Experimental and Numerical Study of Mass Transfer in Single Droplets

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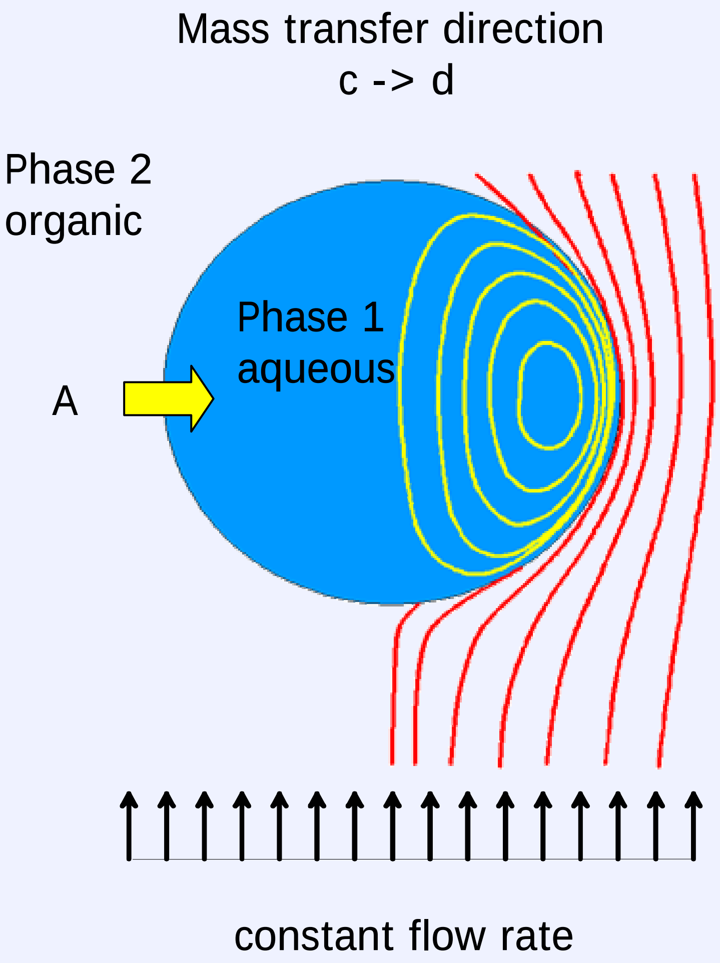
Introduction



Analytical description

- simplification by neglecting the mass transfer resistance in one phase
- no satisfactory description of the interaction of mass transfer and fluid dynamics

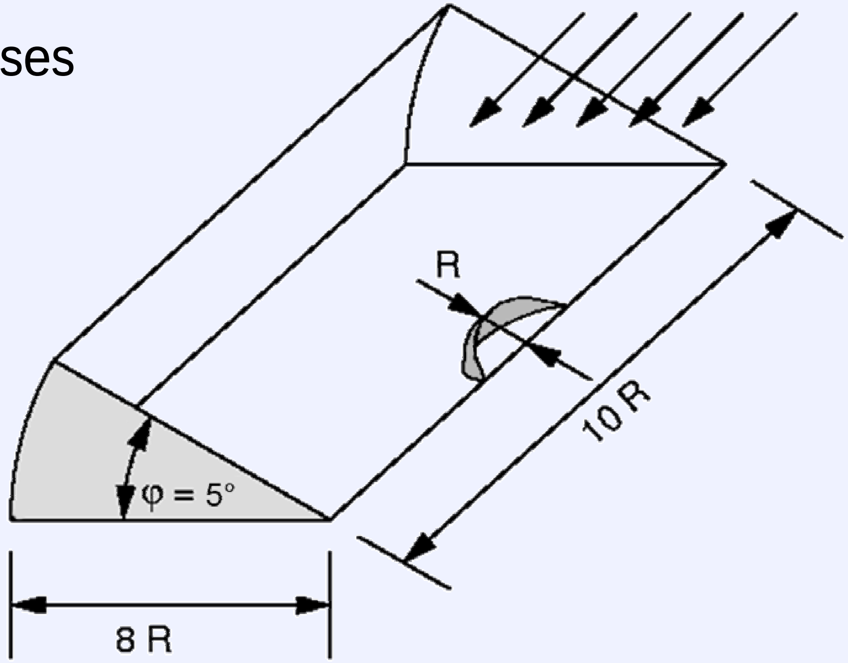
Goal

- quantitativ prediction of the mass transfer rate by CFD → When can simplifications be applied?
- description of mass tranfer enhancement (or limitation) due to
  - chemical reaction
  - Marangoni convection
- validating the code with our experimental data

