Numerical Investigation of Mass Transfer with Two-Phase Slug Flow in a Capillary

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Outline

• Introduction
• Theoretical Background
• Computation Model
• Results
• Conclusions
Introduction

• Demand in biomedical, chemical reaction engineering, food processing etc.
• Development and application of MEMS technology
• The potential in microfluidic technology
• Experiments with microreactor
• A simple type of microreactor with capillary
• Improve mass transfer for immiscible liquids
• CFD method provides more details
Theoretical Background

- Demonstration by using a simple neutralization reaction

\[ \text{CH}_3\text{C}O\text{OH} + \text{KOH} \xrightleftharpoons[k]{\text{H}_2\text{O}} \text{CH}_3\text{C}O\text{OK} + \text{H}_2\text{O} \]

- Assume it is 2\textsuperscript{nd} order reaction

- Takes place without any additional condition

- Easy to be quantified
Experiment Background

- Two phases:
  - Aqueous phase (250 mol/m$^3$ KOH aqueous solution)
  - Organic phase (650mol/m$^3$ acetic acid mixed with kerosene)

Demonstration of Two-Phase slug flow with chemical reaction
Theoretical Background

- Assume: rate constant $k=0.001 \text{m}^3\text{mol}^{-1}\text{s}^{-1}$
- Kinetic equations

  \[ R_{AA} = \frac{d[CH_3COOH]}{dt} = -k[CH_3COOH][KOH] \]

  \[ R_{KOH} = \frac{d[KOH]}{dt} = -k[CH_3COOH][KOH] \]

- Reaction rate

  \[ R = -k[CH_3COOH][KOH] \]
Theoretical Background

- Mass transfer by convection-diffusion

\[
\frac{\partial C_{mn}}{\partial t} + \vec{u} \cdot \nabla C_{mn} - \nabla \cdot (D_{mn} \nabla C_{mn}) - R = 0
\]

- Mass transfer by diffusion

\[
\frac{\partial C_{mn}}{\partial t} - \nabla \cdot (D_{mn} \nabla C_{mn}) - R = 0
\]

Where,

\[
D_{mn} = 7.4 \times 10^{-8} \frac{T \sqrt{\phi_n M_n}}{\mu_n (M_m / \rho_m)^{0.6}}
\]

(Wilke-Chang correlation)
Computation Scheme

**Matlab m file** with all the parameters and constants

**Geometry** generation

**Mesh** generation

**Momentum transport module**
Incompressible N-S equation (steady)

**Mass transport module**
Convection-diffusion equation (unsteady)

**Post processing**
Using Tecplot for visualization

**Matlab m file**
Writing a Tecplot file for post processing
Computation Model

- 2-D Axisymmetric
- Two axes are independent
- Computational domain

Domain 1 represents aqueous phase; Domain 2 represents organic phase

- Mesh
  - Structured mesh
  - Element number: 1500
  - Node number: 3131
Convection-diffusion case

• Solver
  - COMSOL Multiphysics with Matlab package
  - Discretize governing equation with Finite Element Method
  - Assumption: neglecting gravitational force and surface tension effect
  - Solve steady incompressible Navier-Stokes equation
  - Solve convection-diffusion equation with implement of flow field

• Boundary condition for flow field

  ![Diagram showing slip boundary condition](attachment:image.png)

  Slip boundary condition: \( \vec{n} \cdot \vec{v} = 0 \)

  Average flow velocity at \( r=0 \)

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Convection-diffusion case

• Boundary condition for solving mass transport
  - Solve mass transport for two species separately
  - Assume no KOH is transported into organic phase
  - \( \nabla \cdot \mathbf{C}_{KOH} = 0, \nabla C_{KOH} = 0 \)
  - \( \nabla \cdot \mathbf{C}_{KOH} = 0 \) was applied to the boundary 1, 2, 3 and 4

• Solve mass transport of AA in two phases
  - Periodic boundary condition applied to 1 and 6
  - \( \nabla \cdot \mathbf{C}_{AA} = 0 \) was applied to the boundary 2 and 5
Pure diffusion case

