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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

$$CH_3COOH + KOH \xrightarrow{k} CH_3COOK + H_2O$$

- Assume it is 2nd 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$m^3mol^{-1}s^{-1}$
- Kinetic equations

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

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

- 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, $D_{mn} = 7.4 \times 10^{-8} \frac{T\sqrt{\varphi_n M_n}}{\mu_n (M_m / \rho_m)^{0.6}}$

(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)

←

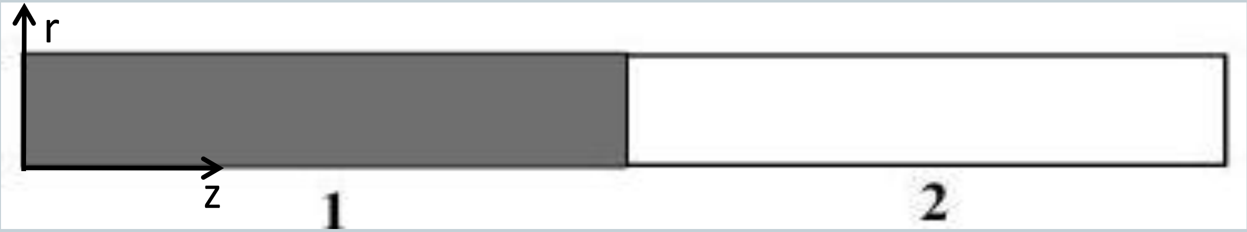
Matlab m file
Writing a Tecplot file for post processing

