Modelling of miscible interfaces

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EPSRC project: Pore-level Network Modelling of the Miscible Displacement, 2009-2012, £264,281

Current projects:

- Mixing dynamics in diffusion-limited reactions, *RFBR-Royal Society*, 2016-2018
- Stability, nonlinear dynamics and control of the behaviour of multiphase hydrodynamic systems, *Russian Science Foundation*, 2014-2018, PI: Prof. T. Lyubimova
- Heat and mass transfer in multicomponent and multiphase media. From space experiments to Earth technologies, *Government of Perm Region*, 2015-2017, PI: Prof. T. Lyubimova

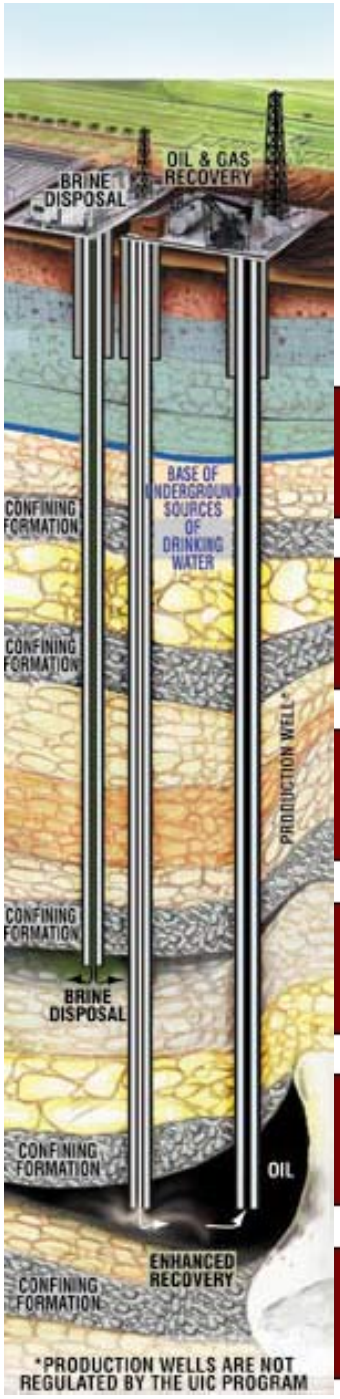
Aim

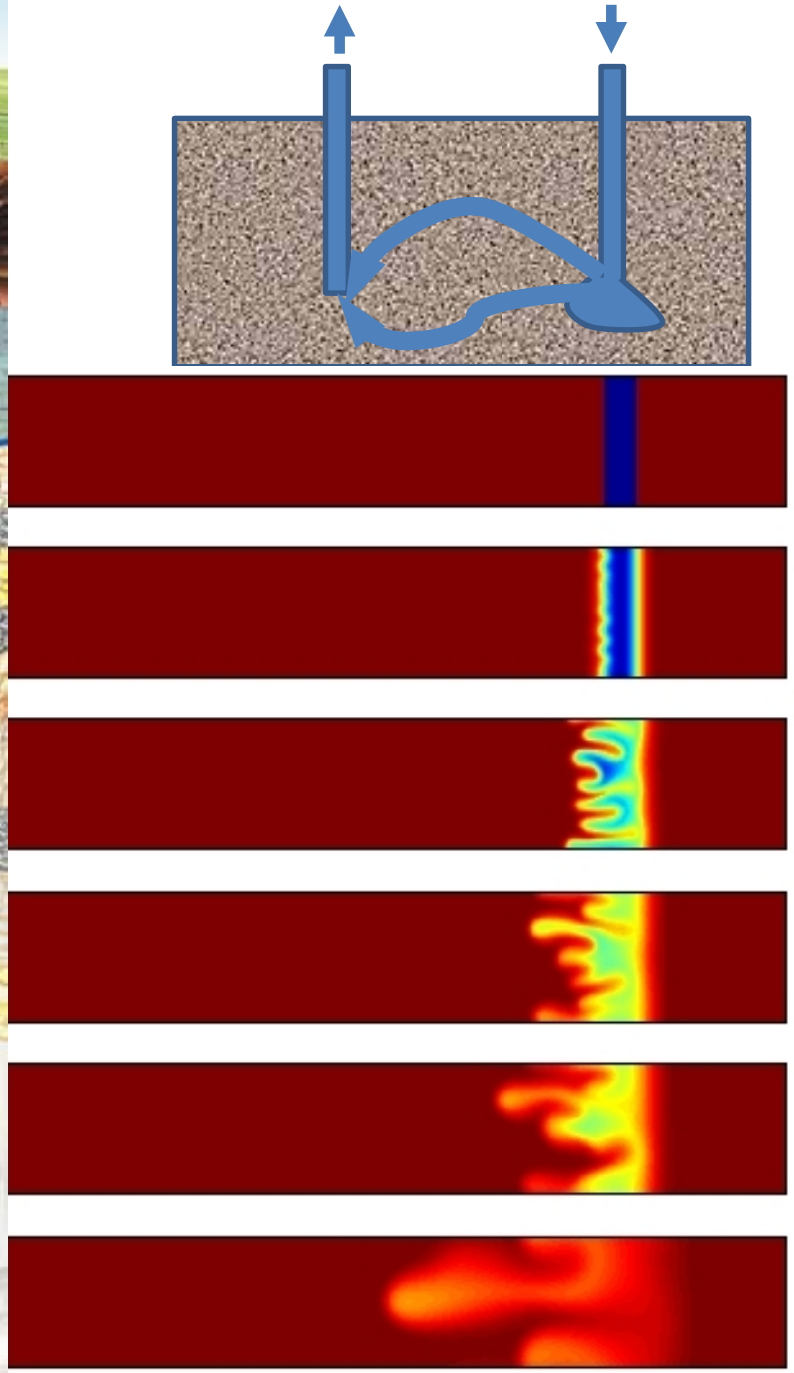
- a theoretical model for accurate description of miscible gas/liquid or liquid/liquid interfaces with account of interfacial diffusion, variations in interface shape, dynamic surface tension, and hydrodynamic flows induced by concentration gradients.