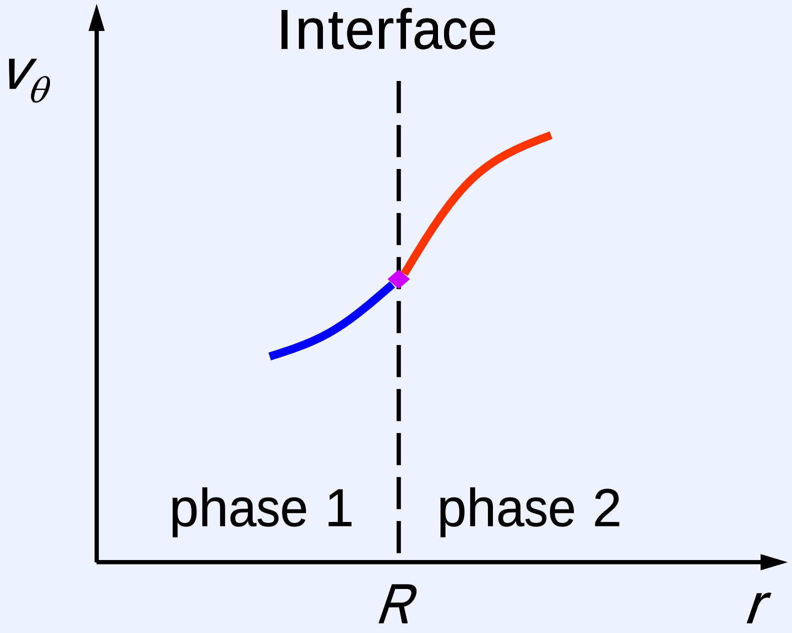
Modelling

- spherical drop in an infinte continuous phase (no deformation)
- rotational symmetry (2D simulation)
- immiscible liquids (Newtonian behaviour, incompressible)
- transfered component soluble in both phases
- constant physical properties
- variable interfacial tension
  ➡ coupled solution of velocity- and concentration field

Inlet
continuous phase



Velocity field



In both phases

- momentum balance
- continuity equation

Interface

- fixed in space $v_{r,1} = v_{r,2} = 0$
- no slip condition $v_{\Theta,1} = v_{\Theta,2}$
- shear stress balance $\eta_1 \left(\frac{\partial v_\Theta}{\partial r} - \frac{v_\Theta}{r} \right)_1 = \eta_2 \left(\frac{\partial v_\Theta}{\partial r} - \frac{v_\Theta}{r} \right)_2 + \frac{1}{R} \frac{\partial \gamma(c)}{\partial \Theta}$

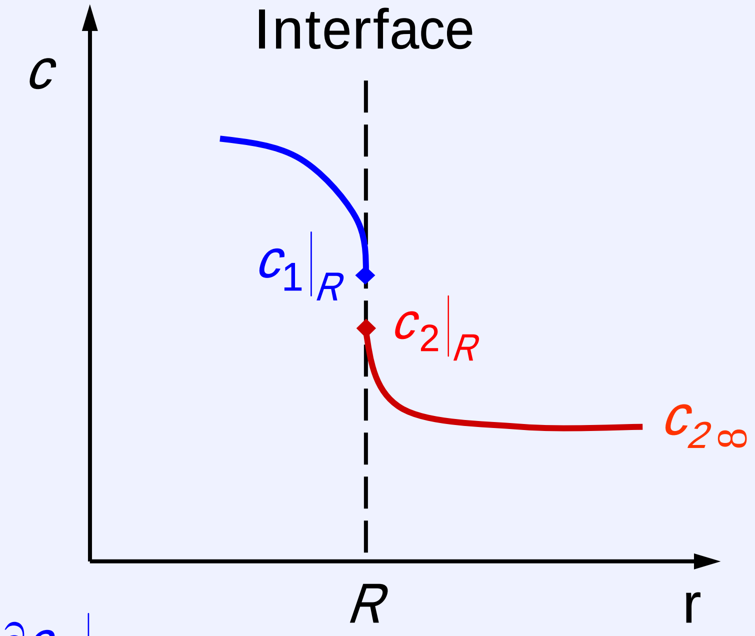
Inlet velocity

- force balance at interface $m\,\dot{\mathbf{v}} = \mathbf{F}_g + \mathbf{F}_A + \mathbf{F}_{drag}$