←

Post processing
Using Tecplot for visualization

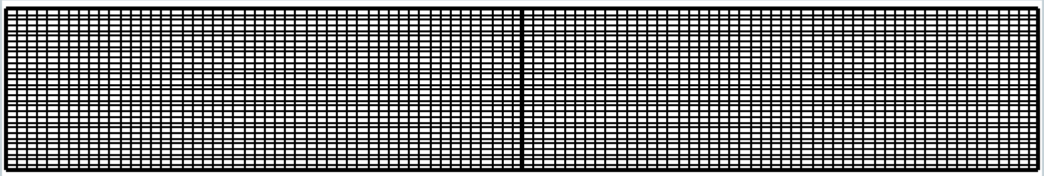
Computation Model

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



Domain 1 represents aqueous phase; Domain 2 represents organic phase

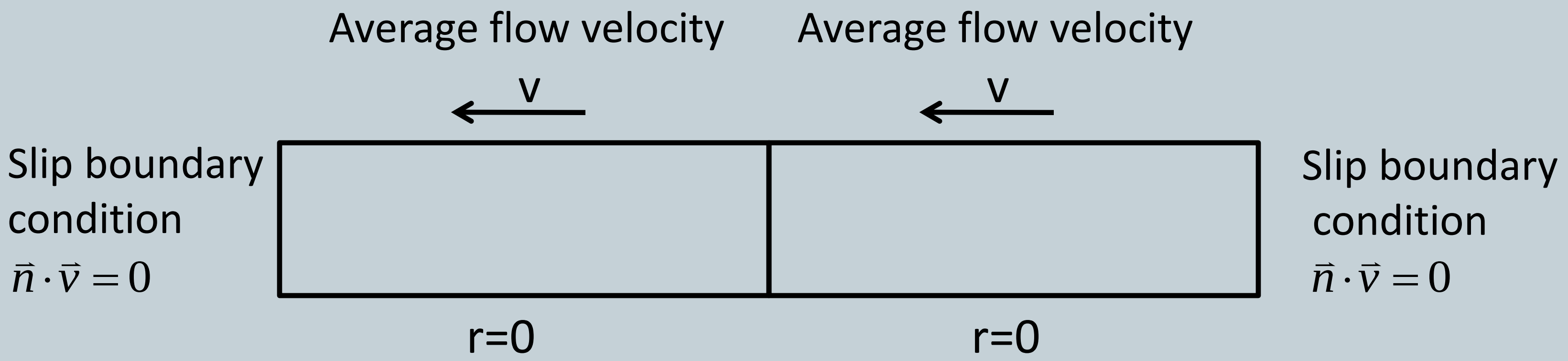
- Mesh



❖ Structured mesh
❖ Element number: 1500
❖ Node number : 3131

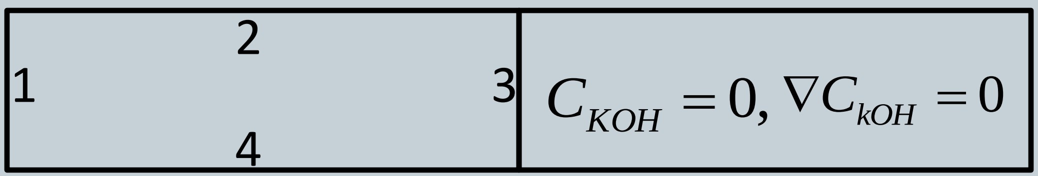
Convection-diffusion case

- 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



Convection-diffusion case

- Boundary condition for solving mass transport
  - ❖ Solve mass transport for two species separately
  - ❖ Assume no KOH is transported into organic phase



  - ❖ $\vec{n} \cdot \nabla C_{KOH} = 0$ was applied to the boundary 1, 2, 3 and 4

  - ❖ Solve mass transport of AA in two phases

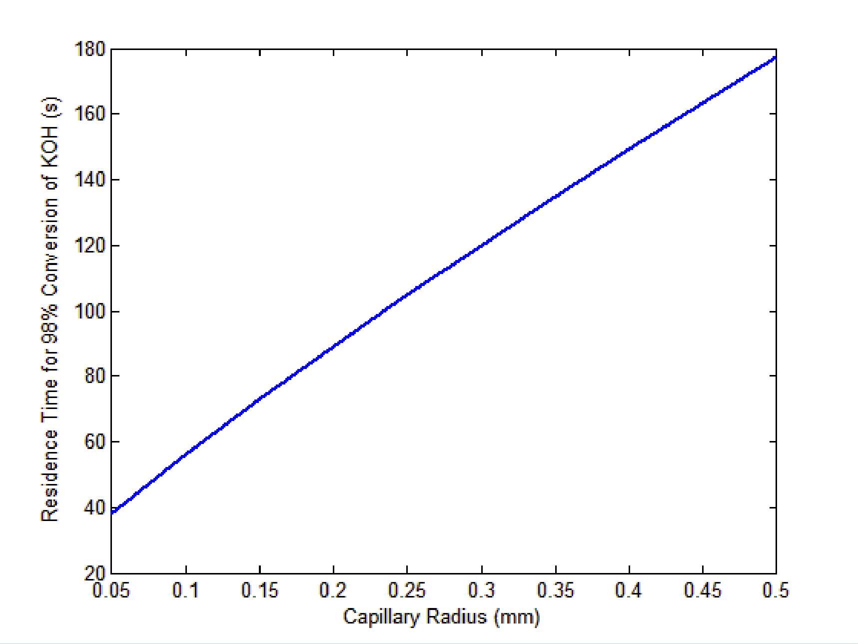
  - ❖ Periodic boundary condition applied to 1 and 6
  - ❖ $\vec{n} \cdot \nabla C_{AA} = 0$ was applied to the boundary 2 and 5

