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

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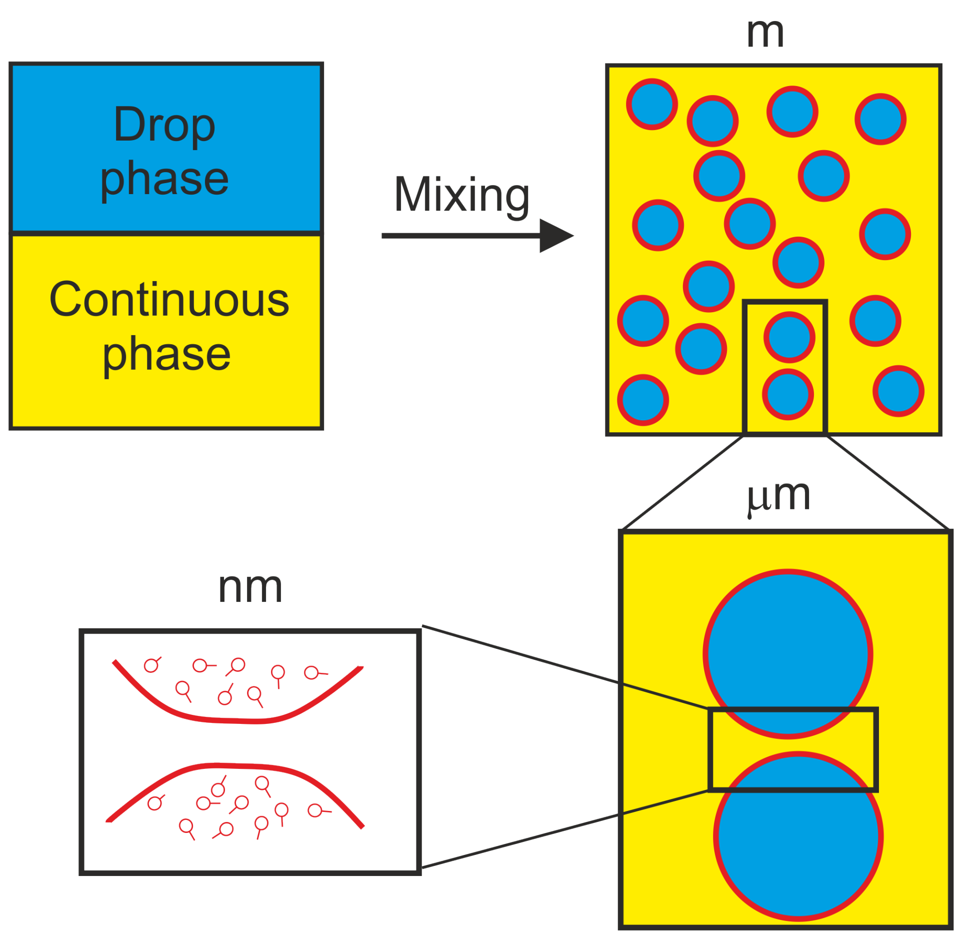
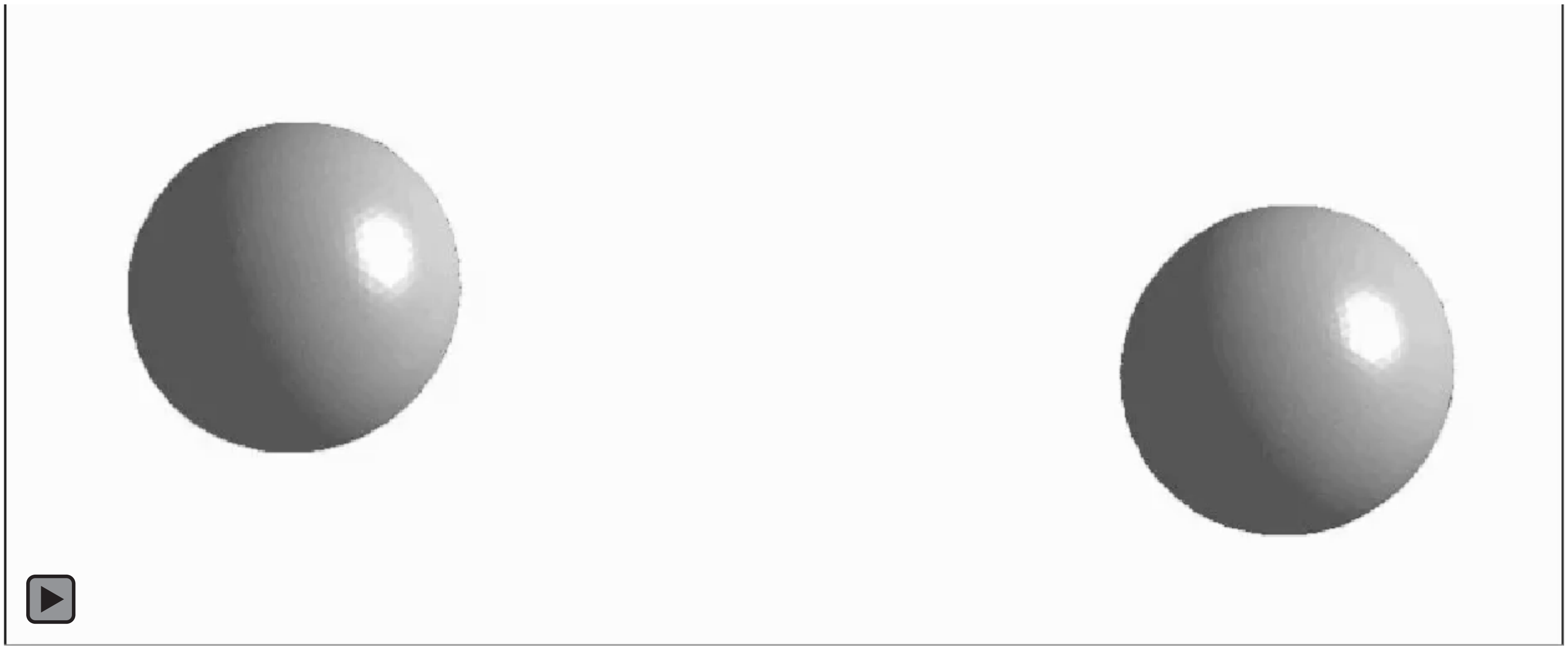
Introduction: Drop coalescence and applications