Concentration field

In both phases

- mass balance
- source terms for chemical reaction



Interface

- thermodynamic equilibrium $m = \left.\frac{c_1}{c_2}\right|_R$
- equality of fluxes $D_1 \left.\frac{\partial c_1}{\partial r}\right|_R = D_2 \left.\frac{\partial c_2}{\partial r}\right|_R$
- concentration dependency of interfacial tension $\gamma = \gamma\,(c)$

Inlet

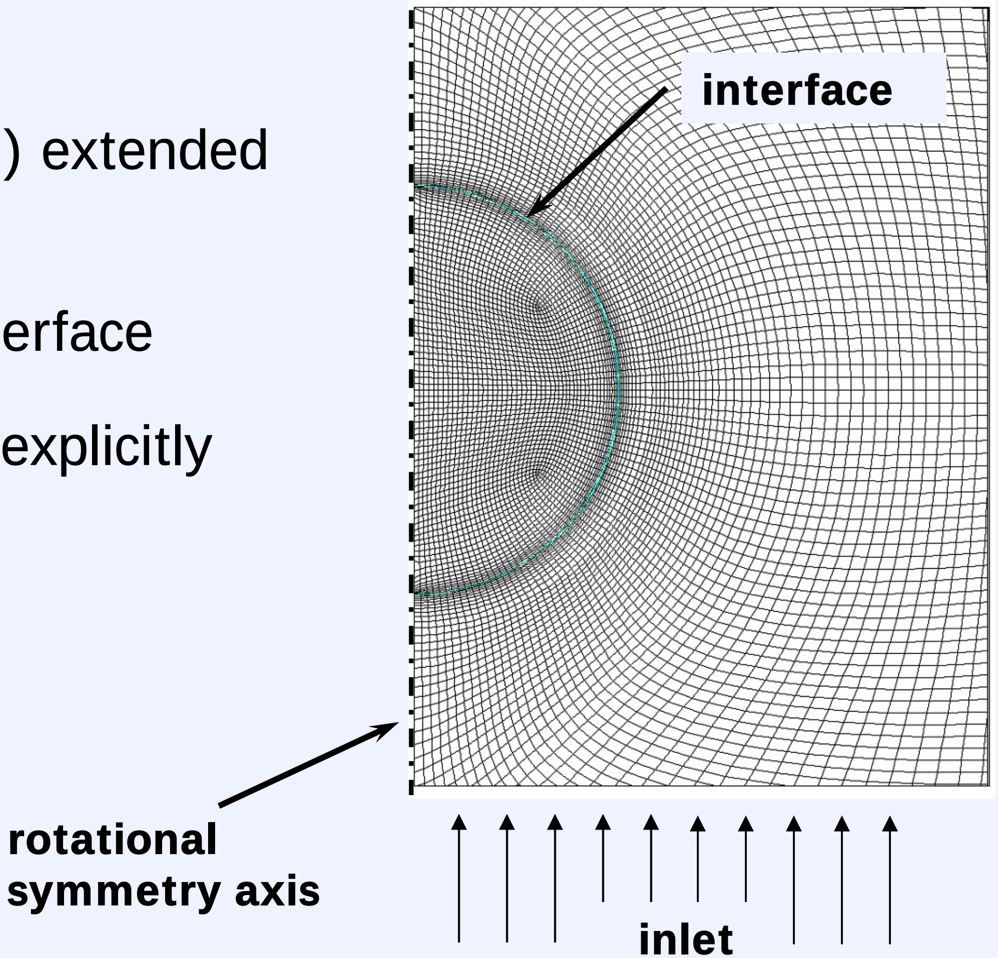
- fixed inlet concentration $c_{2,\infty}$

