Microreactor Engineering

Goran Jovanovic
Oregon State University
School of Chemical, Biological, and Environmental Engineering

Two-Phase-Flow Microchannel Reactors II

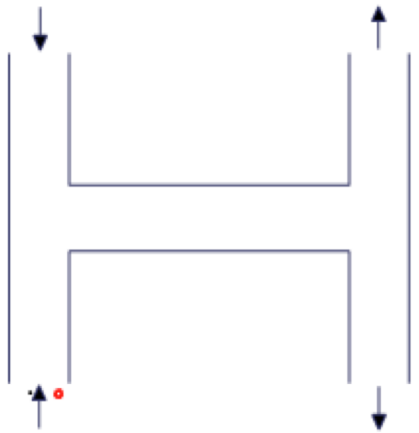
In Affiliation With:

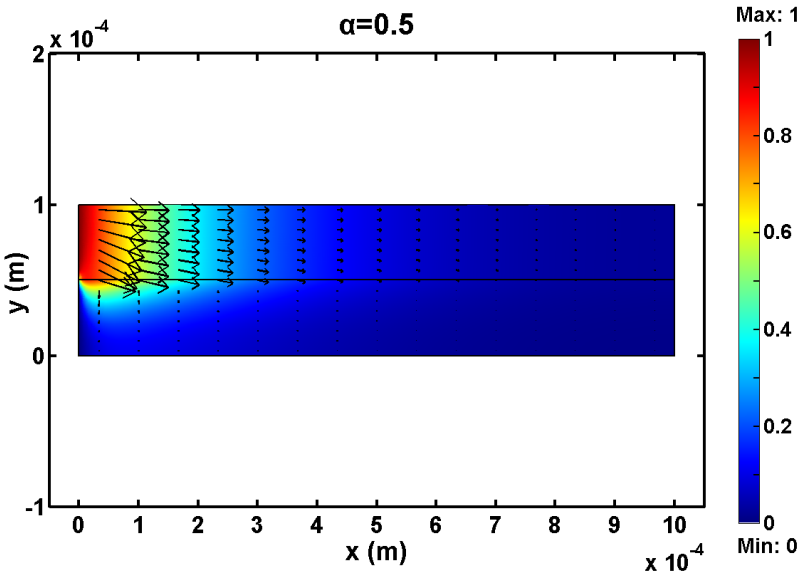
MBI
Microproducts Breakthrough Institute

PTT - LOA
PTT - Laboratories Of America

Problem Outline

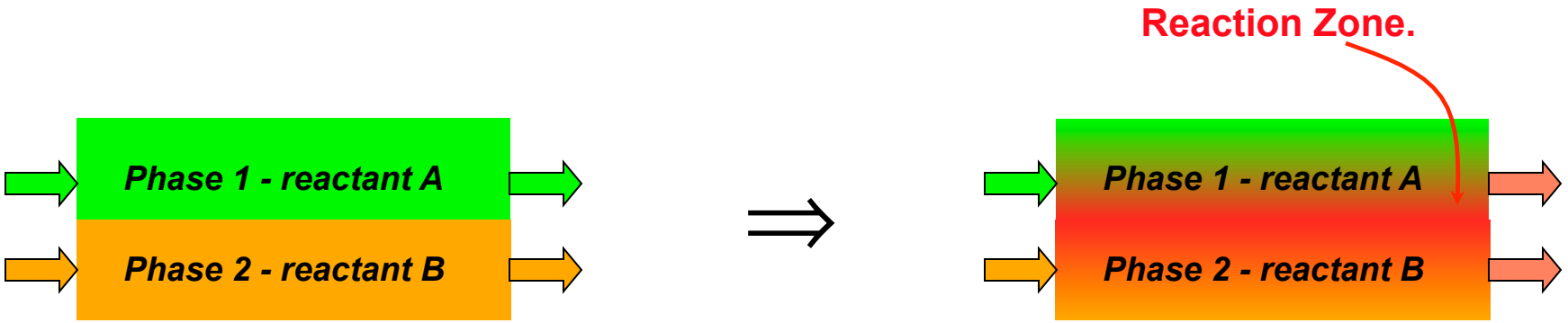
- Investigate phenomena pertinent to convection, diffusion, and second order chemical reaction in two-phase immiscible microreaction systems.
- Develop two-dimensional velocity, and diffusion-reaction models to predict conversion in microreactors in which both reactant can freely diffuse into two immiscible phases with a partition coefficient of 1.





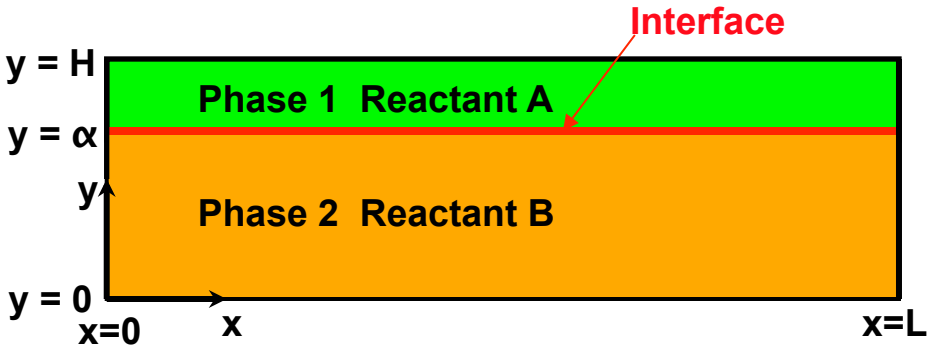
The Most Generic Problem Consideration

$$A + B \Rightarrow R \qquad -r_A = kC_A C_B$$



Reactant *B* diffuse into Phase 1, and
Reactant *A* diffuse into Phase 2.