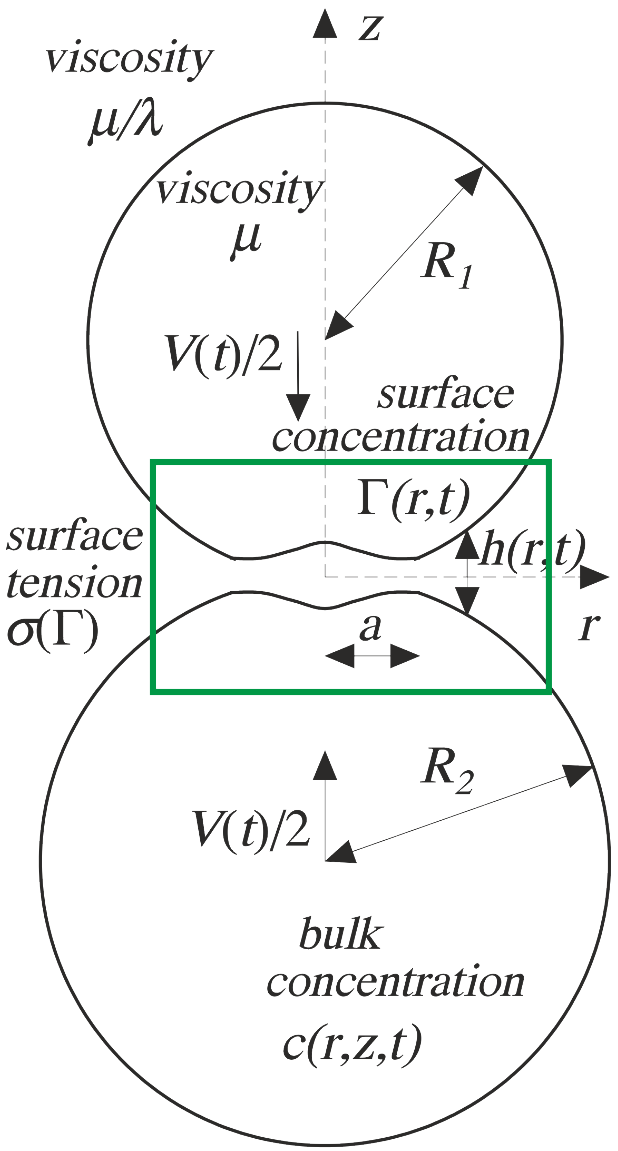
Applications of multiphase systems: Emulsions - Food; drugs; cosmetics; composite materials; chemicals; petroleum; etc.