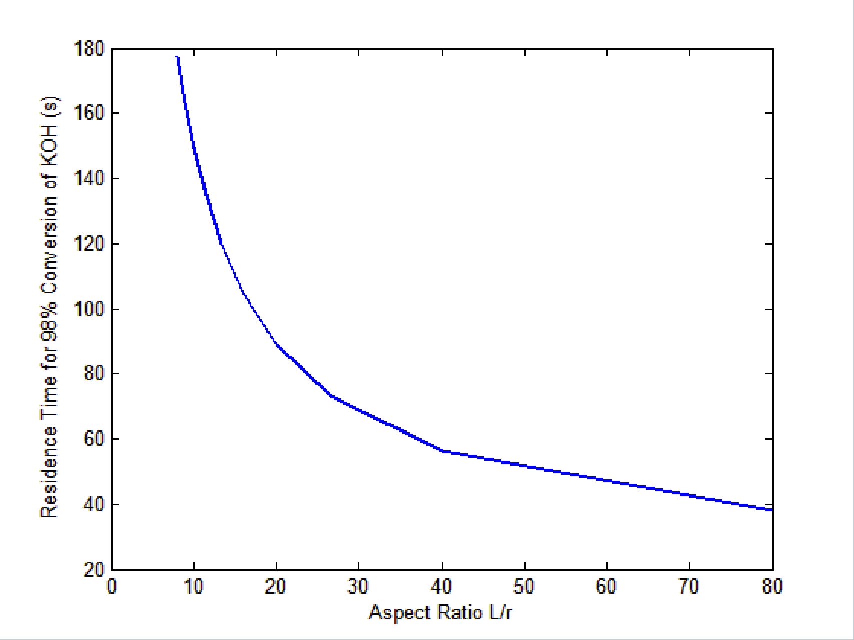
Pure diffusion case

- 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)

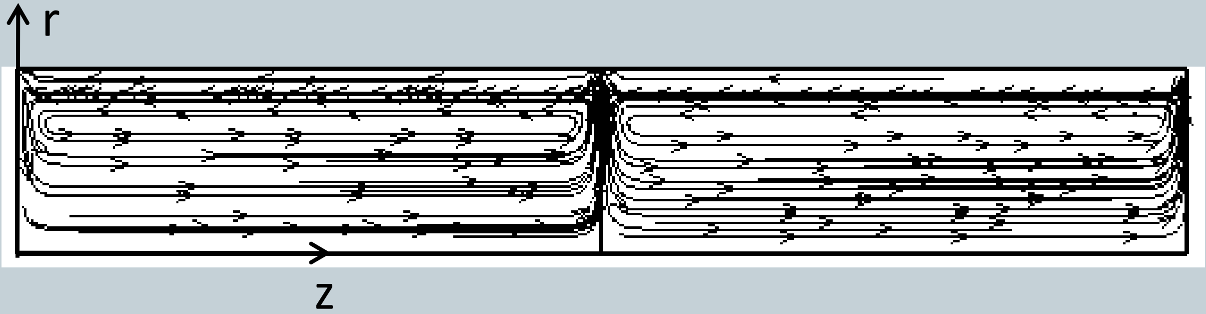
- Slug length: 4mm; Capillary radius (50µm-500µm)
- Residence time to achieve 98% conversion of KOH
- Aspect ratio is the ratio of slug length to capillary radius (L/r)





Results (Convection-diffusion)