Example: *dissolution of a honey droplet in a tea cup,*

or

absorption of CO_2 bubble (in supercritical conditions) by crude oil, or absorption of CO_2 bubble by aqueous amine solution



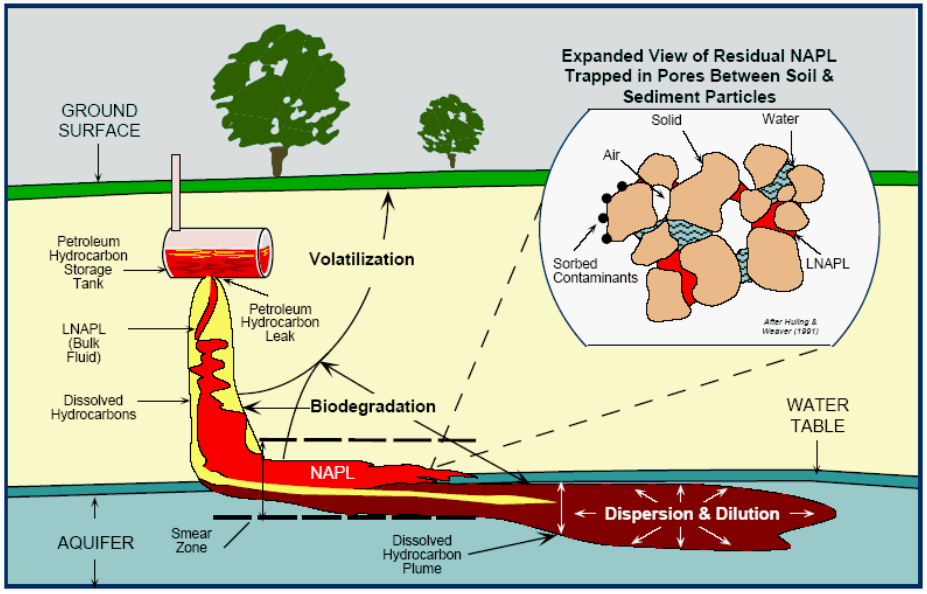


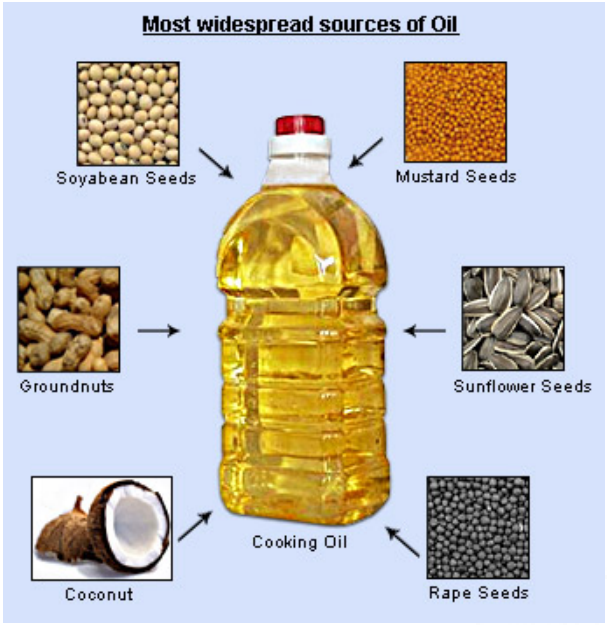
Enhanced Oil Recovery:

(miscible displacement)