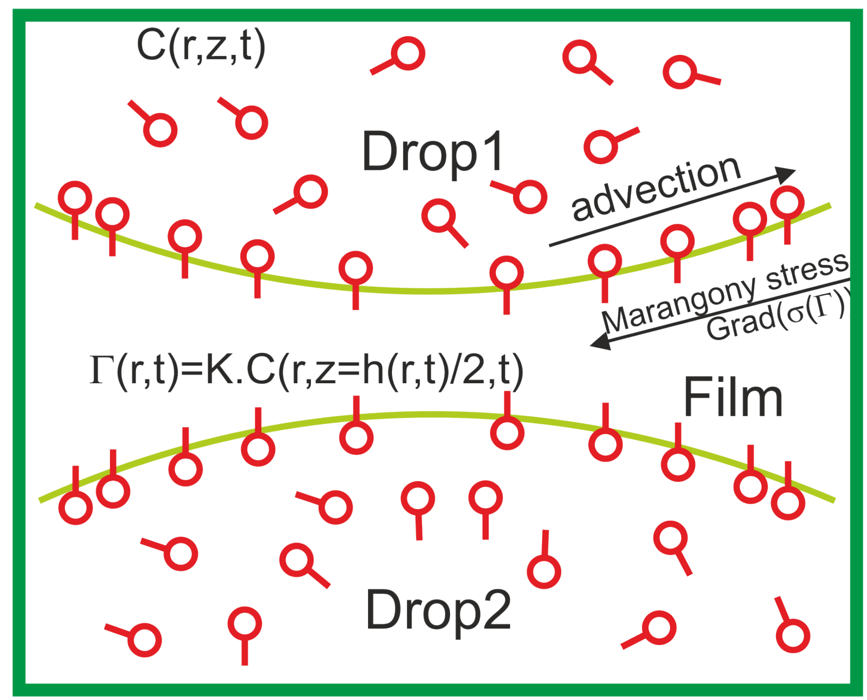


Drop-to-drop interaction in simple shear flow at $Ca = 0.25$

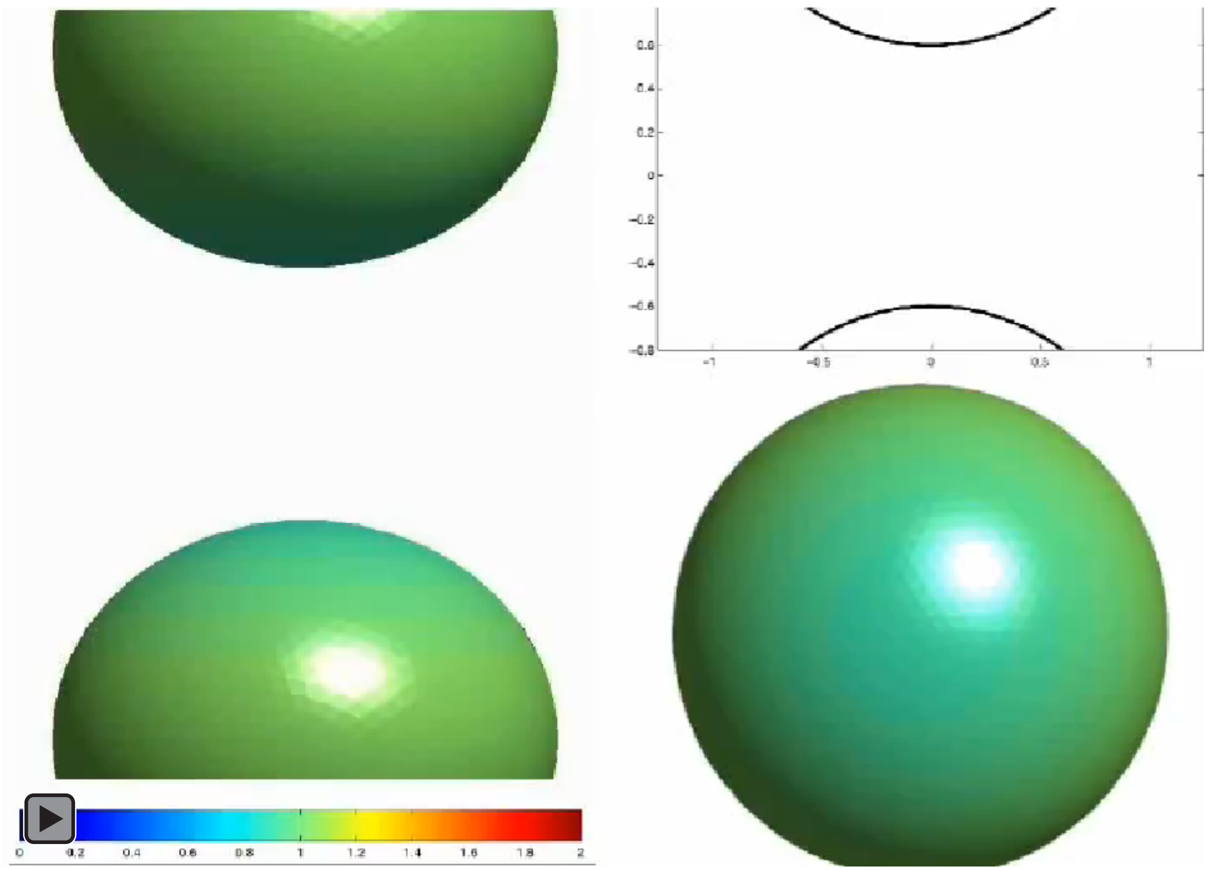


Schematic sketch of the problem





Head-on collision in axisymmetric compressional flow, insoluble surfactant.



Mathematical model: Hydrodynamic part.

In the drops:

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

In the film:

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

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

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

$$\tau = \mu \frac{\partial v_1}{\partial z}; \qquad u_{int} = v_1; \qquad \text{BC at the interface} \qquad (5)$$

Mathematical model: Surfactant transport.

On the interface $z = h/2$:

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

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

In the drops:

$$\frac{\partial C}{\partial t} + \frac{1}{r}\frac{\partial (rCv_1)}{\partial r} + v_3\frac{\partial C}{\partial z} = D\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{\partial^2 C}{\partial z^2}\right) \qquad (8)$$

$$\left(\frac{\partial C}{\partial r}\right)_{r=0} = \left(\frac{\partial C}{\partial z}\right)_{z=\infty} = \left(\frac{\partial C}{\partial r}\right)_{r=\infty} = 0 \qquad C(r, z=0) = \Gamma(r)/K. \qquad (9)$$

$\sigma(r) = \sigma_{pure} - \Gamma(r) R_G T;$ R_G gas constant; T absolute temperature. (10)

Mathematical model: Initial conditions.