Numerical methods

- Finite Volume Method (FVM)
- hexahedral mesh
- CFD tool: STAR-CD (from CD-adapco) extended by user coding
- finest resolution of the grid at the interface
- boundary conditions at interface are explicitly calculated

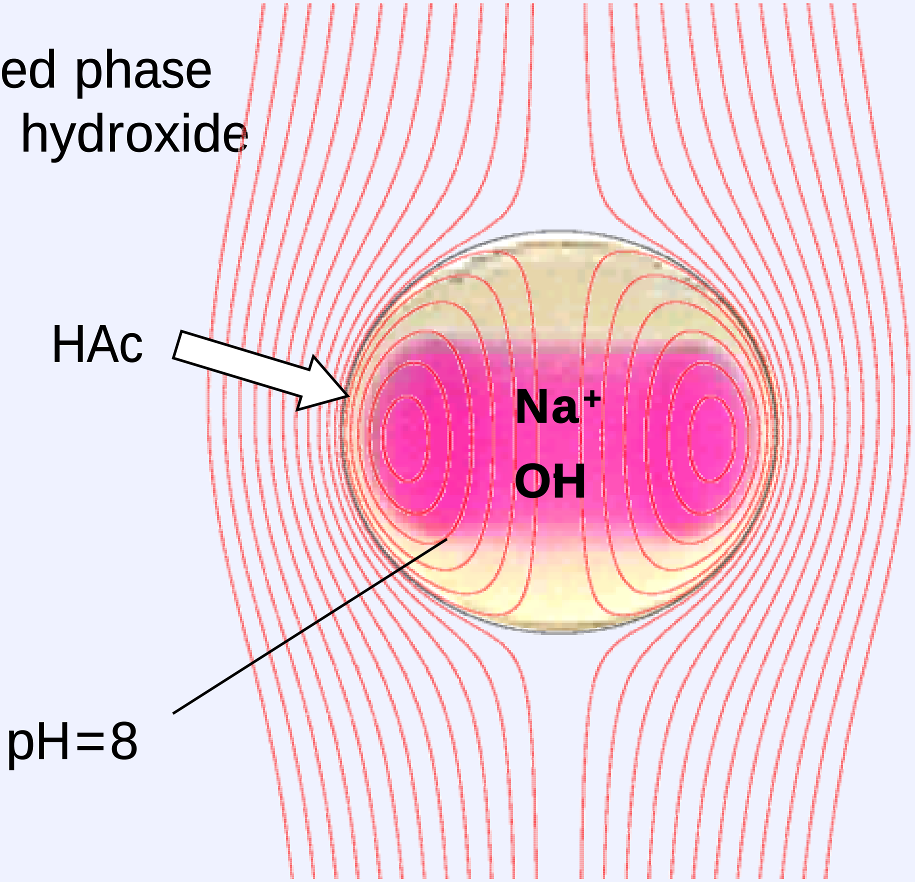
  ➡ time step restriction

number of cells: 31000
drop cells: 13000

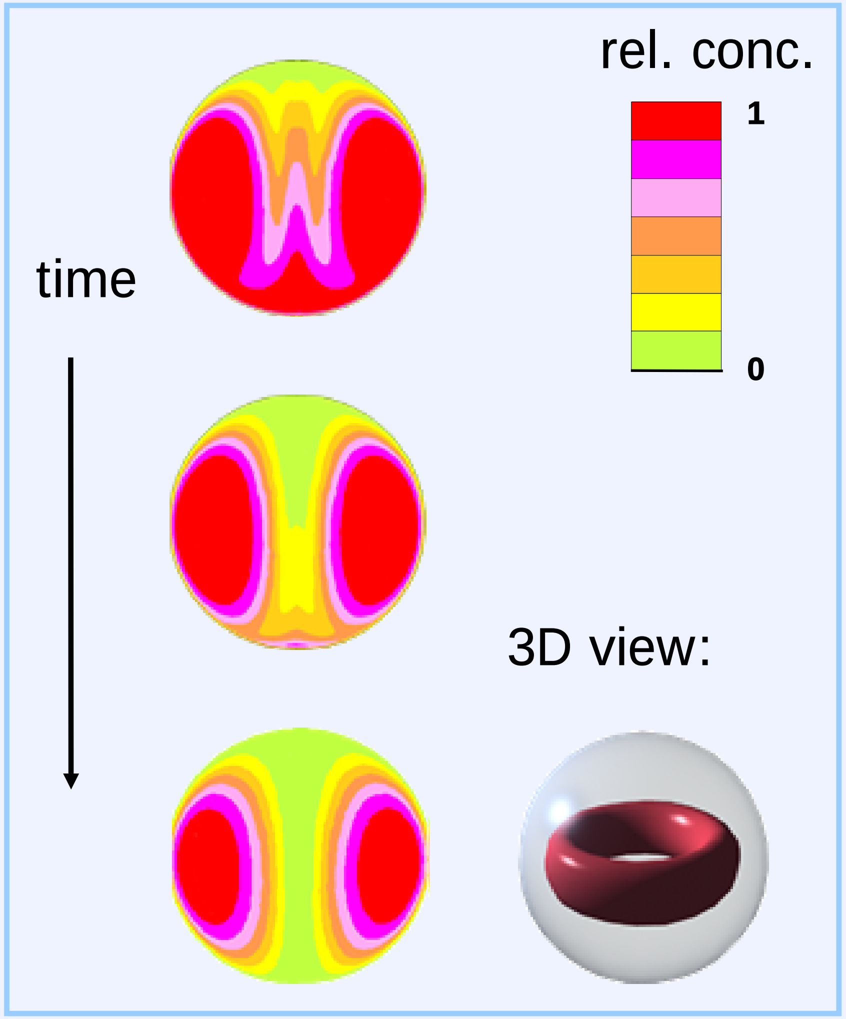


Visualisation of the local concentration front

- continuous phase
  cyclohexanol / acetic acid
- dispersed phase
  sodium hydroxide