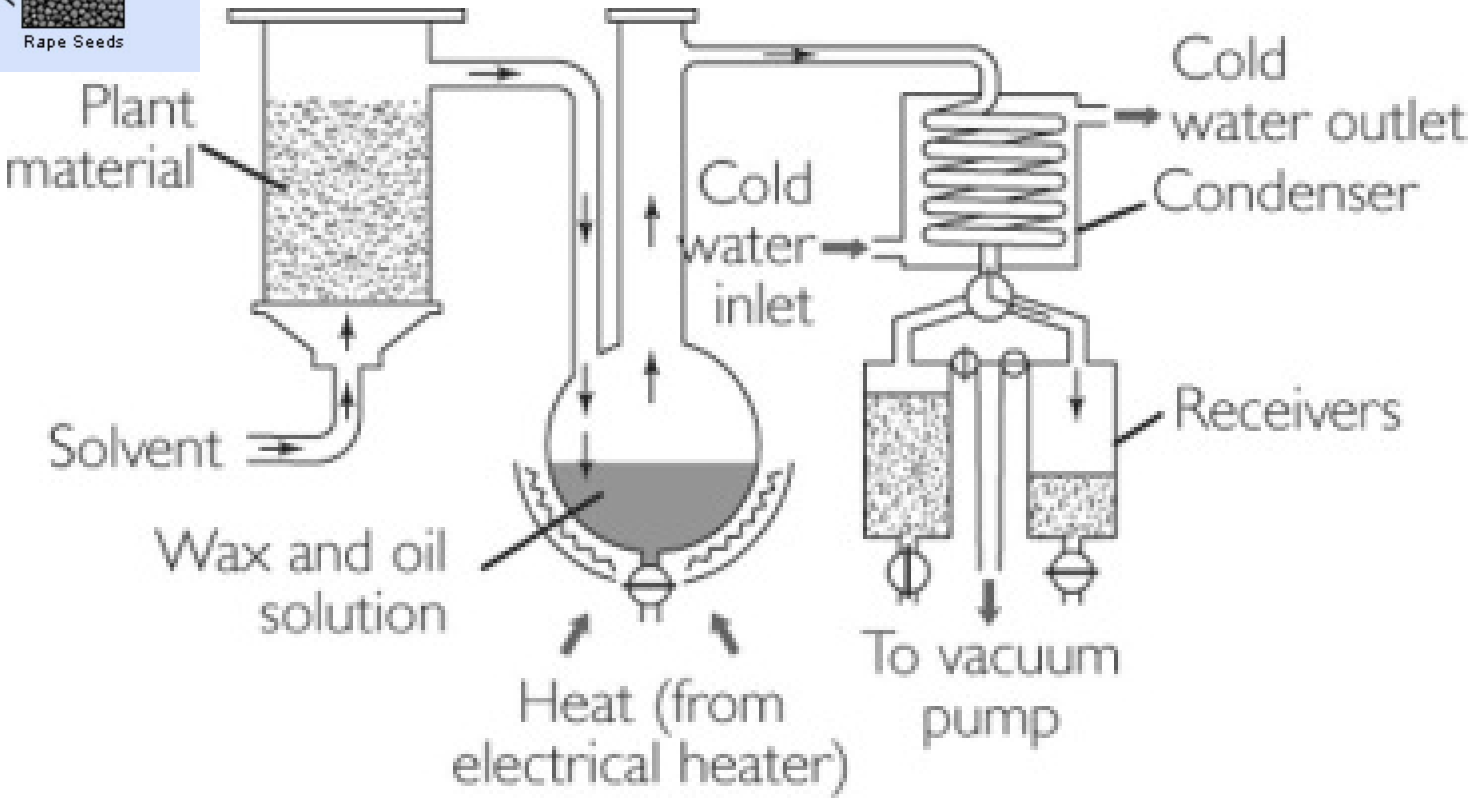
CO_2 sequestration

Enhanced Aquifer Remediation

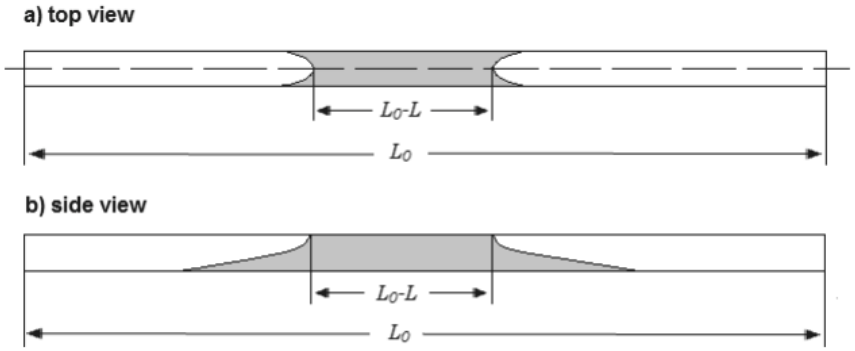




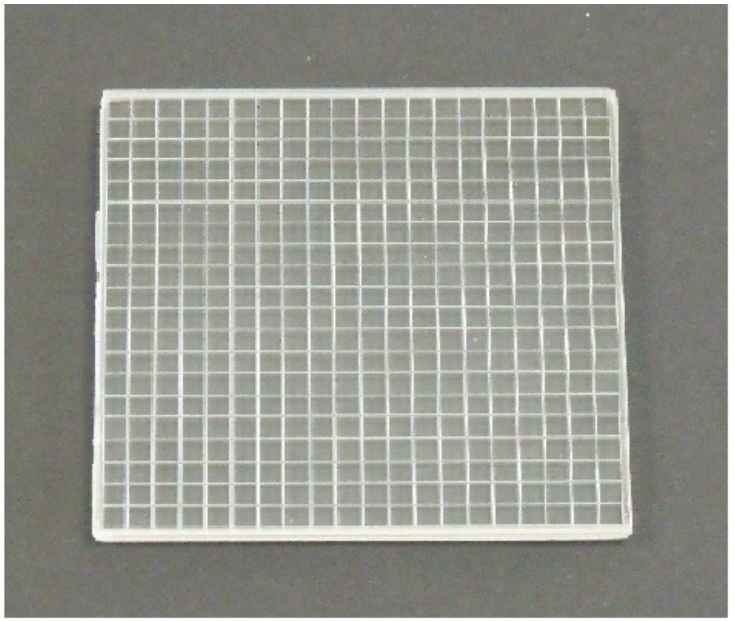
Chemical Extraction of Vegetable/Essential Oils

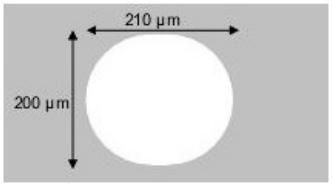


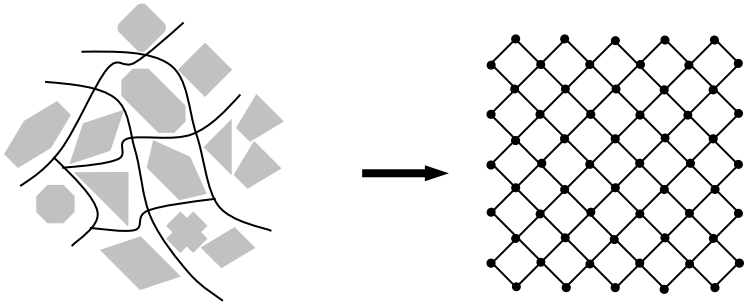