For the film thickness:

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

For the surfactant distribution:

- initially clean interfaces:

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

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

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

Transformation and Parameters:

$$r^* = \frac{r}{R_{eq}a'};\ h^* = \frac{h}{R_{eq}a'^2};\ z^* = \frac{z}{R_{eq}a'},\ a' = \frac{a}{R_{eq}} \qquad \lambda^*;\ K^*;\ Pe^*_{intf};\ Pe^*;\ C^*_{ini}$$

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 V with boundary ∂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

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

where

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

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

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:

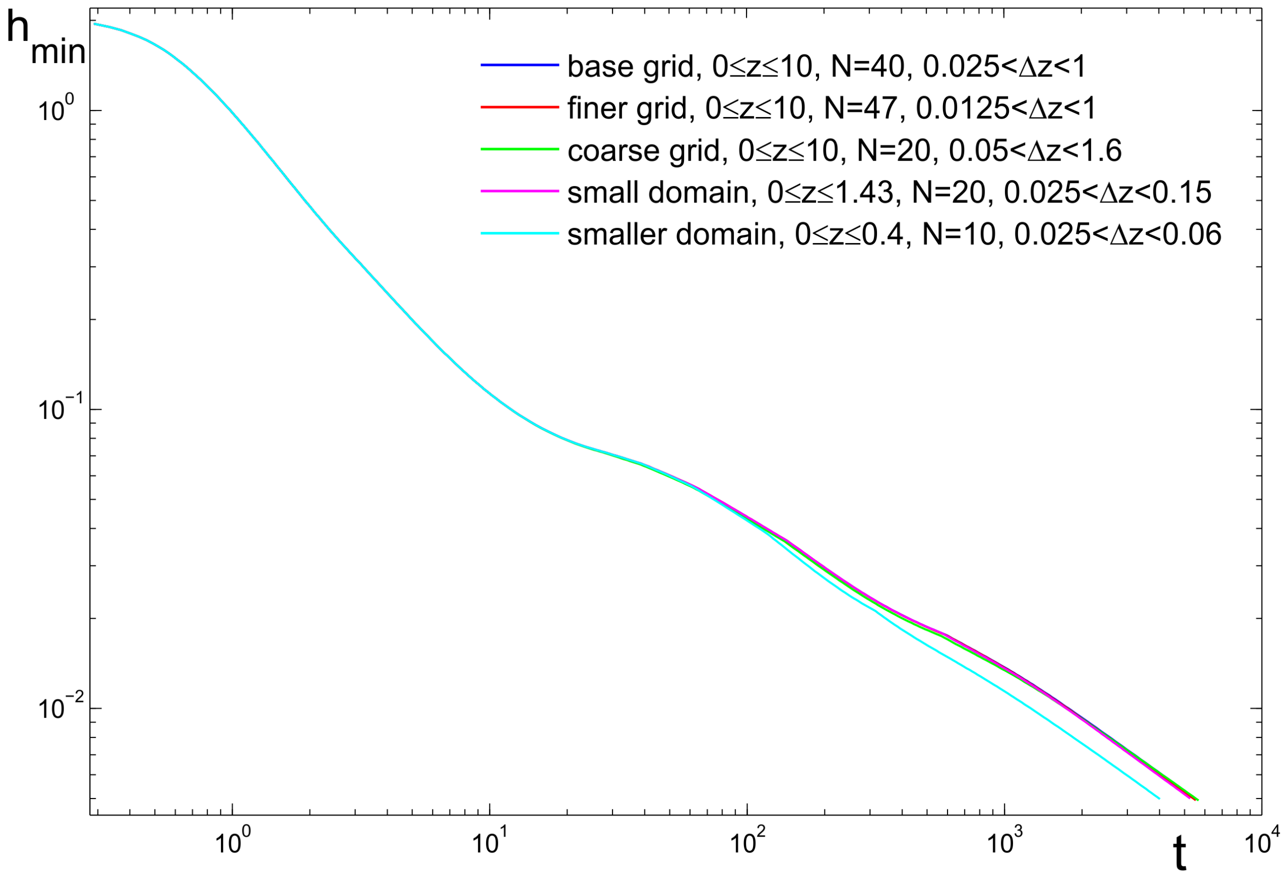
$$(\Delta t)_I \le const \cdot \min_j \left(\frac{\Delta r_j^3}{h_j^2} \right); \quad (\Delta t)_{II} \le \frac{24}{\lambda} \cdot \min_j \left(\frac{\Delta r_j^4}{h_j^5} \right)$$

Adaptive mesh/step are used both for the time as well as space discretization: Δt of order $10^{-4} - 10^{-9}$ and in the film region Δr 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 $h(r,t)$.