• Solver
  - Solve diffusion equation
  - COMSOL Multiphysics with Matlab package
  - Discretize governing equation with Finite Element Method
  - Solve mass transport for two species separately

• Boundary condition
  - Periodic boundary condition at interface
  - No mass flux through the capillary wall
  - Holds r=0 at central axis
Results (Pure diffusion case)

- Slug length: 4mm; Capillary radius (50µm-500µm)
- Residence time to achieve 98% conversion of KOH
- Aspect ratio is the ratio of slug length to capillary radius (L/r)
Results (Convection-diffusion)

- Streamline plot

- Internal circulation formed inside each slug
- Mass transported not only by diffusion but also by convection
- Increases effective interfacial area
- Increase concentration gradient
Results (Convection-diffusion)

- Capillary radius: 250µm
- Slug length: 4mm
- L/r=16
- Residence time to achieve 98% conversion of KOH
Results (Convection-diffusion)

- Average concentration varies with time

The variation of average concentration of two species at $v=0.002\text{m/s}$ with capillary radius of 250 µm

The variation of average concentration of two species at $v=0.014\text{m/s}$ with capillary radius of 250 µm

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Concentration distribution

- Capillary radius of 250 µm
  - $C_{\text{KOHmax}}=250 \text{ mol/m}^3$ at $t=0s$
  - $C_{\text{KOHmax}}=42.99 \text{ mol/m}^3$ at $u=0.002 \text{m/s}$ at $t=15s$
  - $C_{\text{KOHmax}}=14.15 \text{ mol/m}^3$ at $u=0.008 \text{m/s}$ at $t=15s$
  - $C_{\text{KOHmax}}=12.14 \text{ mol/m}^3$ at $u=0.014 \text{m/s}$ at $t=15s$

The concentration distribution and maximum concentration value of KOH during the titration for different velocity at residence time $t=15s$
Concentration distribution

- Average velocity: 0.002 m/s   Slug length: 4 mm
- Capillary radius: 250 µm
- \( C_{AA\text{min}} = 0 \, \text{mol/m}^3 \) \( C_{AA\text{max}} = 650 \, \text{mol/m}^3 \) at \( t=0 \, \text{s} \)
- \( C_{AA\text{min}} = 100.32 \, \text{mol/m}^3 \) \( C_{AA\text{max}} = 387.46 \, \text{mol/m}^3 \) at \( t=10.3 \, \text{s} \)
- \( C_{AA\text{min}} = 171.19 \, \text{mol/m}^3 \) \( C_{AA\text{max}} = 235.59 \, \text{mol/m}^3 \) at \( t=25.2 \, \text{s} \)

The concentration distribution of AA in two phases

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Concentration distribution

- Average velocity: 0.014 m/s    Slug length: 4 mm
- Capillary radius: 250 µm

- $C_{AA_{min}} = 0 \text{mol/m}^3$     $C_{AA_{max}} = 650 \text{mol/m}^3$ at $t=0$ s

- $C_{AA_{min}} = 207.89 \text{mol/m}^3$    $C_{AA_{max}} = 217.77 \text{mol/m}^3$ at $t=10.3$ s

- $C_{AA_{min}} = 199.21 \text{mol/m}^3$    $C_{AA_{max}} = 199.67 \text{mol/m}^3$ at $t=25.2$ s

The concentration distribution of AA in two phases
Results (Convection-Diffusion)

- Average flow velocity: 0.014 m/s
- Slug length: 4 mm
- Residence time to achieve 98% conversion of KOH
Conclusions

• COMSOL Multiphysics with Matlab package allows for rapid analysis
• Average flow velocity, slug size and capillary size all have effect on mixing efficiency
• Residence time decreases with increasing average flow velocity for a fixed aspect ratio
• Residence time increases with increasing the aspect ratio for a fixed average flow velocity
• Two-phase slug flow has potential benefit on immiscible fluids mixing
Acknowledge

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Thank you for your attention!

Question?