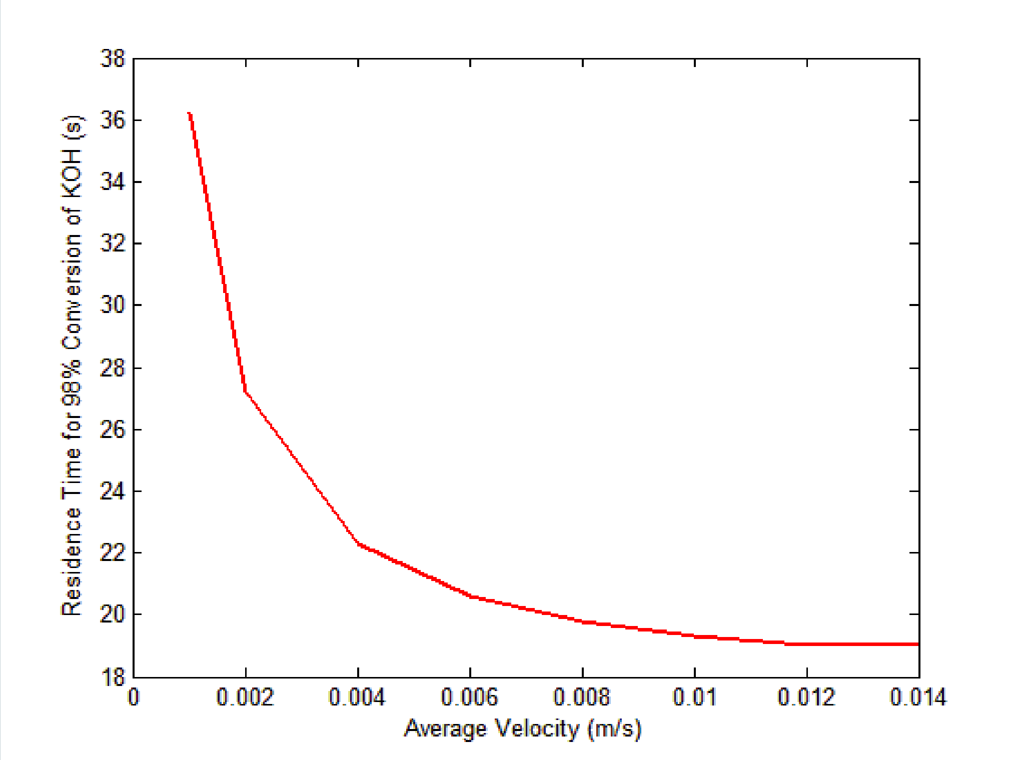
- Streamline plot



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

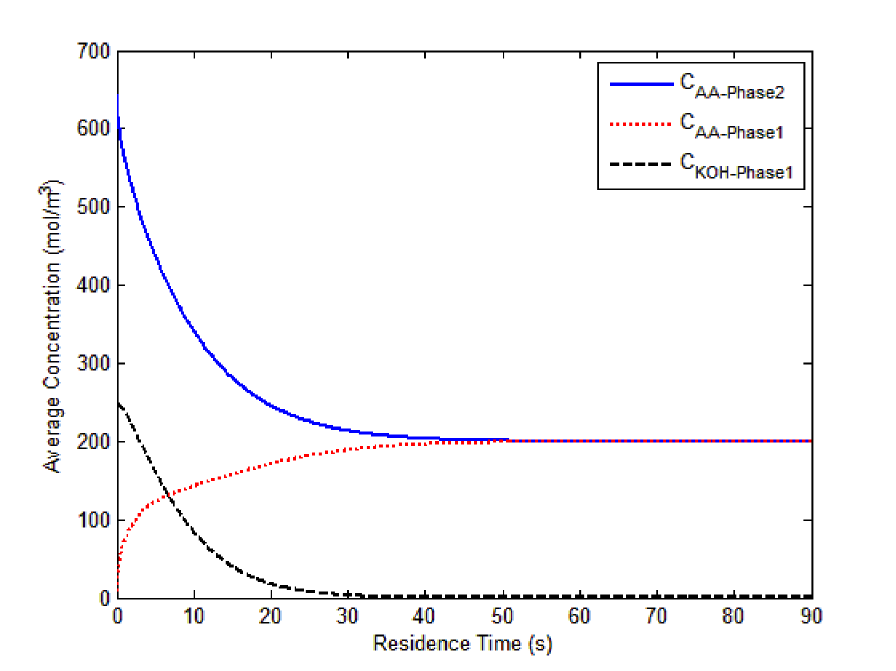
Results (Convection-diffusion)