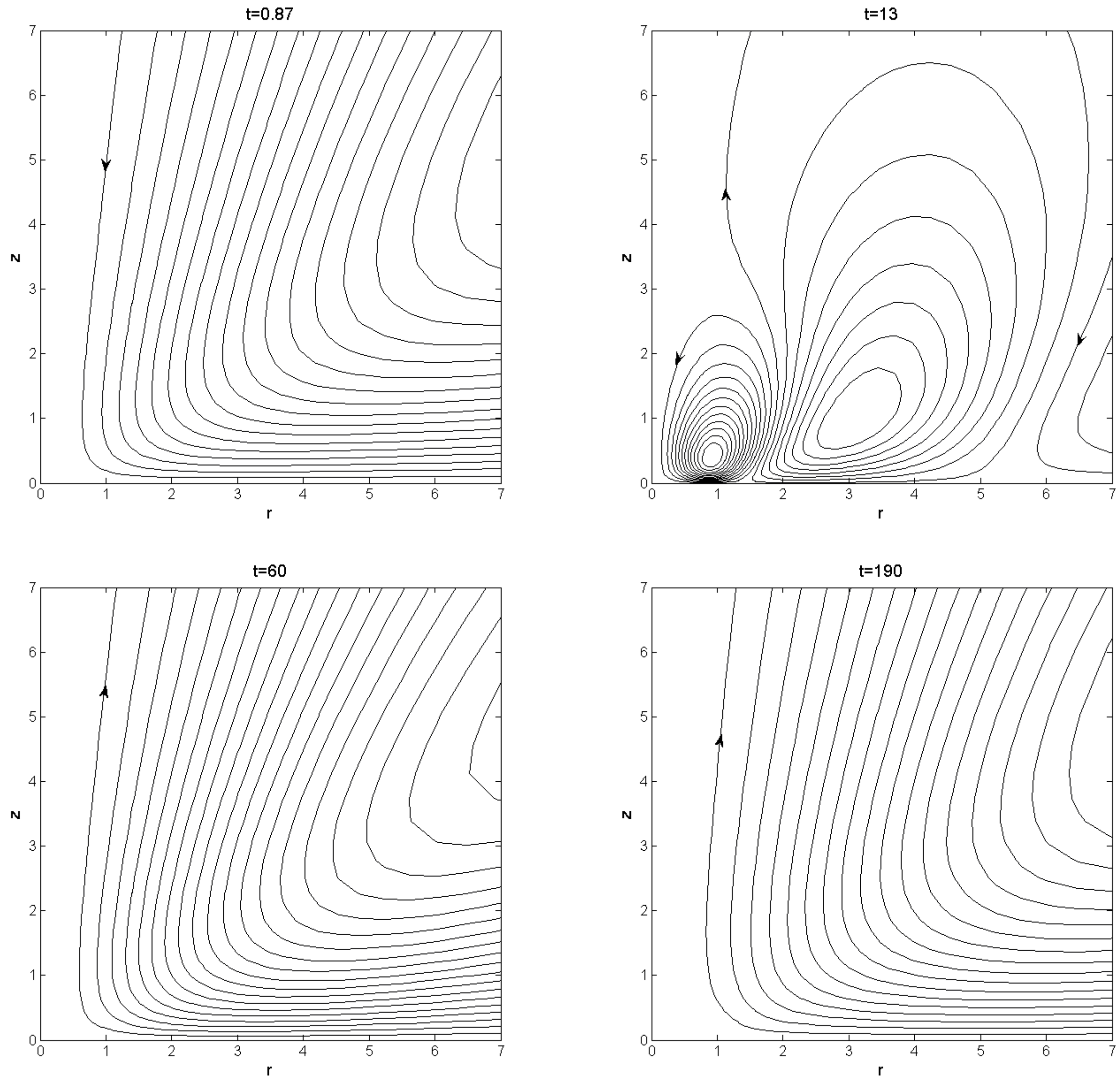
The convection-diffusion equation for the surfactant concentration in the drops, $C(r,z,t)$ is solved by Euler implicit or Crank-Nikolson scheme with respect z and Euler explicit with respect r.