Mass Balance Equation (two-dimen., steady-state)

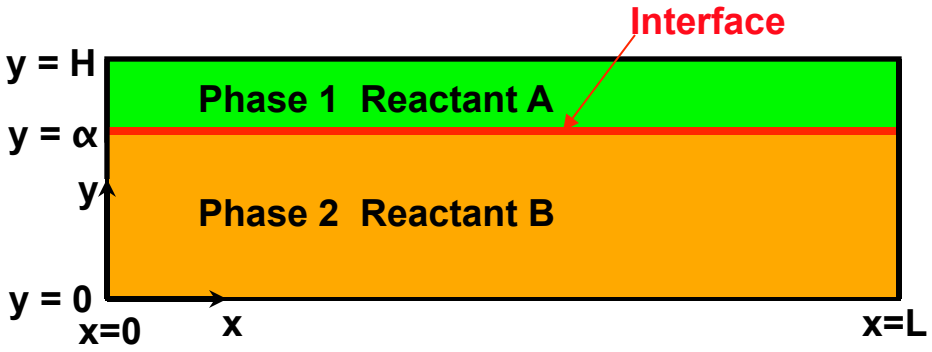


Convection-Diffusion-Reaction Equations for Phase 1

reactant A: $$-u_1 \frac{\partial C_{A1}}{\partial x} + D_{A1} \frac{\partial^2 C_{A1}}{\partial x^2} + D_{A1} \frac{\partial^2 C_{A1}}{\partial y^2} - kC_{A1}C_{B1} = 0$$

reactant B: $$-u_1 \frac{\partial C_{B1}}{\partial x} + D_{B1} \frac{\partial^2 C_{B1}}{\partial x^2} + D_{B1} \frac{\partial^2 C_{B1}}{\partial y^2} - kC_{A1}C_{B1} = 0$$

Mass Balance Equation (two-dimen., steady-state)



Boundary Conditions for Phase 1 Mass Balance Equation

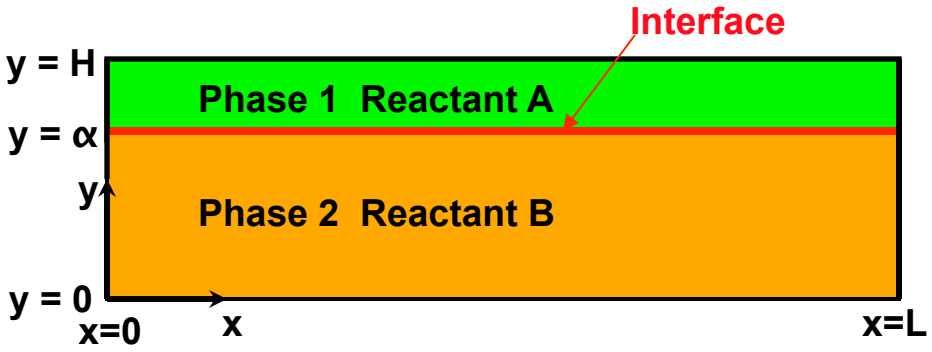
$$@\ x = 0, \quad C_{A1} = C_{A0},\ C_{B1} = 0$$

$$@\ x = L, \quad \frac{\partial C_{A1}}{\partial x} = 0 \quad \frac{\partial C_{B1}}{\partial x} = 0$$

$$@\ y = \alpha H,\ C_{A1} = C_{A2},\ C_{B1} = C_{B2}$$

$$@\ y = H, \quad \frac{\partial C_{A1}}{\partial y} = 0 \quad \frac{\partial C_{B1}}{\partial y} = 0$$

Mass Balance Equation (two-dimen., steady-state)

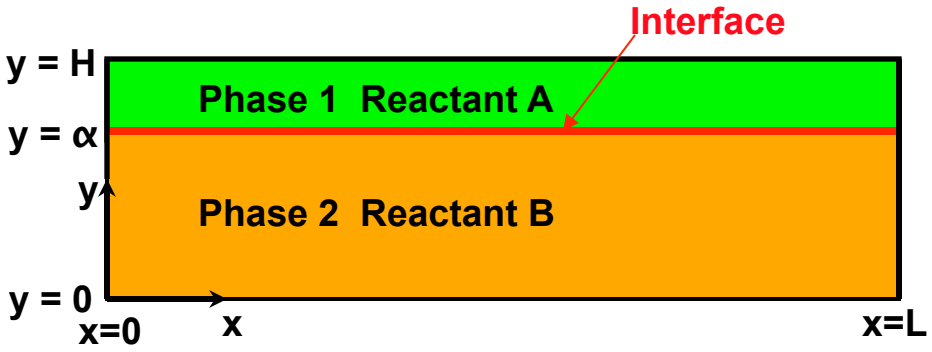


Convection-Diffusion-Reaction Equations for Phase 2

reactant A: $$-u_2 \frac{\partial C_{A2}}{\partial x} + D_{A2} \frac{\partial^2 C_{A2}}{\partial x^2} + D_{A2} \frac{\partial^2 C_{A2}}{\partial y^2} - kC_{A2}C_{B2} = 0$$

reactant B: $$-u_2 \frac{\partial C_{B2}}{\partial x} + D_{B2} \frac{\partial^2 C_{B2}}{\partial x^2} + D_{B2} \frac{\partial^2 C_{B2}}{\partial y^2} - kC_{A2}C_{B2} = 0$$

Mass Balance Equation (two-dimen., steady-state)



Boundary Conditions for Phase 2 Mass Balance Equation

$$@\ x=0,\quad C_{A2}=0,\ C_{B2}=C_{Bo} \qquad @\ x=L,\quad \frac{\partial C_{A2}}{\partial x}=0 \qquad \frac{\partial C_{B2}}{\partial x}=0$$

$$@\ y=0,\quad \frac{\partial C_{A2}}{\partial y}=0 \qquad \frac{\partial C_{B2}}{\partial y}=0$$

$$@\ y=\alpha H;\ D_{A1}\frac{\partial C_{A1}}{\partial y}=D_{A2}\frac{\partial C_{A2}}{\partial y}, \qquad D_{B1}\frac{\partial C_{B1}}{\partial y}=D_{B2}\frac{\partial C_{B2}}{\partial y}$$