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

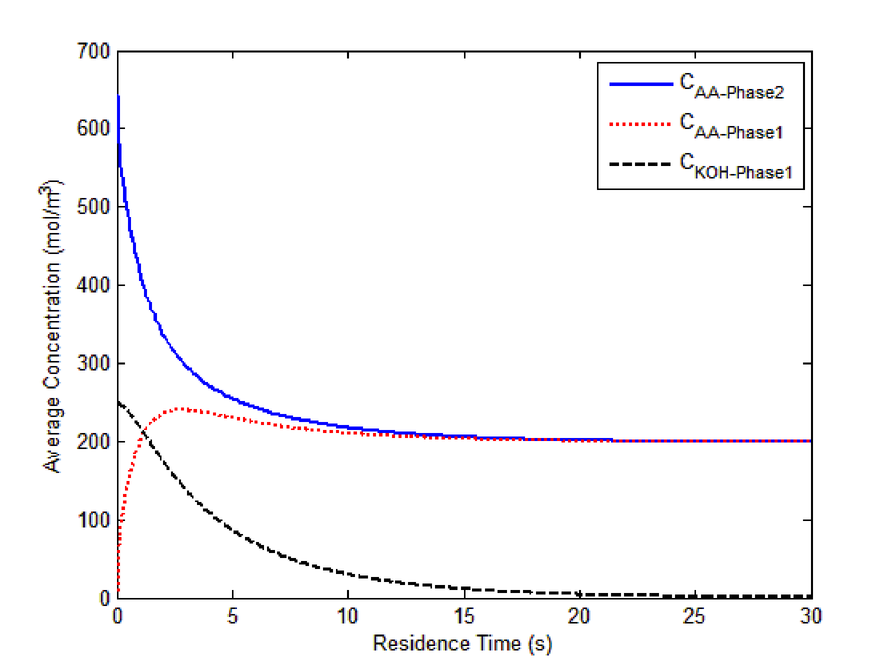


Results (Convection-diffusion)

- Average concentration varies with time



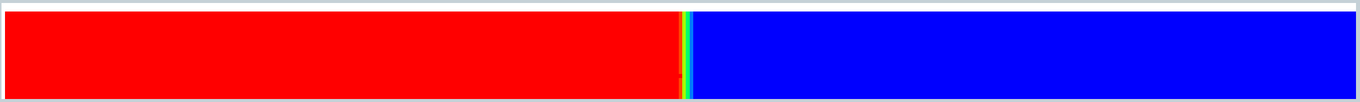
The variation of average concentration of two species at **v=0.002m/s** with capillary radius of 250 µm



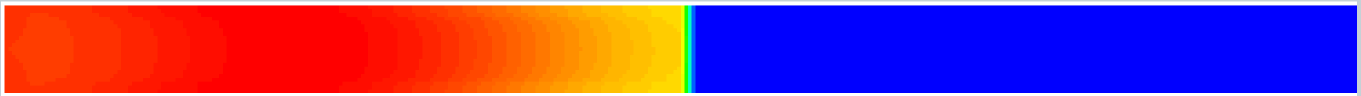
The variation of average concentration of two species at **v=0.014m/s** with capillary radius of 250 µm