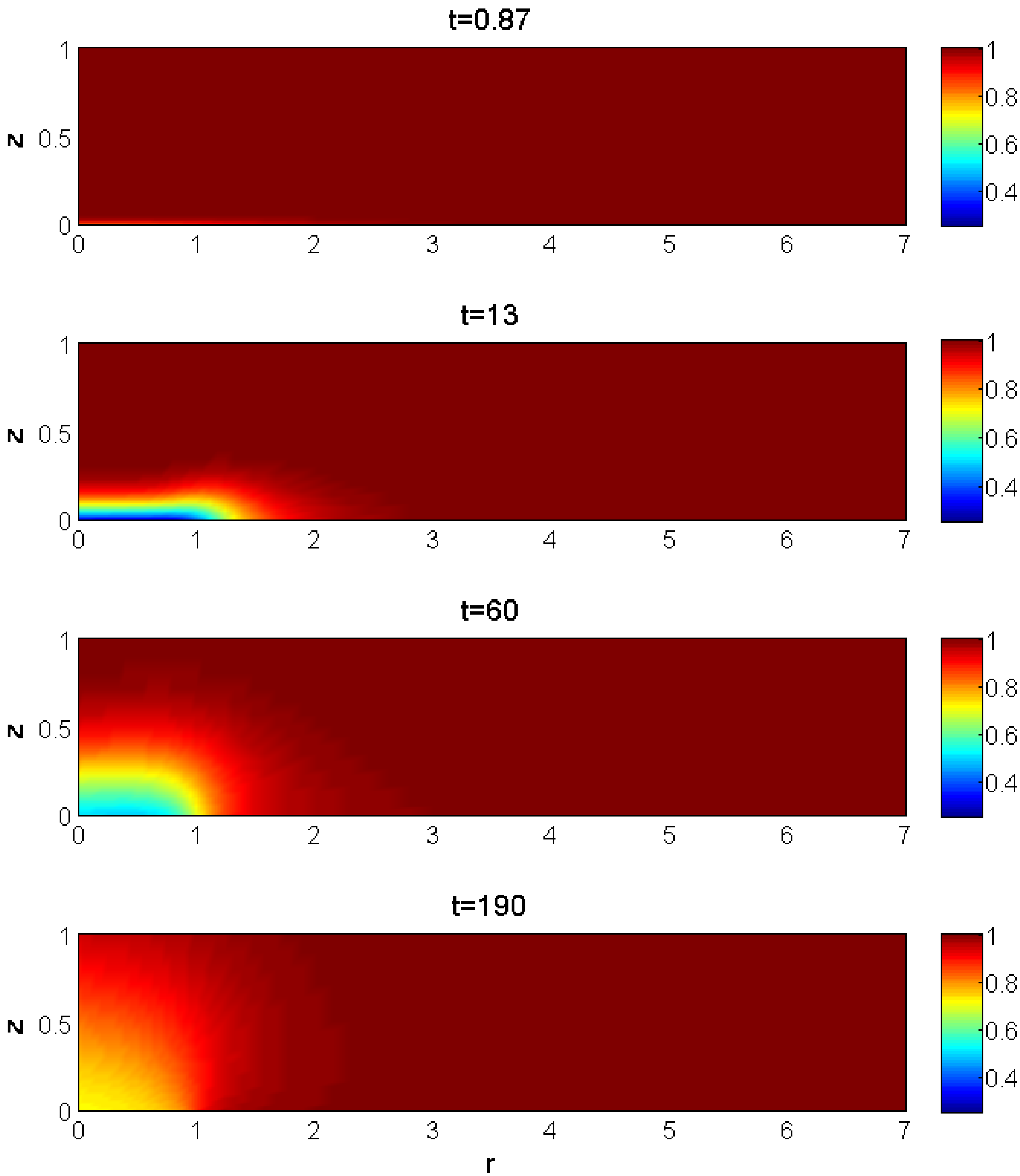
Numerical tests. Evolution of the minimal film thickness, h_{min}



$$\lambda = 1;\ K = 0.2;\ Pe = 1000;\ Pe_{int} = \infty$$

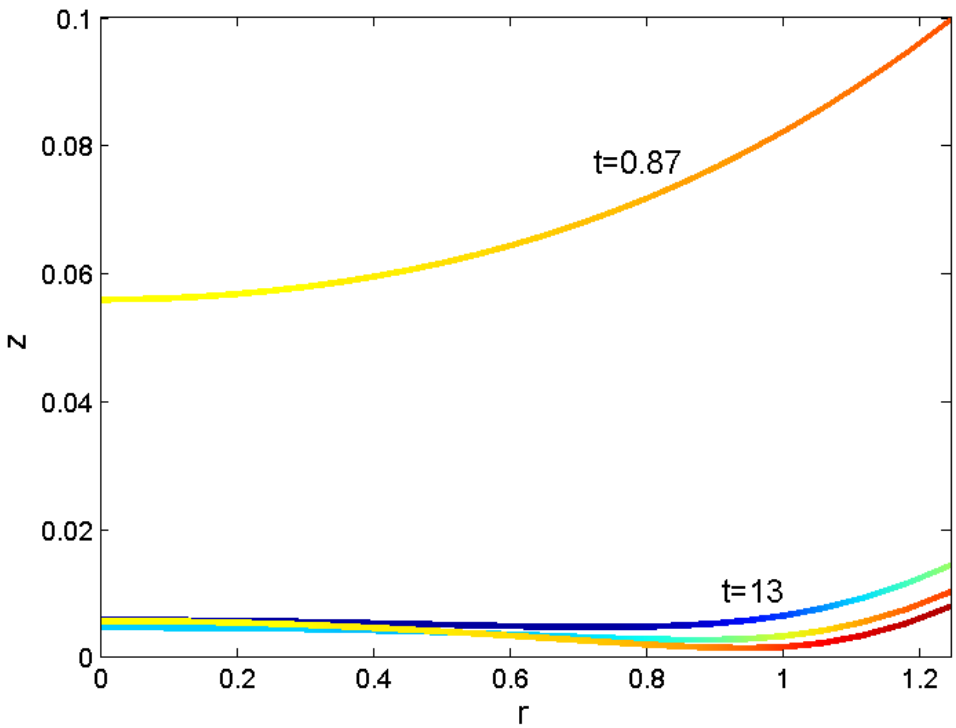
Numerical results. Flow in the drops, $\lambda = 1;\ K = 0.2;\ Pe = 1000;\ Pe_{int} = \infty$