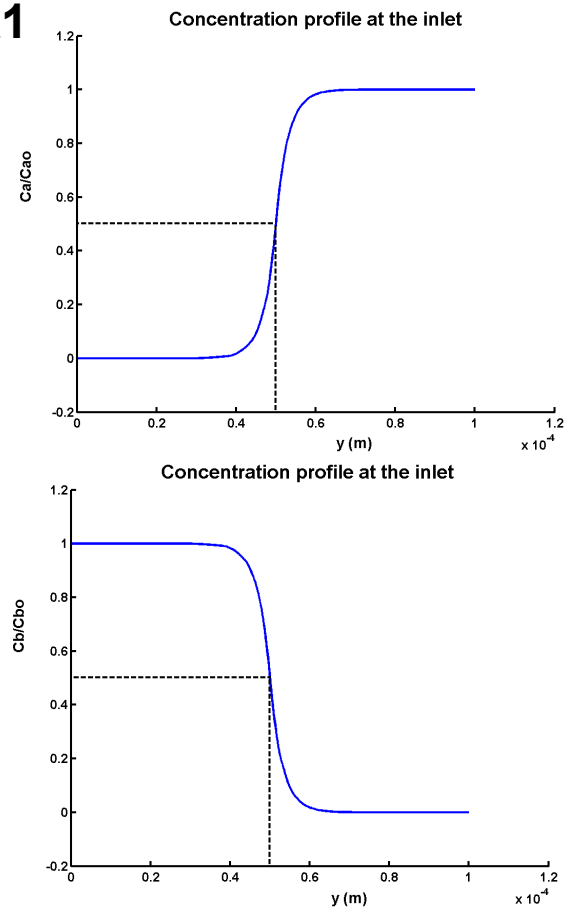
Typical Numerical Issues

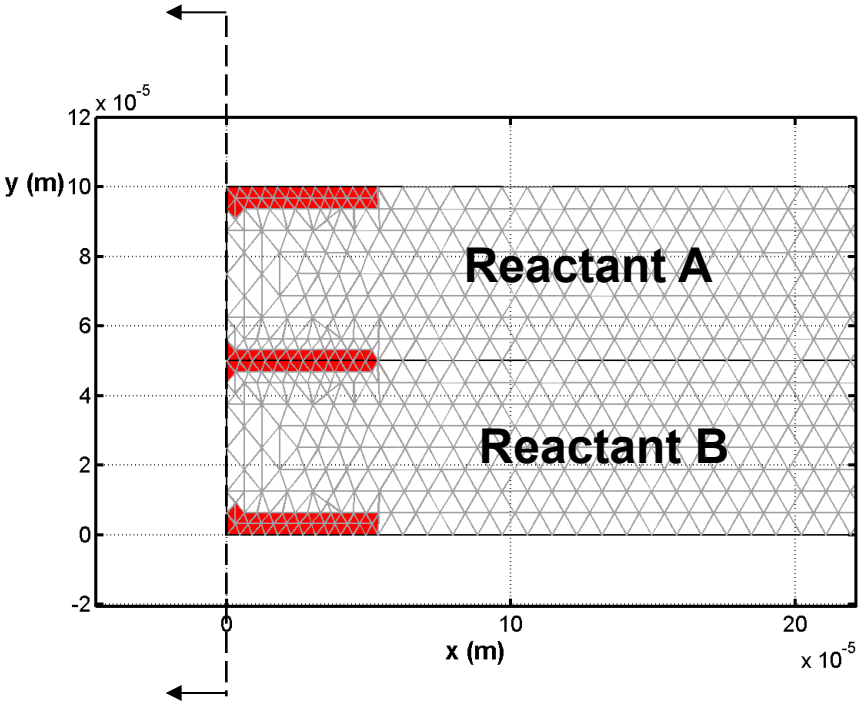
1. How to solve numerical instability at the interface, near the inlet?