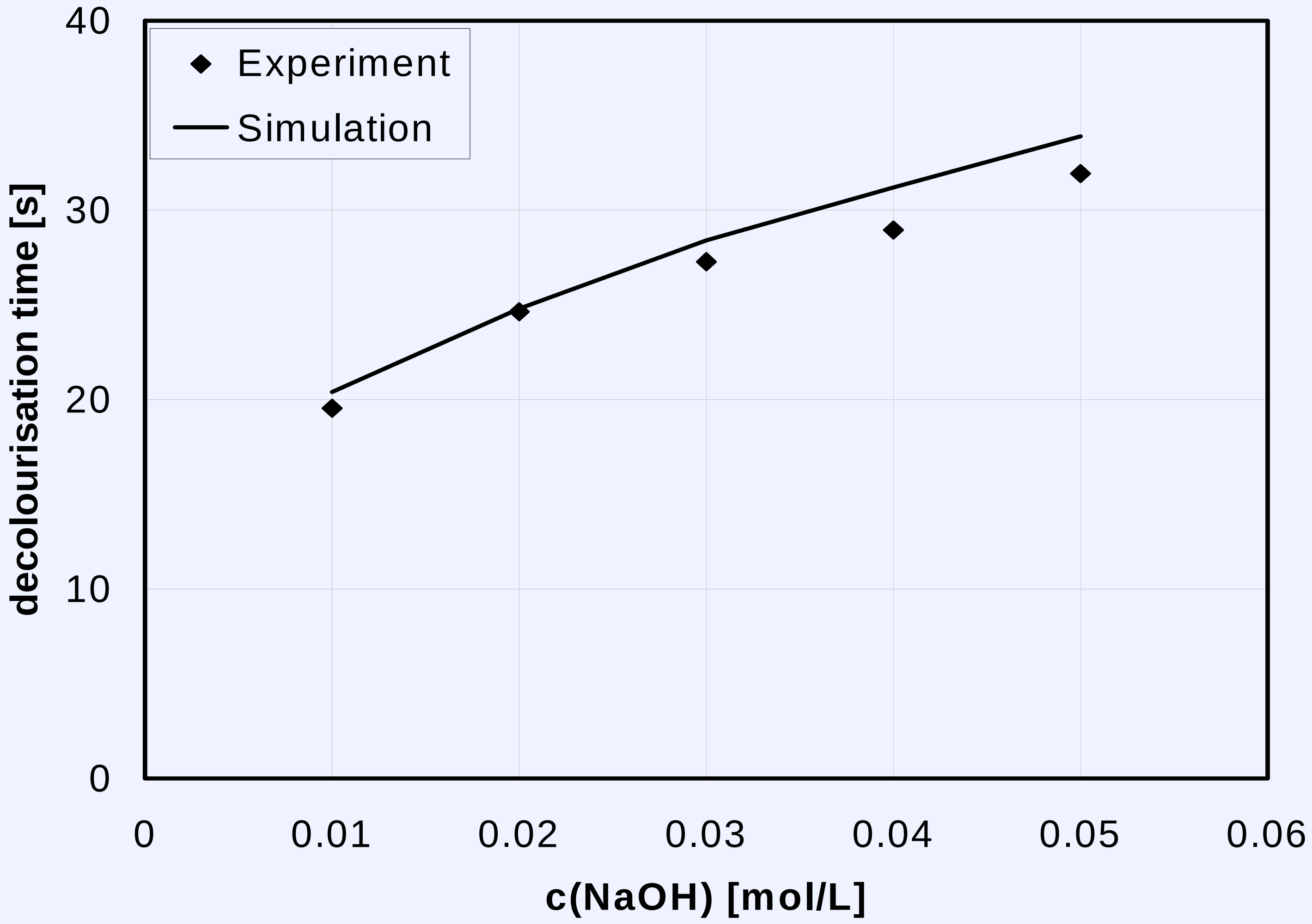
indicator: phenolphthalein



Visualisation of the local concentration front

