Experimental and Numerical Study of Mass Transfer in Single Droplets

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Contents

1. Introduction
2. Modelling
3. Chemical reaction
4. Marangoni convection
5. Conclusions
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
- quantitatively prediction of the mass transfer rate by CFD
- When can simplifications be applied?
- description of mass transfer enhancement (or limitation) due to
  - chemical reaction
  - Marangoni convection
- validating the code with our experimental data
**Modelling**

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

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**2. Modelling**
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 \( m \dot{v} = F_g + F_A + F_{drag} \)
**Concentration field**

**In both phases**
- mass balance
- source terms for chemical reaction

**Interface**
- thermodynamic equilibrium
  \[ m = \frac{c_1}{c_2} \]
- equality of fluxes
  \[ D_1 \frac{\partial c_1}{\partial r} \bigg|_R = D_2 \frac{\partial c_2}{\partial r} \bigg|_R \]
- 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

![Diagram of rotational symmetry axis and inlet with interface and 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

3D view:

rel. conc.

0
1

pH=8

HAc

Na+

OH

3. Chemical reaction
Visualisation of the local concentration front
Decolourisation times - without Marangoni convection

cyclohexanol - acetic acid - NaOH(aq), \( c \rightarrow d, d_p = 2.5 \text{ mm}, c_{HAc} = 0.28 \text{ mol/L} \)

![Graph showing decolourisation times for different concentrations of NaOH with experimental and simulation data points.](image-url)
Visualisation of the local concentration front

4. Marangon convection
Marangoni-effect

flow direction

4. Marangoni convection
Mean solute concentration – with Marangoni convection

toluene – acetone – water, $d \rightarrow c$, $d_p = 2 \text{ mm}$, $c_{A0} = 7.5 \text{ g/l}$

\[ Fo = \frac{t D_1}{R^2} \]

\[ c* = \frac{c_d}{c_0} \]

no Marangoni

Marangoni
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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