2. How to determine the velocity profile?

Typical Numerical Issues

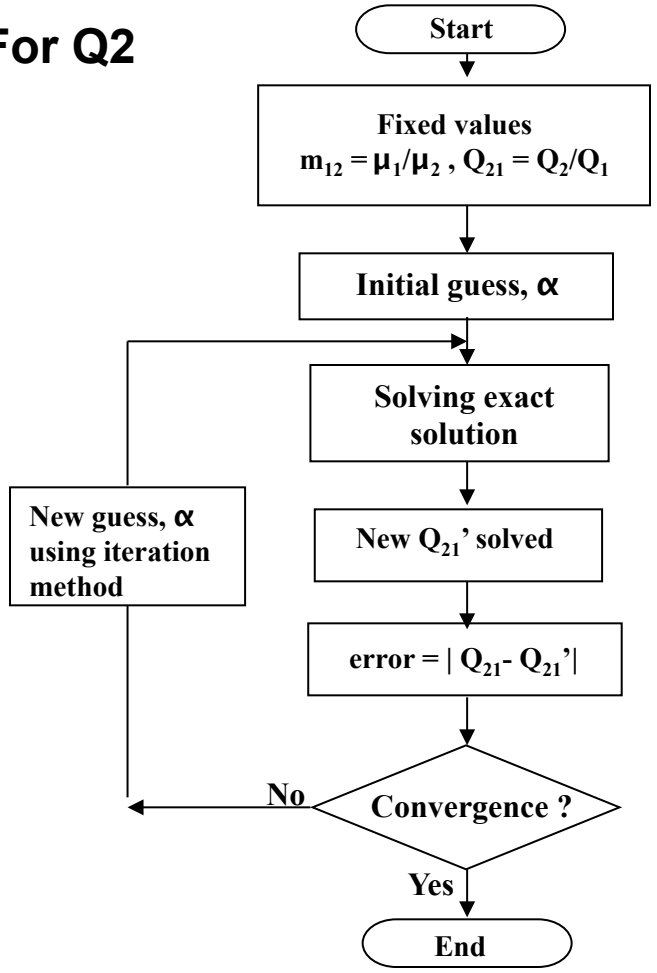
For Q1

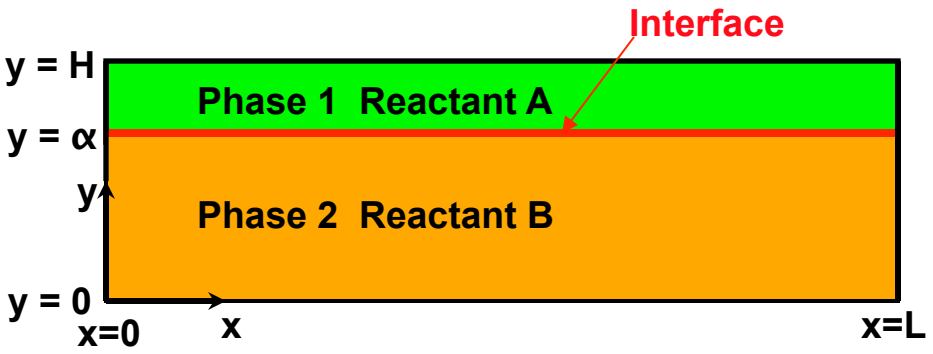




Typical Numerical Issues

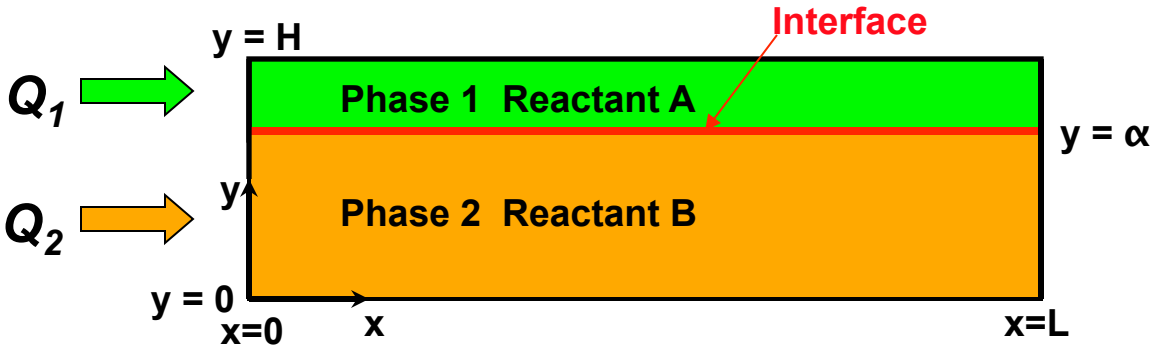
For Q2





$$A + B \Rightarrow R \qquad -r_A = kC_AC_B$$

Typical numerical values for simulation



$$A + B \Rightarrow R \qquad -r_A = kC_A C_B$$

$$D_{A1} = 5 \times 10^{-8} \left[m^2 / s \right] \qquad D_{B1} = 1 \times 10^{-9} \left[m^2 / s \right]$$

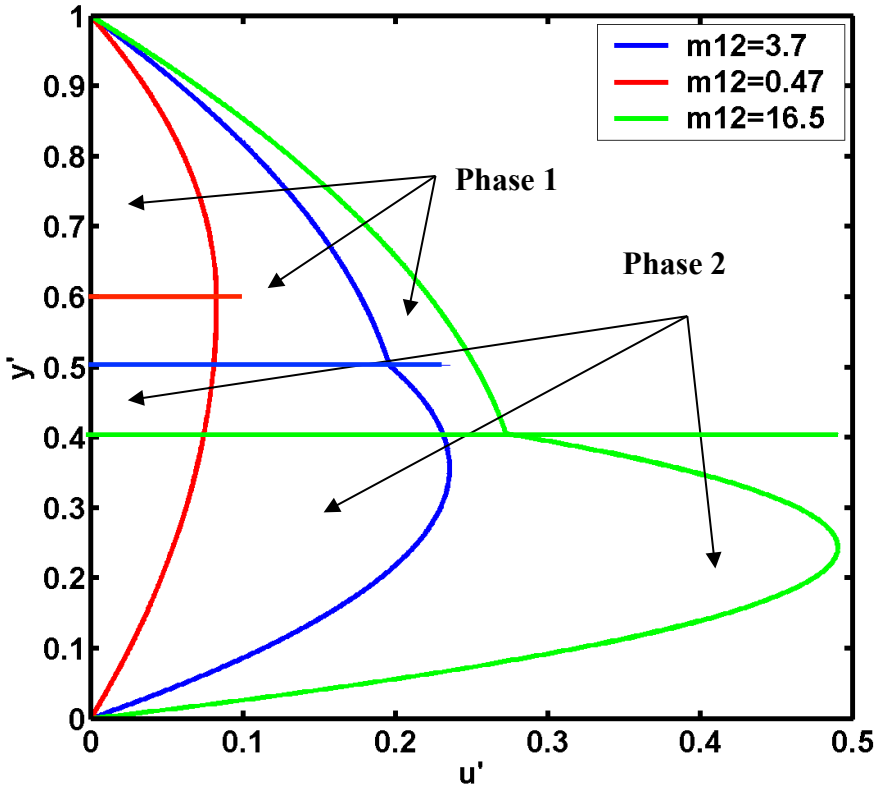
$$D_{A2} = 5 \times 10^{-10} \left[m^2 / s \right] \qquad D_{B2} = 1 \times 10^{-8} \left[m^2 / s \right]$$

$$\rho_1 = 800 \left[kg / m^3 \right] \qquad \rho_2 = 1000 \left[kg / m^3 \right]$$