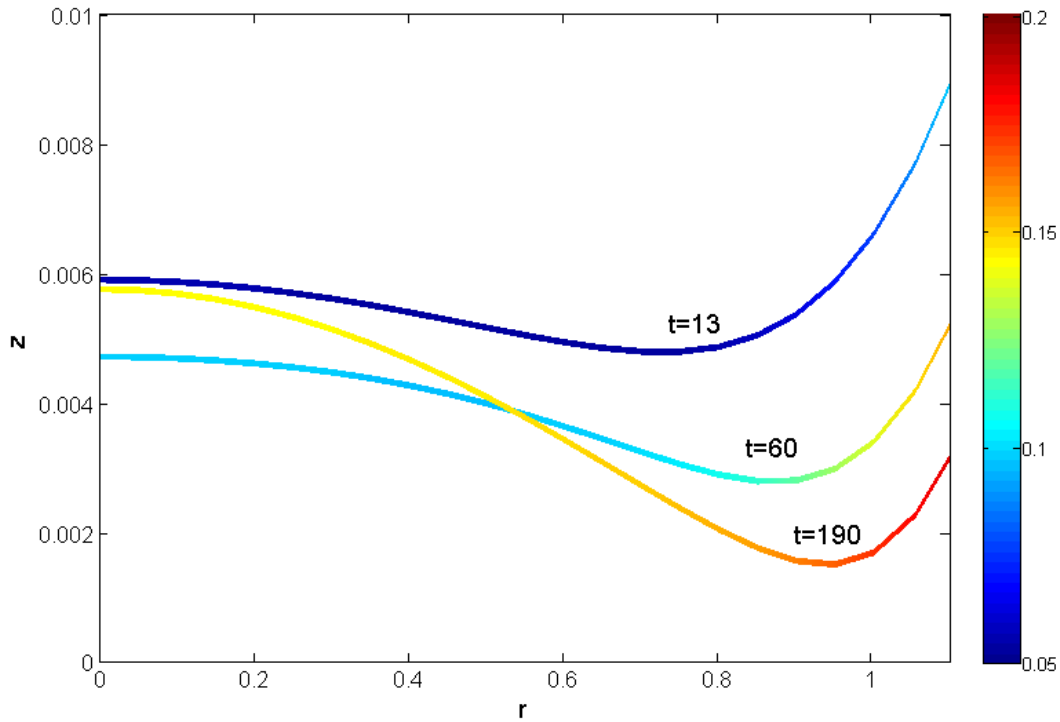


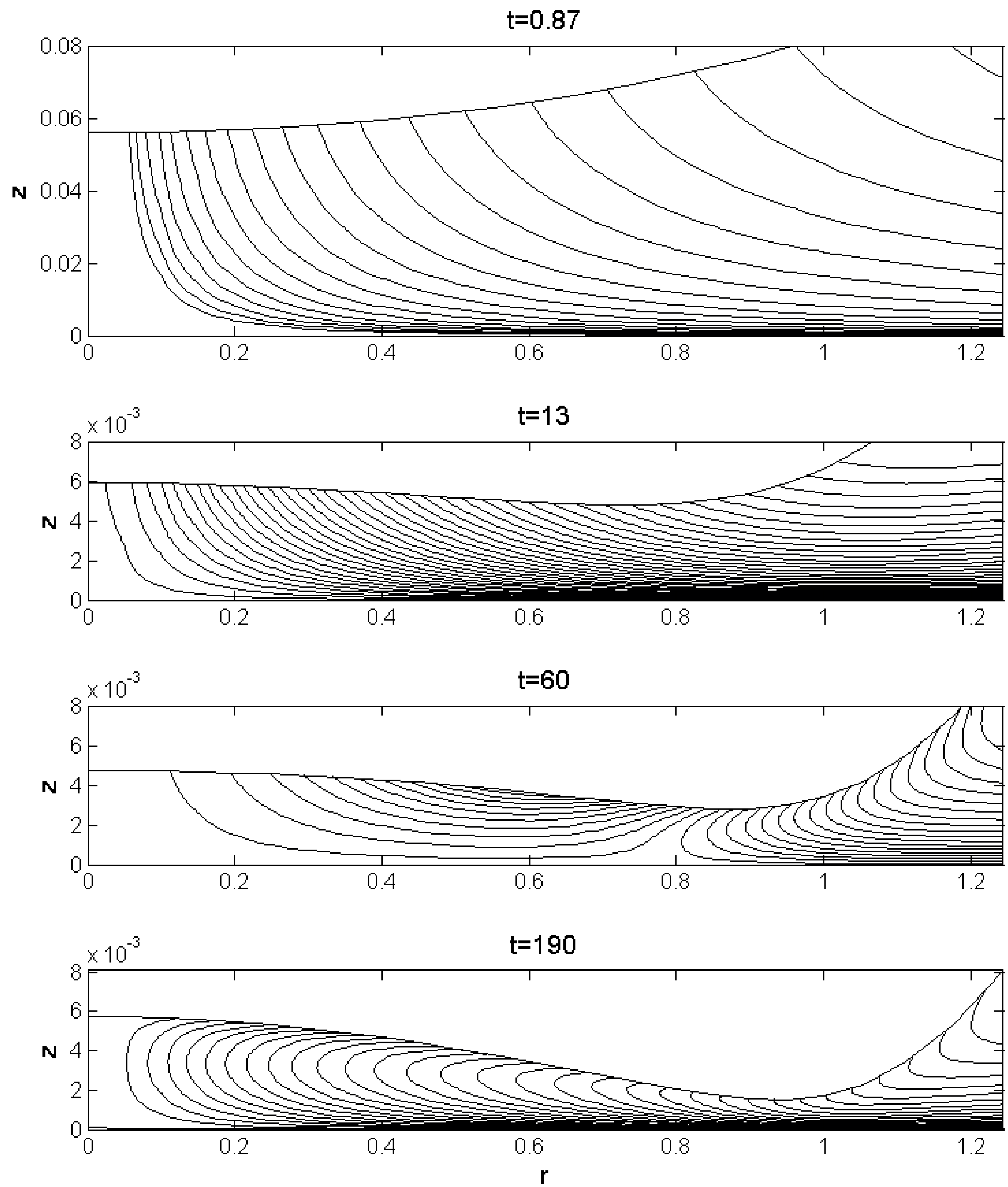


t=0.87
t=13
t=60
t=190
z
r
0
0.5
1
2
3
4
5
6
7
0.4
0.6
0.8

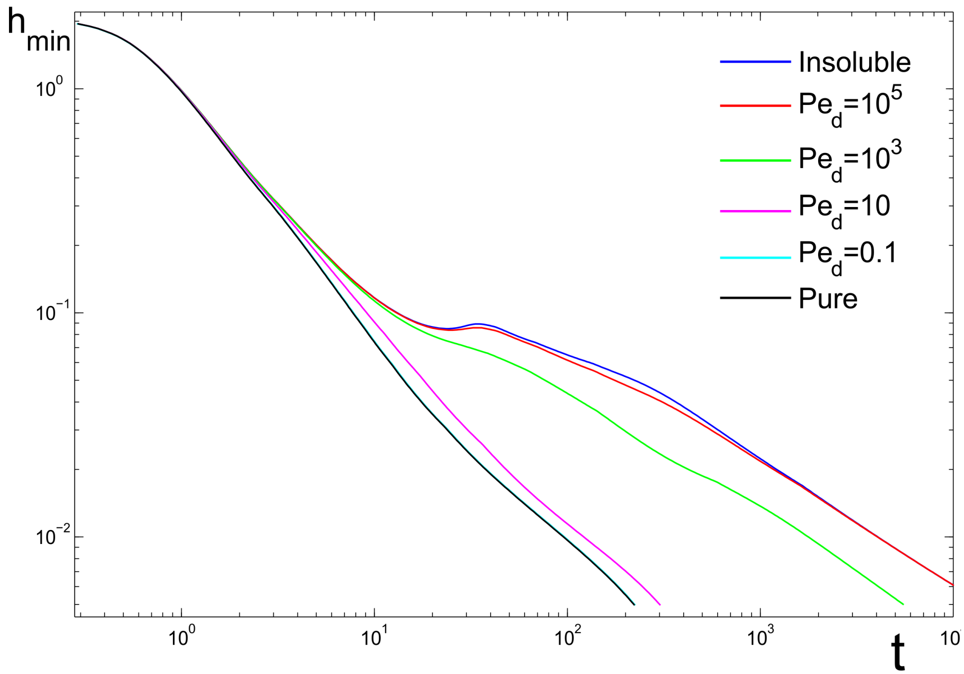
Film profile and the concentration on the interface.