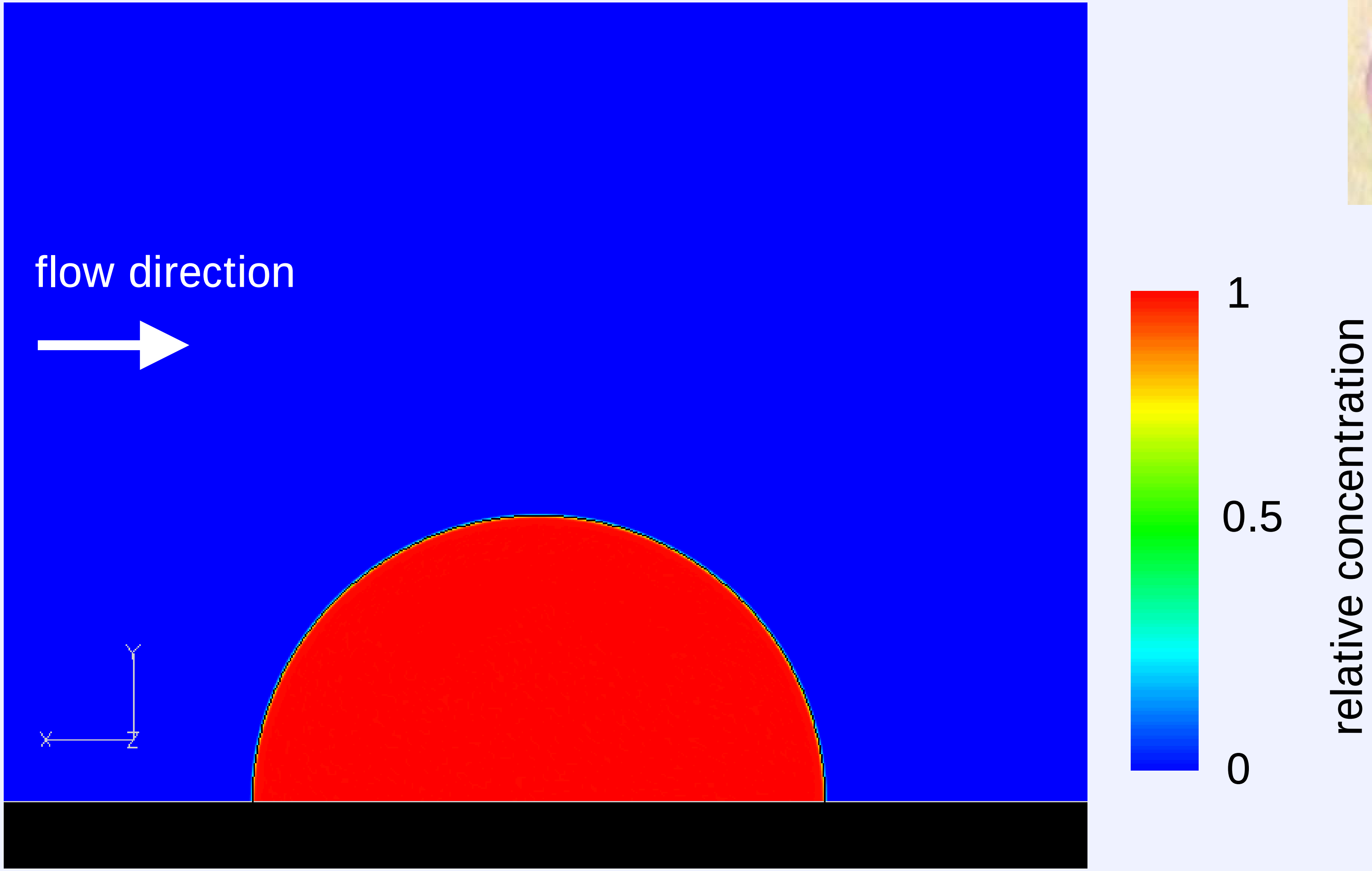
Decolourisation times – without Marangoni convection

