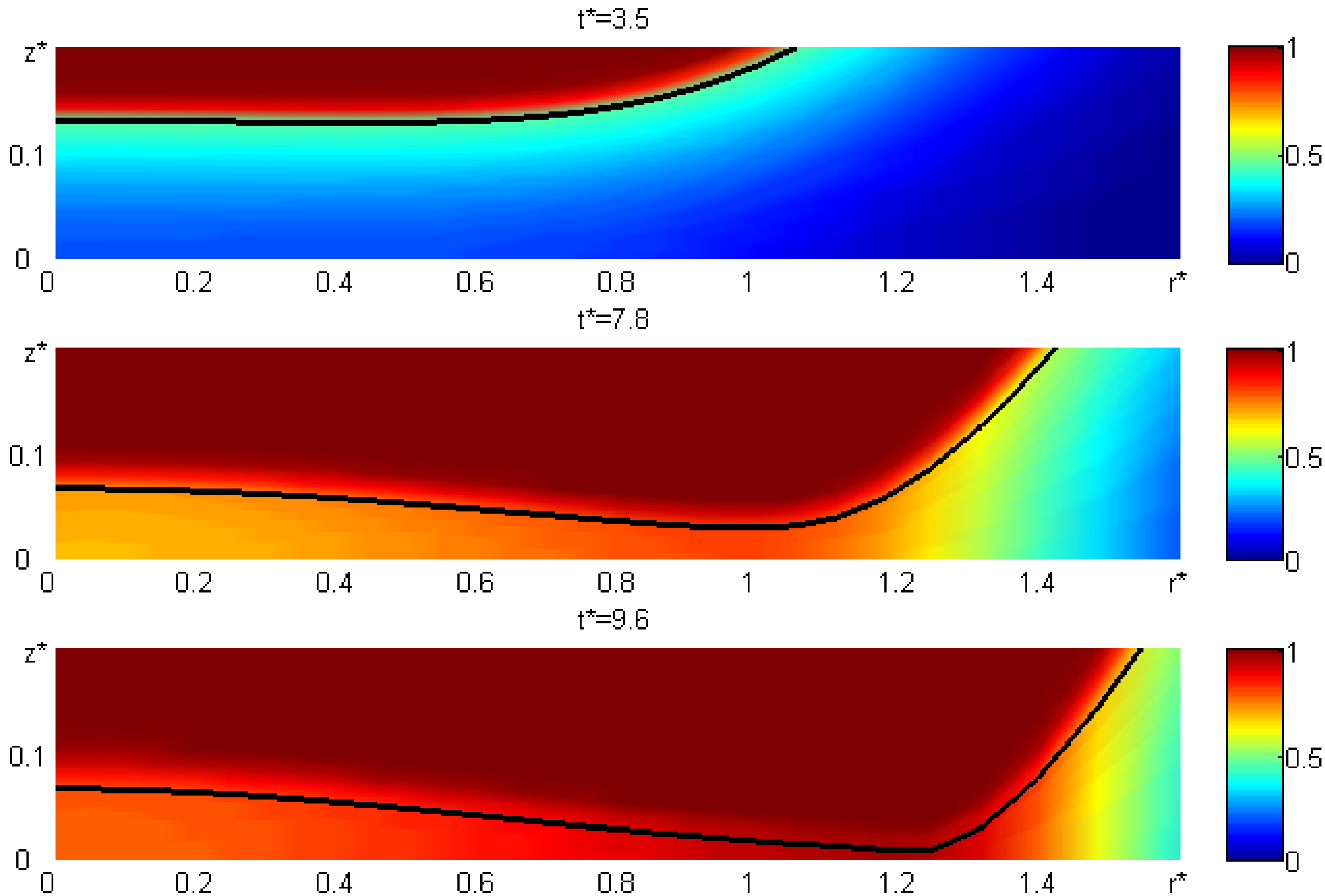
The convection-diffusion equations for the solute concentration in the drops and in the film are solved simultaneously. Second order FD approximation in r and z in combination of hybrid (implicit/explicit) time integration is developed.