$$\mu_1 = 0.8 \left[kg / m \cdot s \right] \qquad \mu_2 = \mu_1 / m_{12}$$

$$k = 2.0 \left[m^3 / kmol \cdot s \right]$$

Velocity Profile



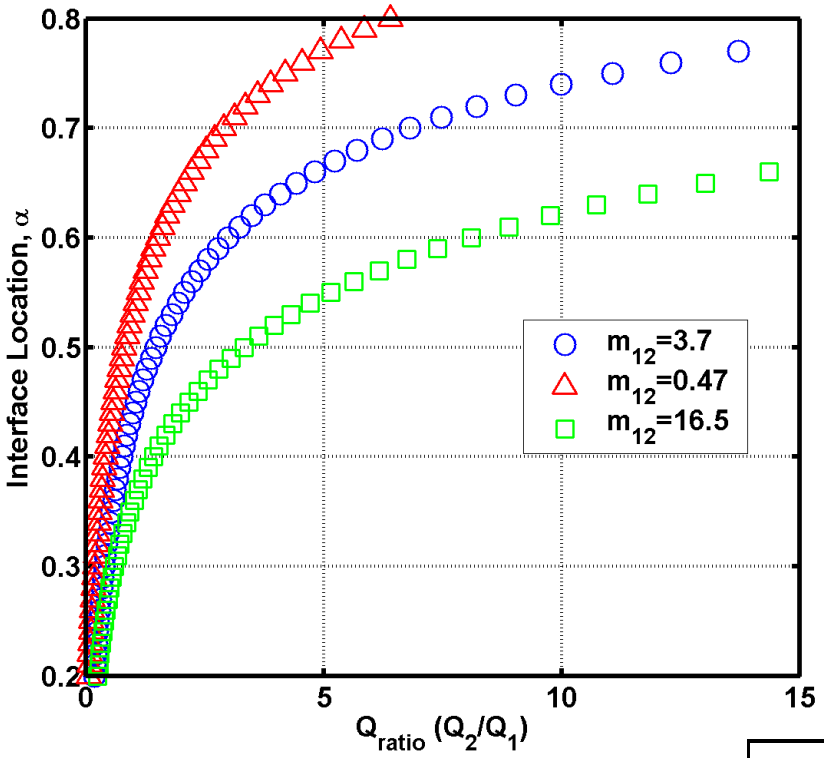
Fully developed velocity profiles

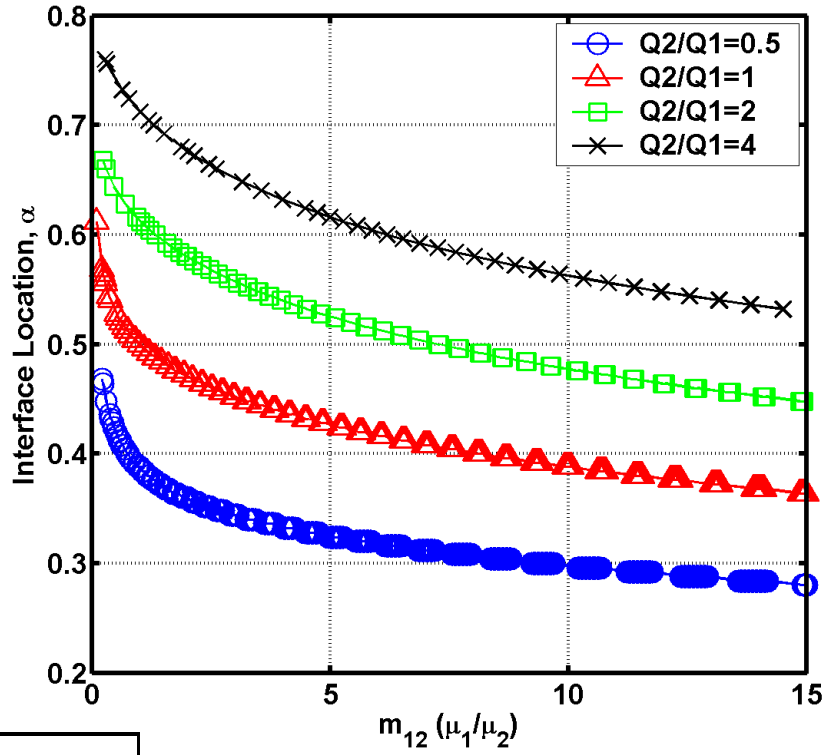
Interface locations of two phase flow

Fixed volume flow rate ratio (Q_2/Q_1 =1.5)