Experiment



A schematic view of the solute/solvent mixture saturating the capillary tube





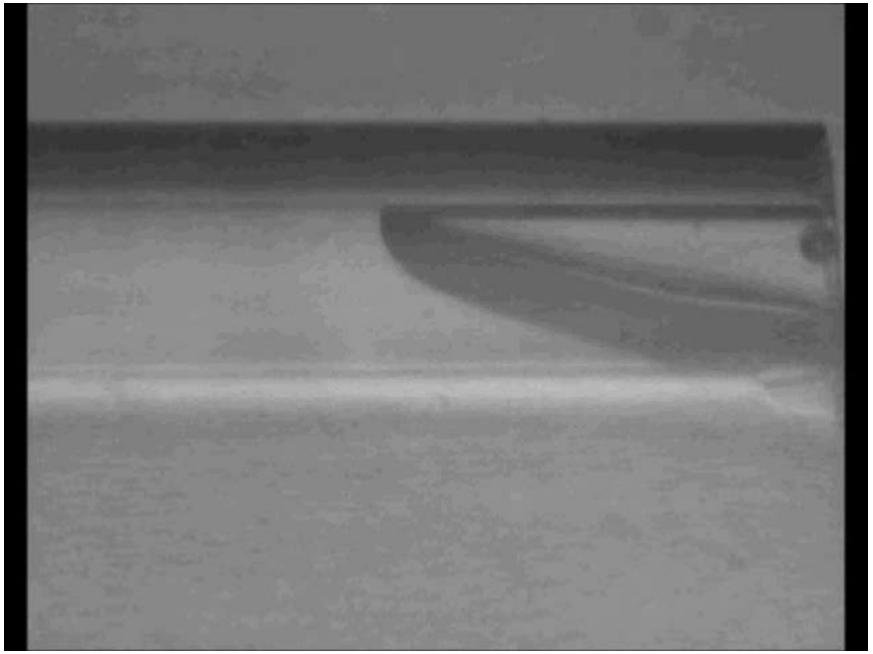


Network approach

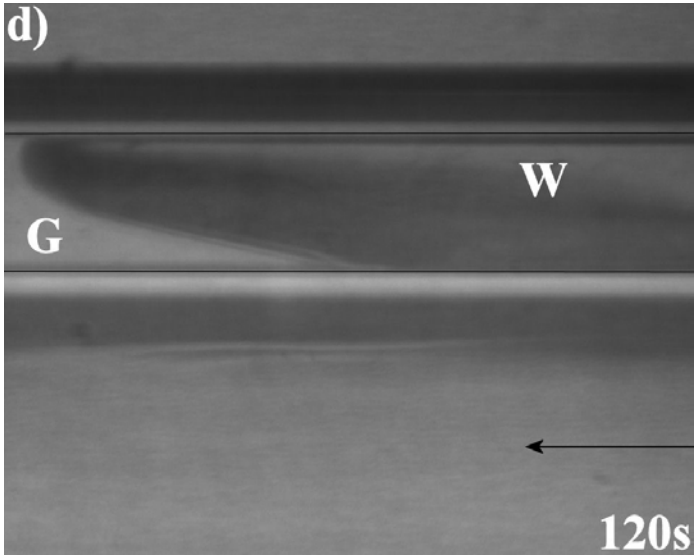
Regular pore-shape glass micromodel with dimensions 45x45x4mm; Isotropic wet-etching technique.