Numerical tests. Evolution of the minimal film thickness, h_{min}

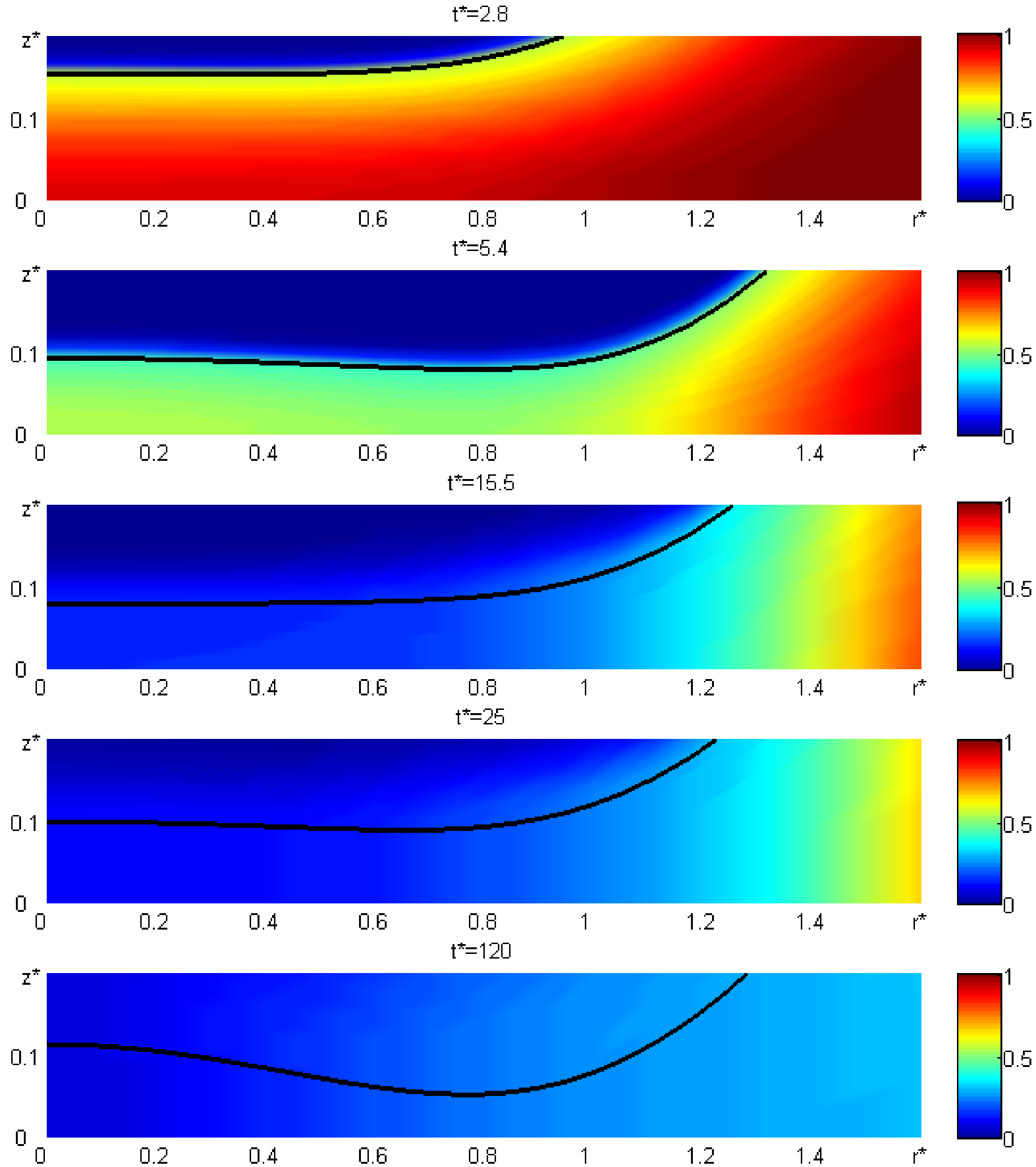


$$\lambda = 1; \quad P = 1; \quad Pe = 250; \quad Pe_d = 25000; \quad Ma = 1$$

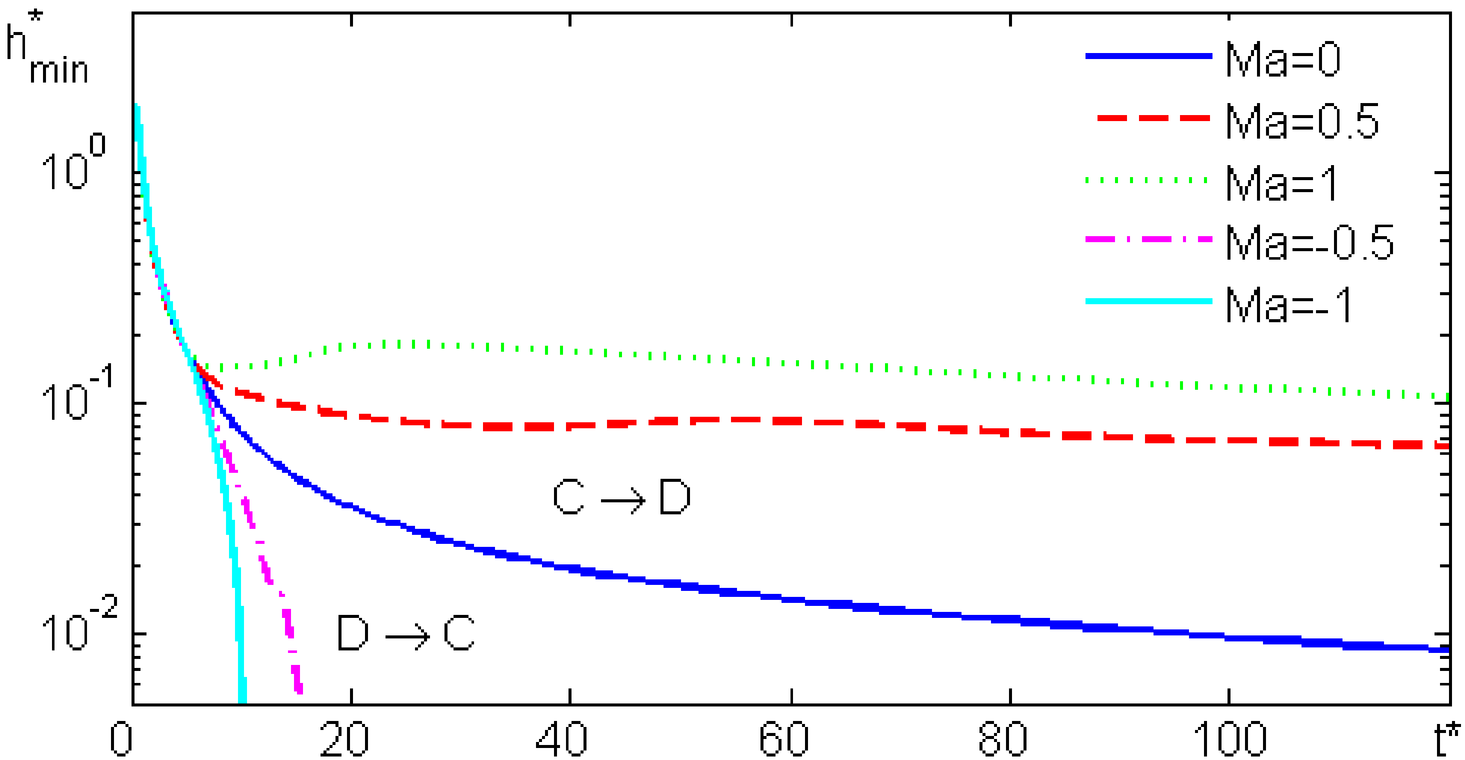
Numerical results. The solute distribution at $\lambda = 1; P = 1; Pe = 250;$ $Pe_d = 25000;\ Ma = -1(D \to C)$



The solute distribution at $Ma = 1(C \to D)$



Evolution of the minimal film thickness, h_{min} at $\lambda = 1;\ P = 1;\ Pe = 250;\ Pe_d = 25000$ and different values of Ma



Future work:

- **Investigation of the effect of the parameters.**

- **The case of surface active solutes.**

Thank you for your patience and attention!