$$m_{12} = \frac{\mu_1}{\mu_2}$$

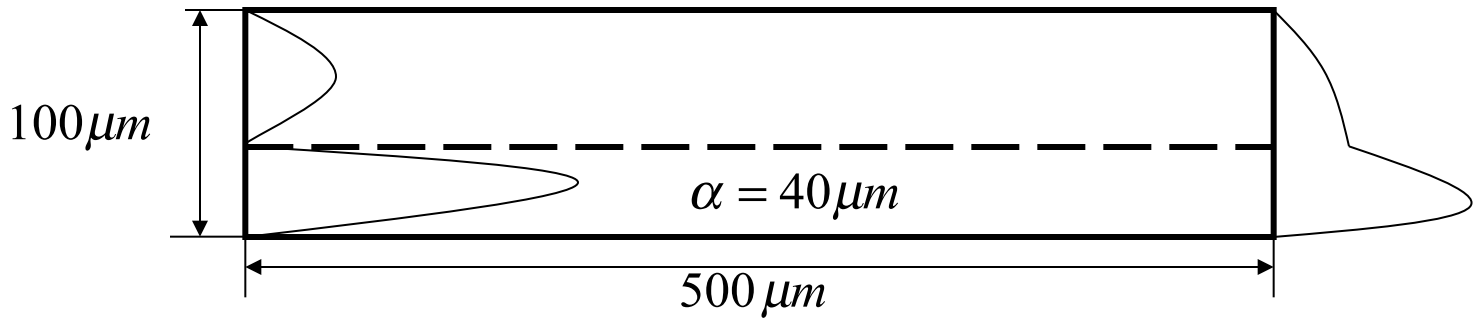
Interface Location



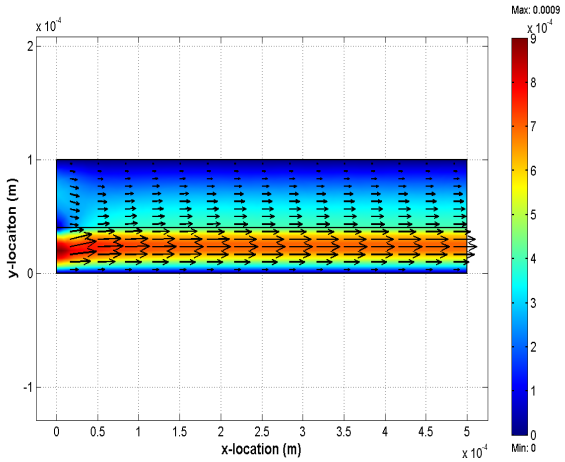


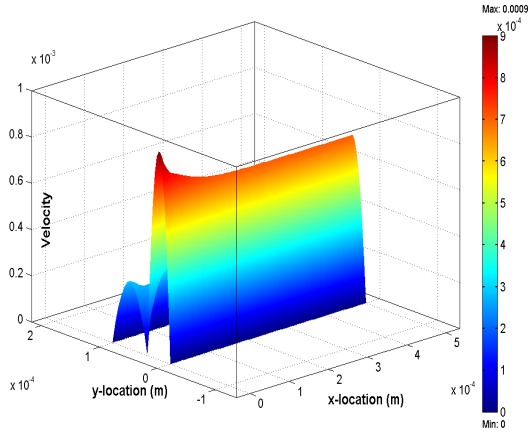
$$m_{12} = \frac{\mu_1}{\mu_2}$$

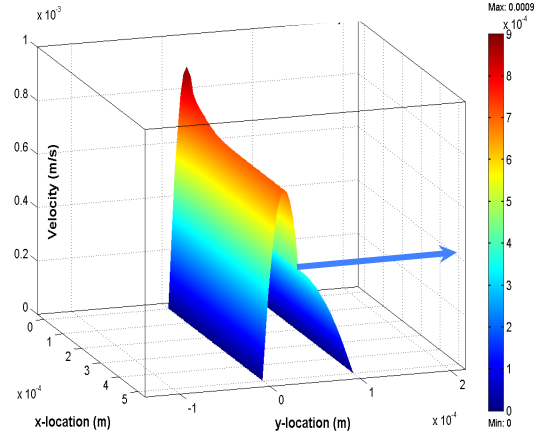
Flow Development Length -x



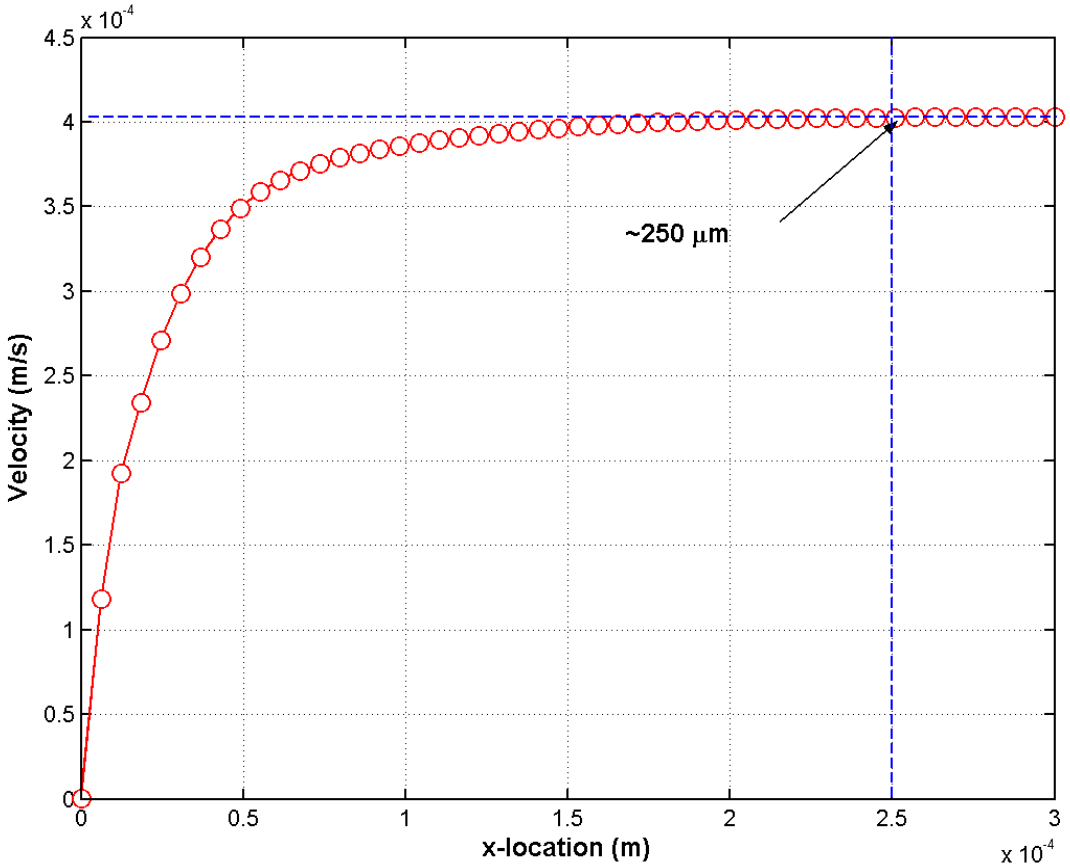
$$m_{12} = 16.5; \quad \frac{Q_2}{Q_1} = 1.5; \quad \alpha = 40[\mu m]; \quad x \approx 500[\mu m]$$