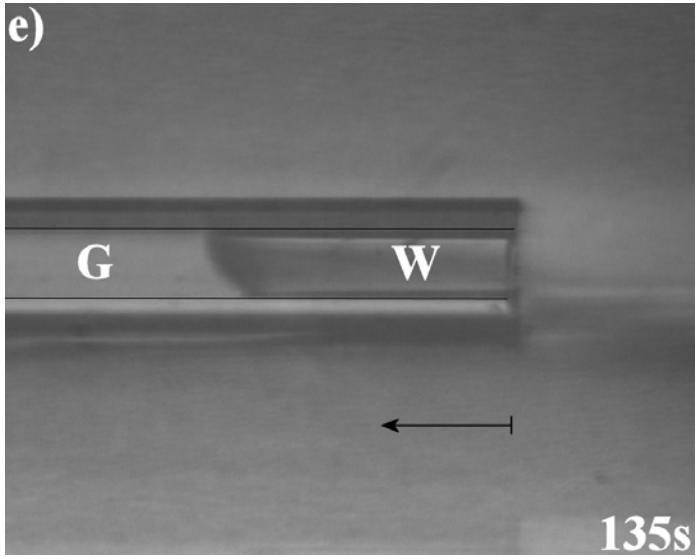
Journal of Colloid and Interface Science, 383, 2012, 184-197.
Transport in Porous Media, 100(3), 2013, p. 407-424.

Glycerol - water



Glycerol - water interfaces in a square tube, d=0.4 mm, L=10 cm, T=20^{o}C; real time =10 x time in video





Glycerol-water interfaces in square tubes with d=0.4 mm and d=0.2 mm, T=30^{o}C

Boussinesq approximation of the Cahn-Hilliard-Navier-Stokes equations

We use the ***phase-field approach*** is used as *a physics-based method* for description of thermo- and hydrodynamic evolution of miscible multiphase systems (either liquid/liquid or gas/liquid)

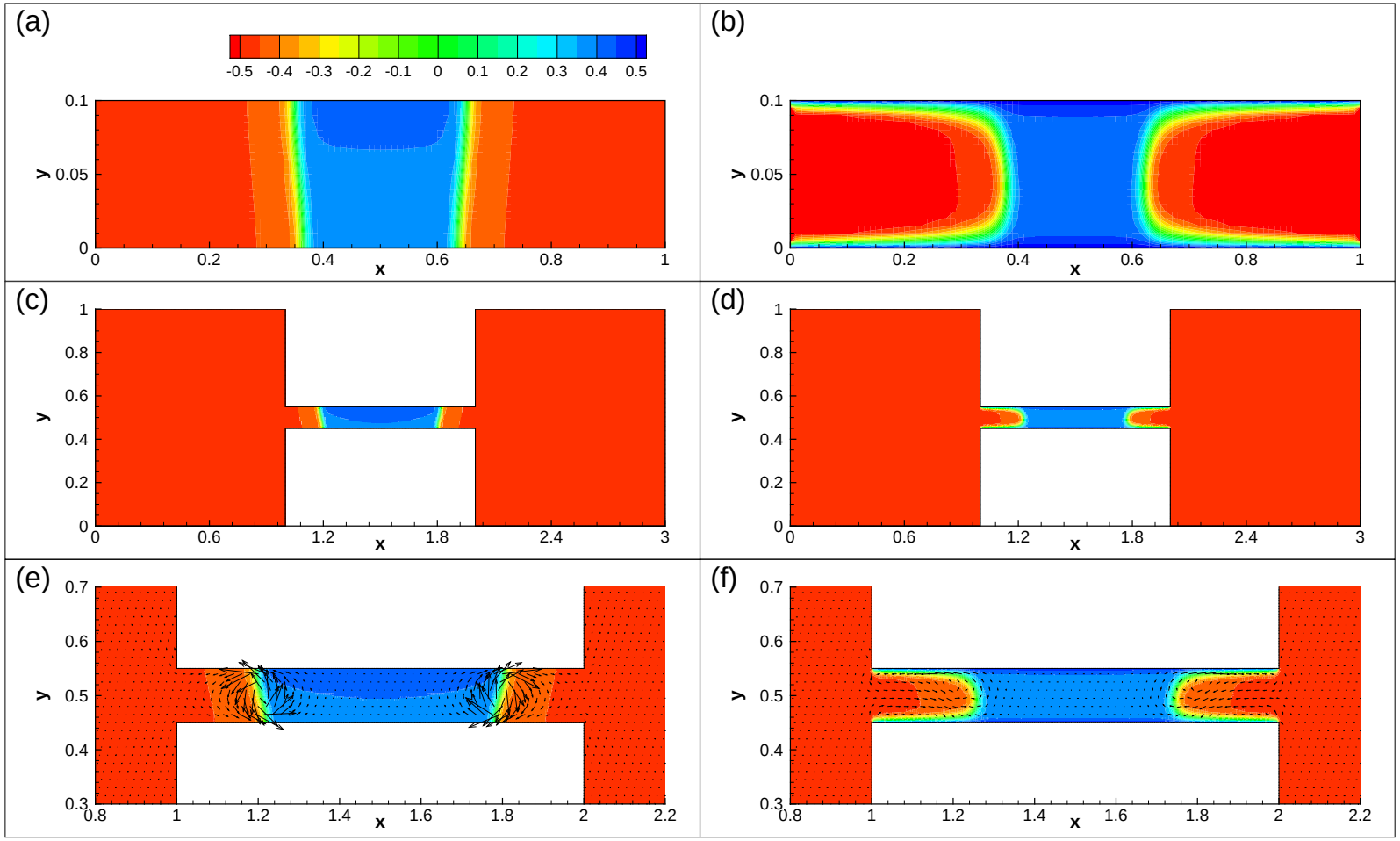
Phys. Rev. E 82, 056312 (2010)