cyclohexanol – acetic acid – NaOH(aq), c → d, d_p = 2.5 mm, c_{HAc} = 0.28 mol / L



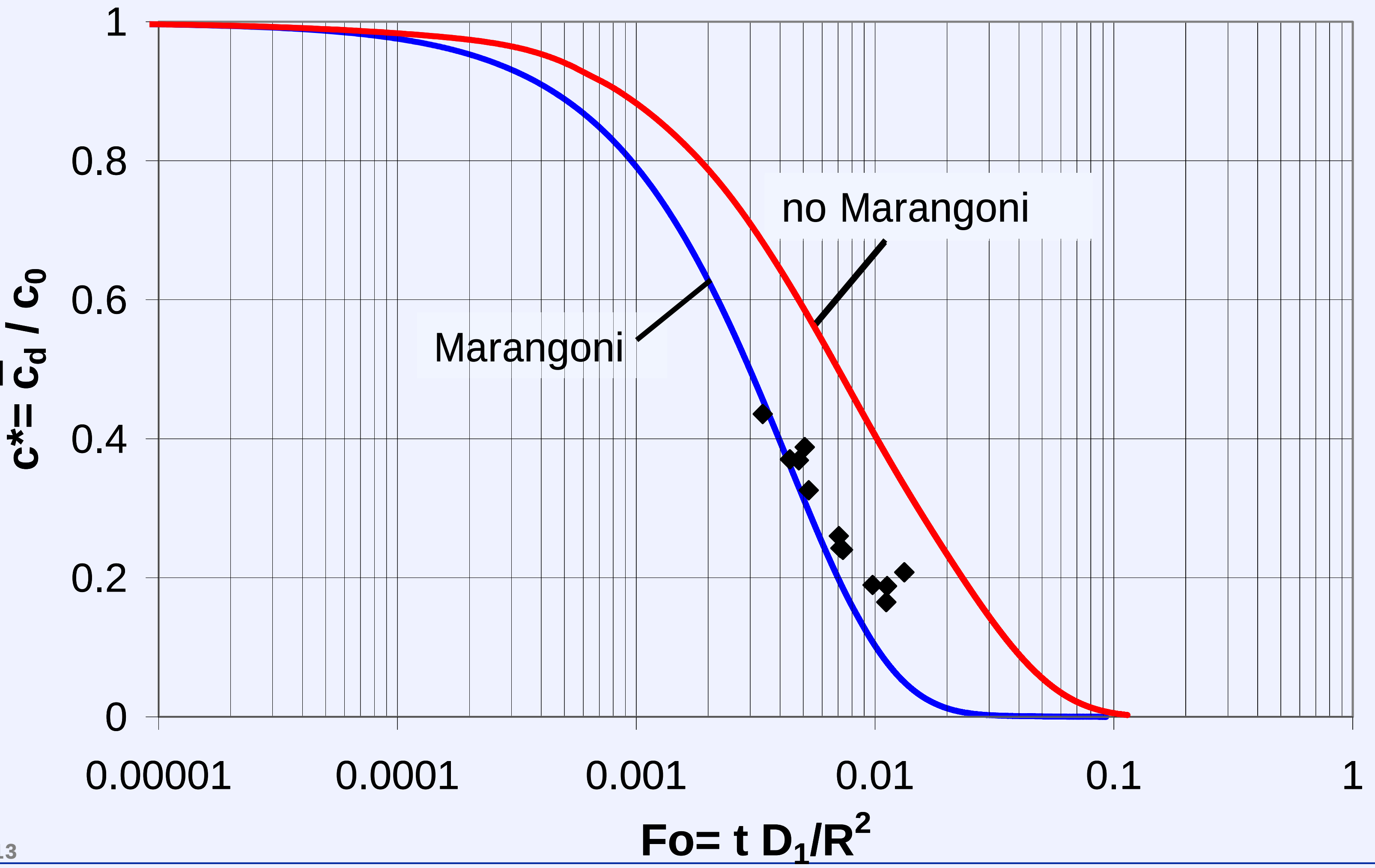
Visualisation of the local concentration front