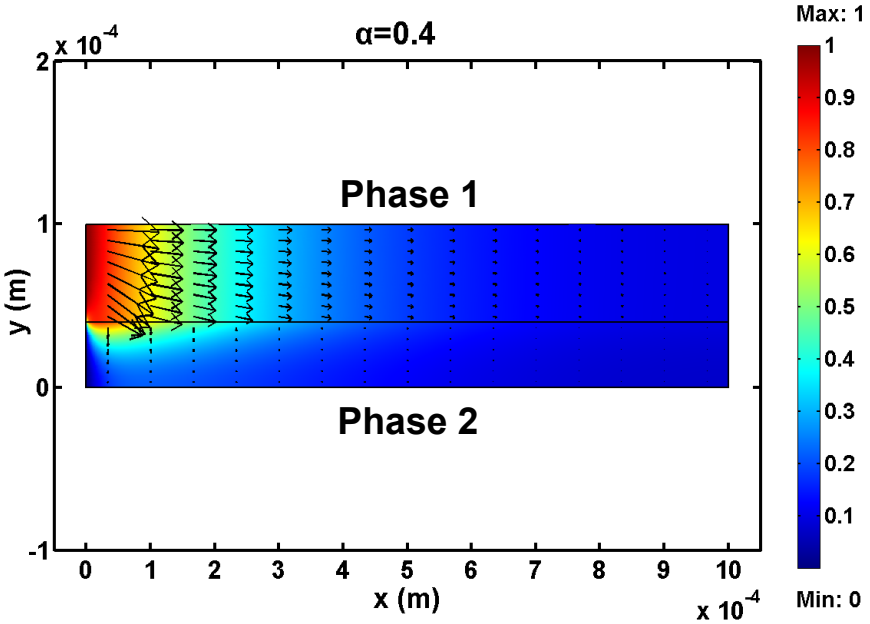


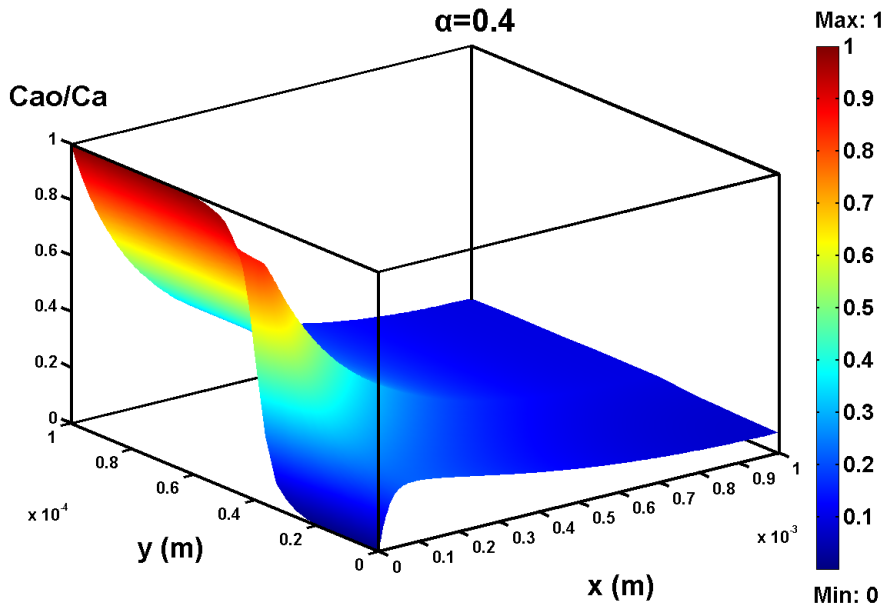
Flow Development Length -x



Concentration contours *(α =0.4; Q_2/Q_1=1.5; H=100μm)*

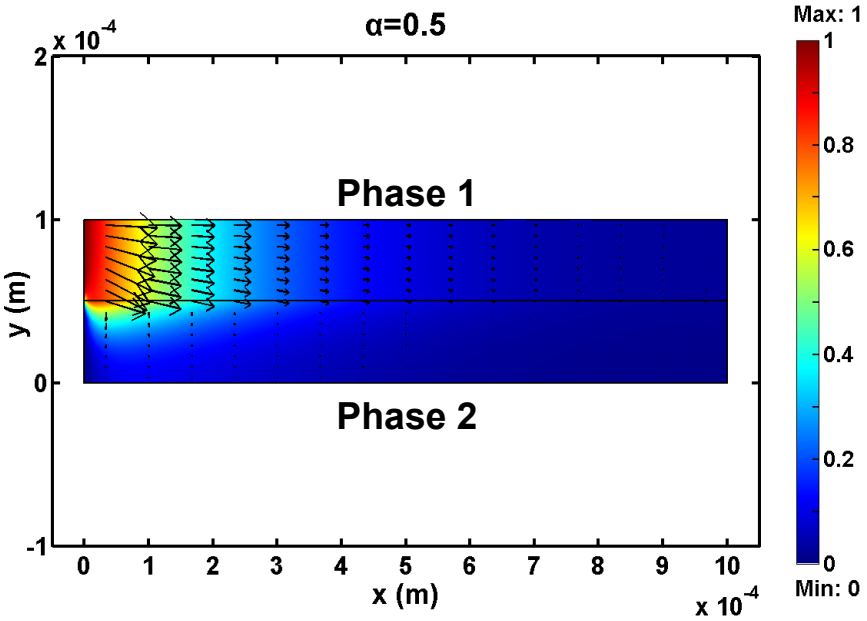
$$m_{12} = \frac{\mu_1}{\mu_2} = 16.5$$

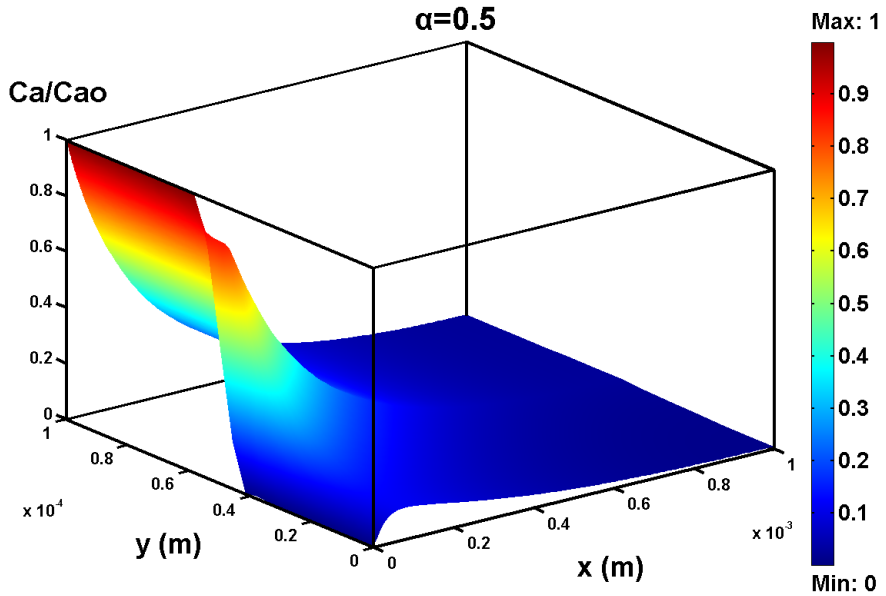




Concentration contours *(α =0.5; Q_2/Q_1=1.5; H=100μm)*