Concentration distribution

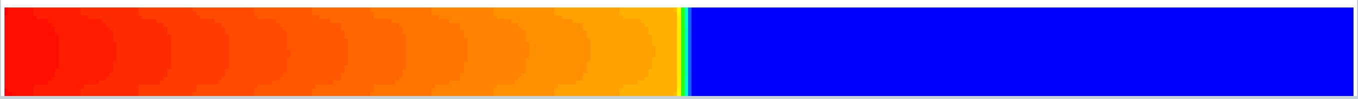
- Capillary radius of 250 µm



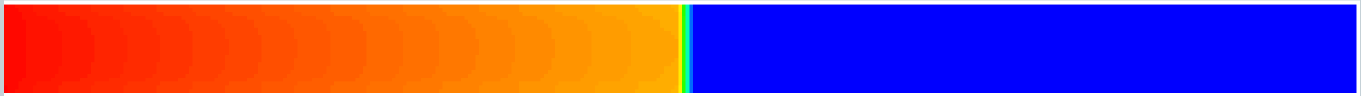
- C_{KOHmax}=250 mol/m^3 at t=0s



- C_{KOHmax}=42.99 mol/m^3 at u=0.002m/s at t=15s



- C_{KOHmax}=14.15 mol/m^3 at u=0.008m/s at t=15s

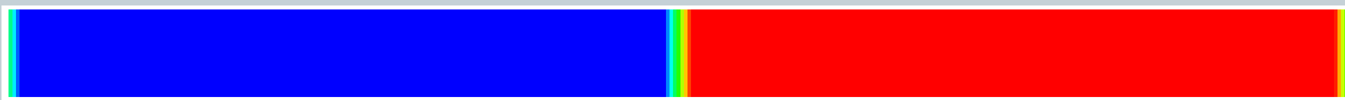


- C_{KOHmax}=12.14 mol/m^3 at u=0.014m/s at t=15s

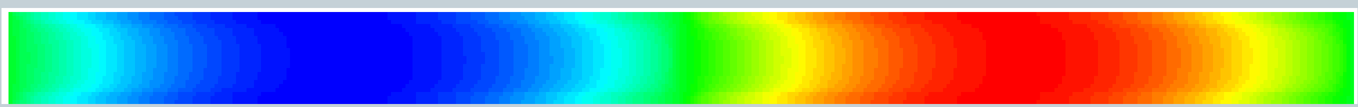
The concentration distribution and maximum concentration value of KOH during the titration for different velocity at residence time **t=15s**

Concentration distribution

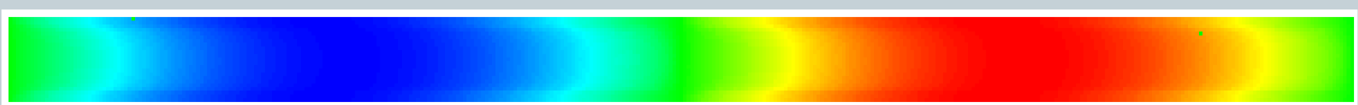
- Average velocity: 0.002m/s   Slug length: 4mm
- Capillary radius: 250 µm



- C_{AAmin}=0mol/m^3 C_{AAmax}=650mol/m^3 at t=0s



- C_{AAmin}=100.32mol/m^3 C_{AAmax}=387.46mol/m^3 at t=10.3s

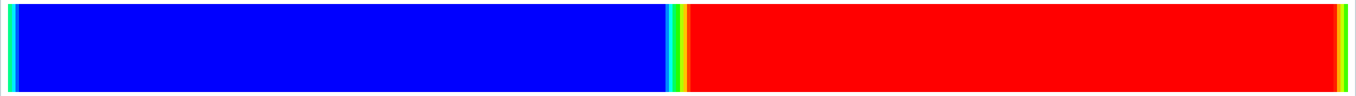


- C_{AAmin}=171.19mol/m^3 C_{AAmax}=235.59mol/m^3 at t=25.2s

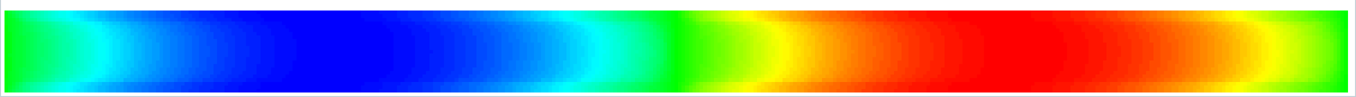
The concentration distribution of AA in two phases

Concentration distribution

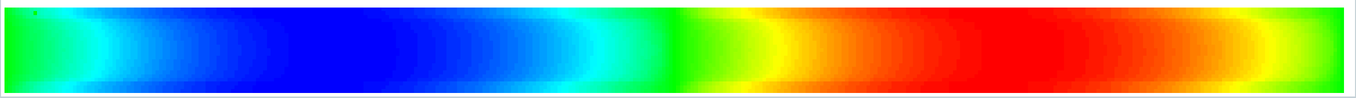
- Average velocity: 0.014m/s   Slug length: 4mm
- Capillary radius: 250 µm