$$\rho_1\left(\frac{\partial \vec{u}}{\partial t}+(\vec{u}\cdot\nabla)\vec{u}\right)=-\nabla\Pi+\eta\Delta\vec{u}-C\nabla\mu+2\varphi C\rho_1\vec{g},$$

$$\rho_1\left(\frac{\partial C}{\partial t}+(\vec{u}\cdot\nabla)C\right)=\alpha\Delta\mu,\quad \mu\equiv\frac{df_0(C)}{dC}+\varphi\rho_1(\vec{g}\cdot\vec{r})-\varepsilon\Delta C,$$

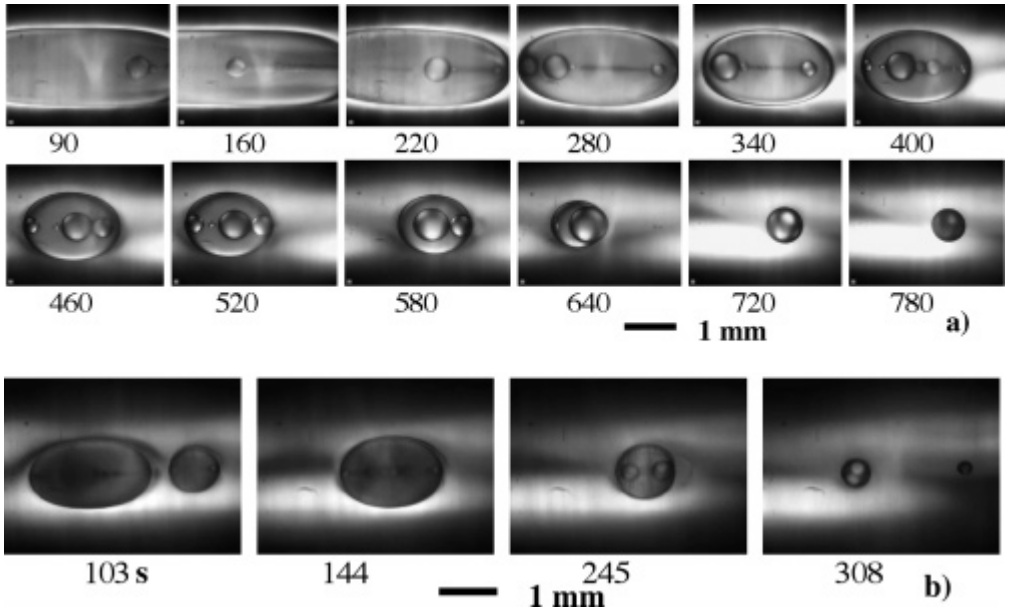
$$\nabla\cdot\vec{u}=0$$

Phase-field modelling



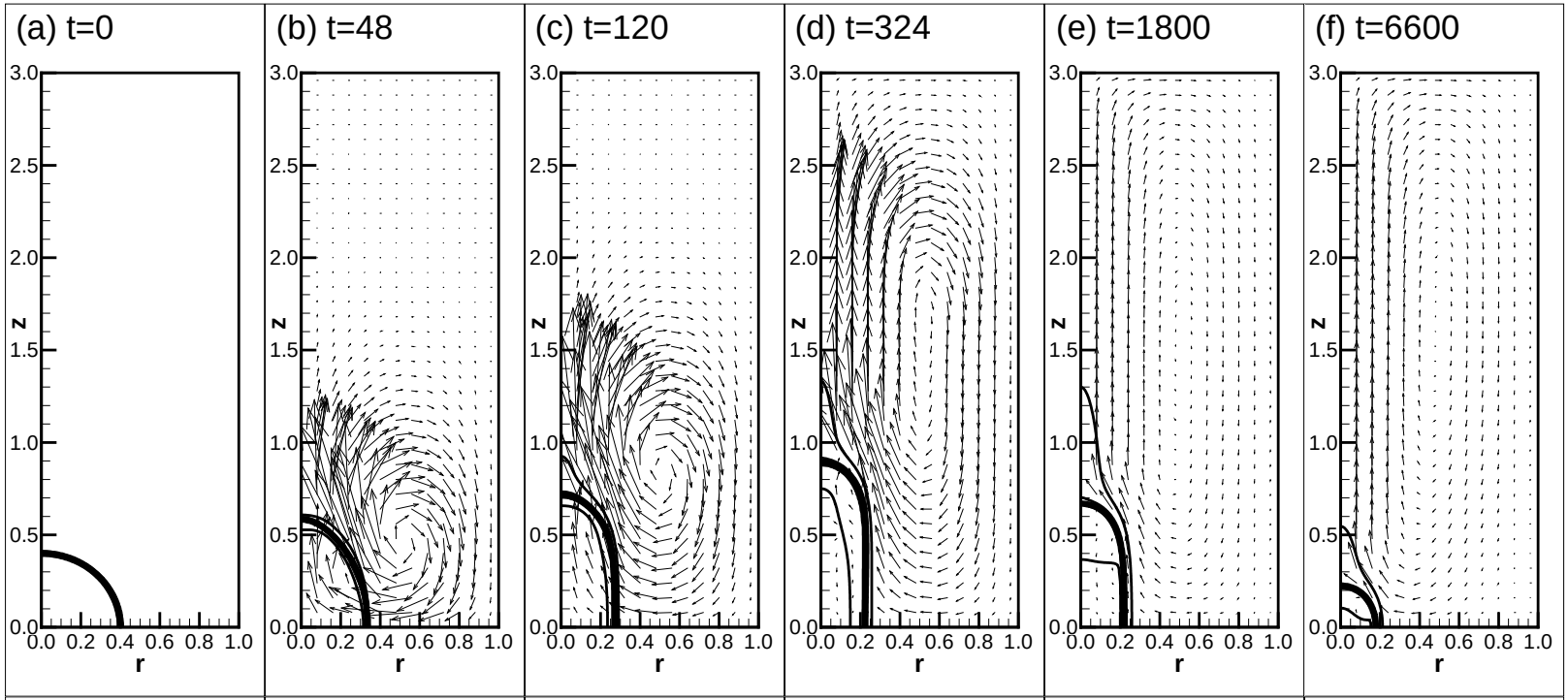
Journal of Colloid and Interface Science, 2016, v. 464, p. 48-58