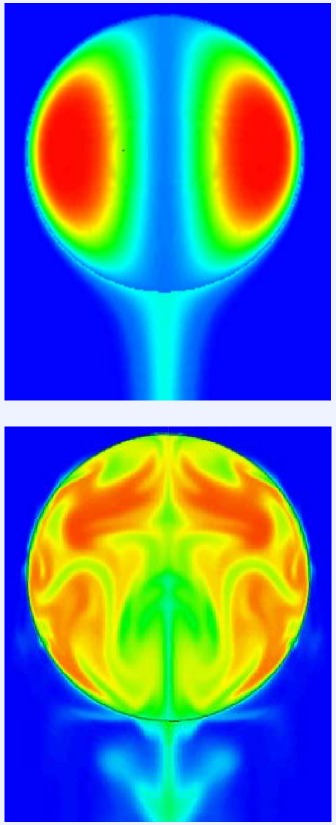
Marangoni-effect



Mean solute concentration – with Marangoni convection

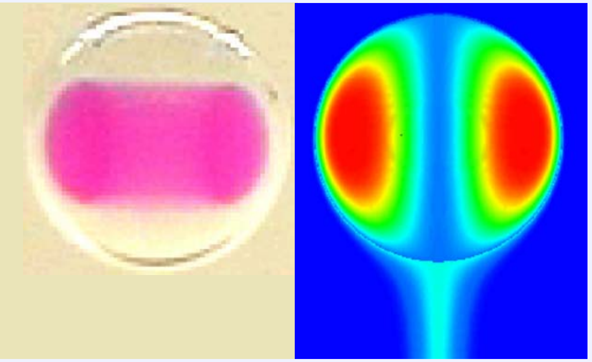
toluene – acetone – water, d → c, d_p = 2 mm, c_{A0} = 7.5 g/l





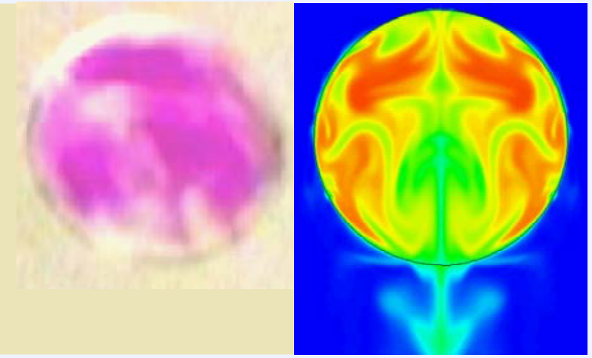
Conclusions

Chemical reaction



- good agreement between experimental and numerical calculated decolourisation times
- currently the investigations extend to:
  - reactions with comparable speed to mass transfer
  - heterogenous reactions

Marangoni convection



- for systems with Marangoni convection the behaviour is predicted qualitatively
- partly quantitative disagreement results from 3-dimensional nature of the phenomenon

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