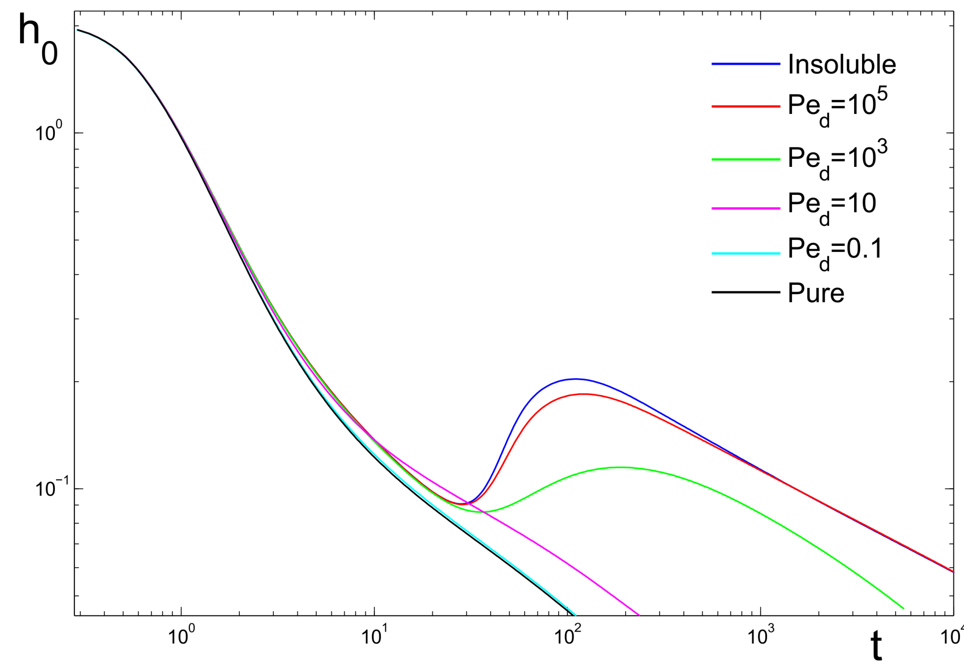





t=0.87
0.08
0.06
z 0.04
0.02
0
0
0.2
0.4
0.6
0.8
1
1.2
t=13
x 10^-3
8
6
z 4
2
0
t=60
x 10^-3
t=190
x 10^-3
r

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!