- C_{AAmin}=0mol/m^3 C_{AAmax}=650mol/m^3 at t=0s



- C_{AAmin}=207.89mol/m^3 C_{AAmax}=217.77mol/m^3 at t=10.3s

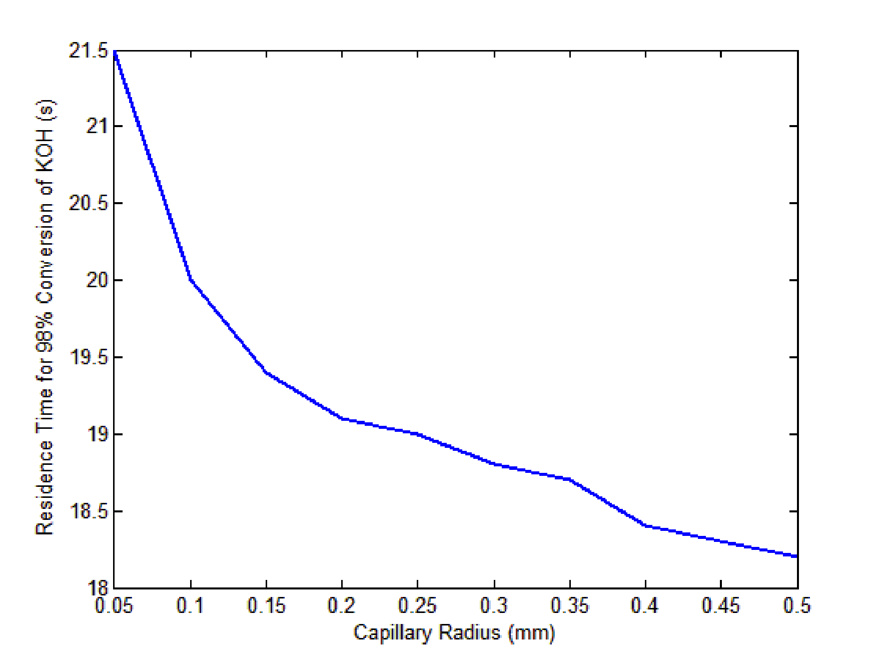


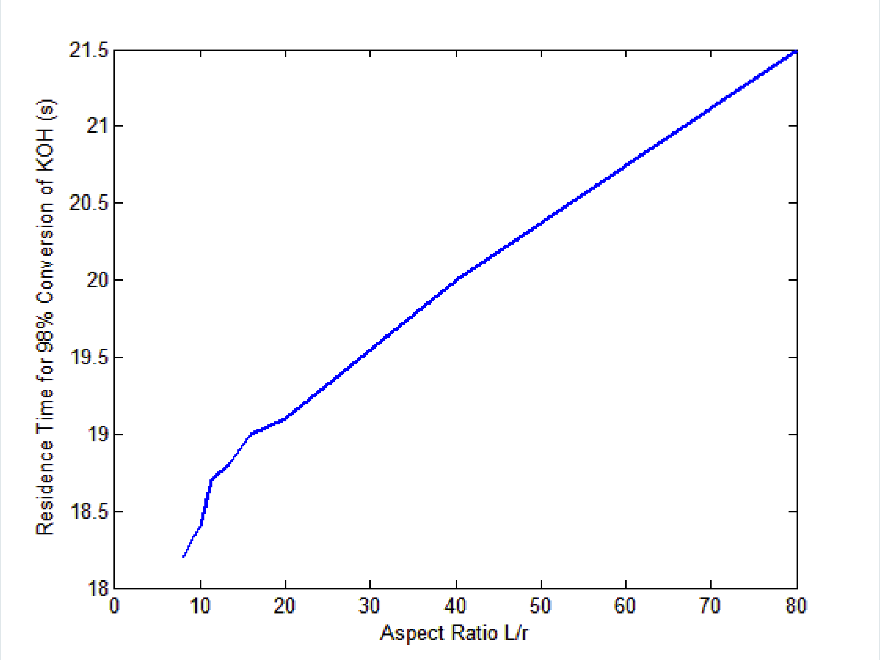
- C_{AAmin}=199.21mol/m^3 C_{AAmax}=199.67mol/m^3 at t=25.2s

The concentration distribution of AA in two phases

Results (Convection-Diffusion)

- Average flow velocity :0.014m/s
- Slug length: 4mm
- 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

Dr. Brian H. Dennis

Thank you for your attention!

Question?