Dissolution of a liquid droplet in a spinning tube

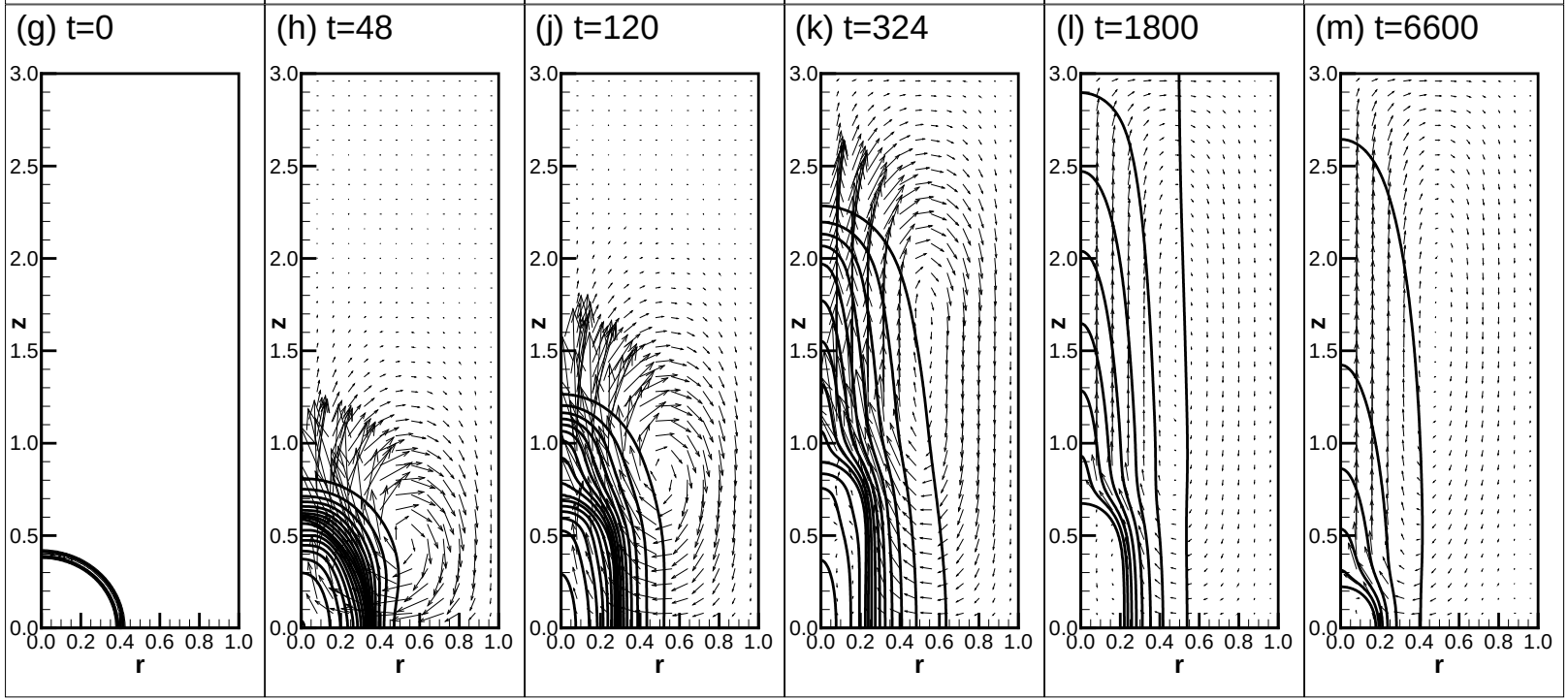


Pojman et al. Langmuir 2006, (a) Pure IBA in pure water below the critical temperature. Rotation: 8000 rpm. Times are in seconds. (b) Pure IBA injected into pure water. Initial and final temperatures: 27.5 °C. Rotation rate: 10 000 rpm. Times are in seconds.

The fields of concentration and velocity

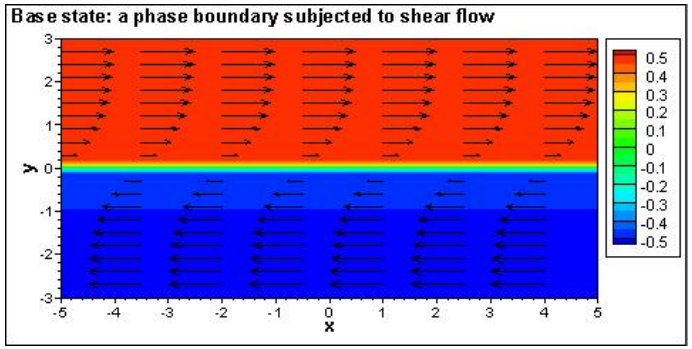


Chemical potential and velocity

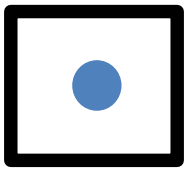


J. Colloid Interface Sci, 482 (2016) 193-204

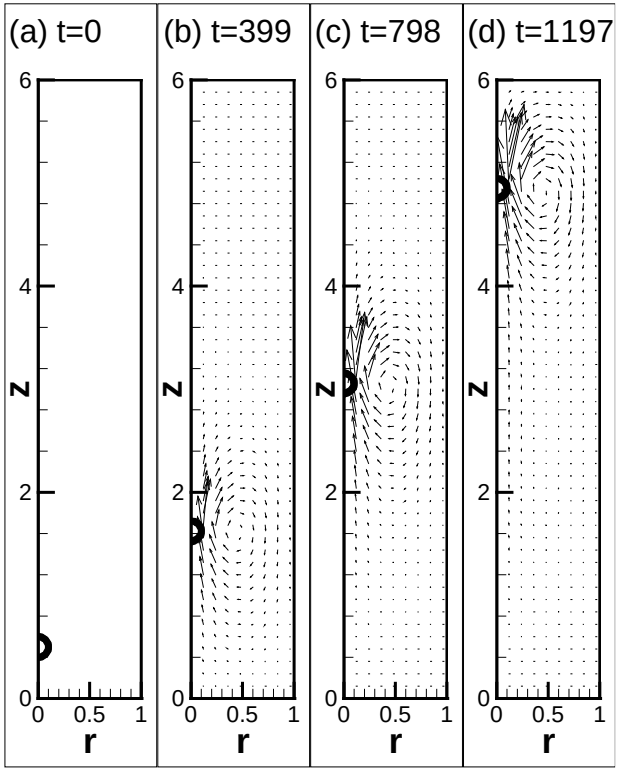
Other works



Linear stability of a phase boundary and propagation and decay of gravity-capillary waves on a phase boundary
Eur. Phys. J. E (2015) 38: 77
Phys. Rev. E 88 (2013) 022404



Phase equilibrium in a closed container: the shape of the phase boundary depends on the container size
Phys. Rev. E 95, 022803 (2017)



Rise of a liquid/gaseous inclusion in liquids with an account of its absorption/dissolution by ambient liquid phase

Review: *Curr. Opin. Colloid Interface Sci.* (2014) 19: 300-308