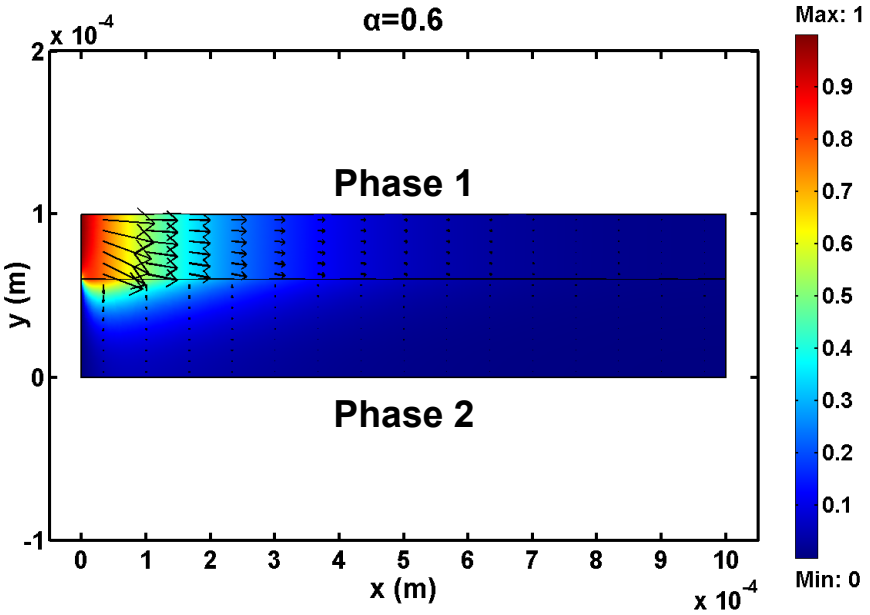
$$m_{12} = \frac{\mu_1}{\mu_2} = 3.7$$





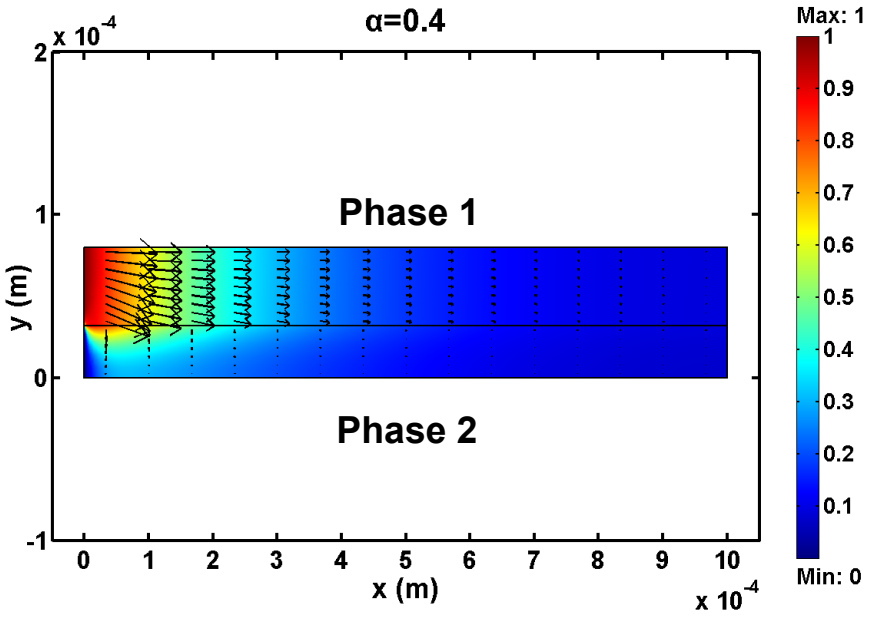
Concentration contours *(α =0.6; Q_2/Q_1=1.5; H=100μm)*

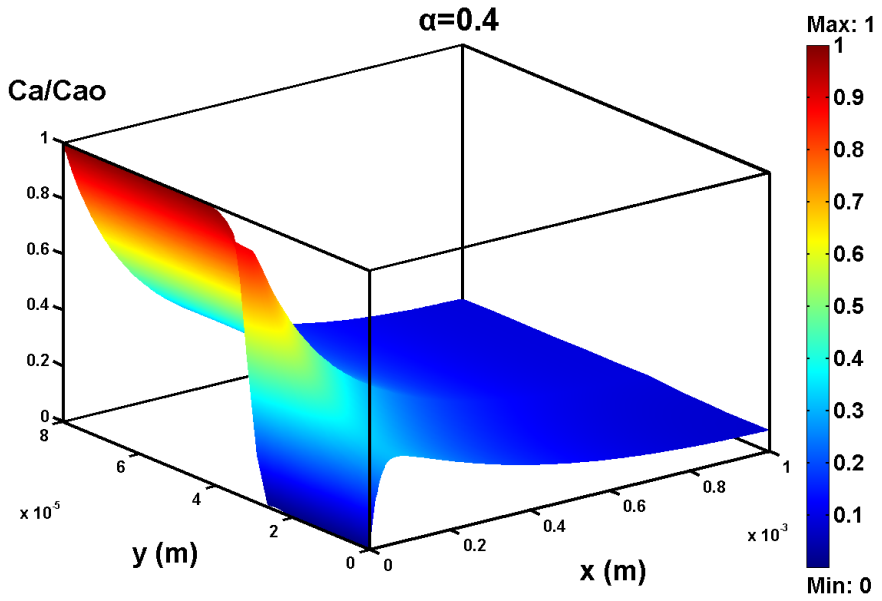
$$m_{12} = \frac{\mu_1}{\mu_2} = 0.47$$



Concentration contours *(α =0.4; Q_2/Q_1=1.5; H=80μm)*

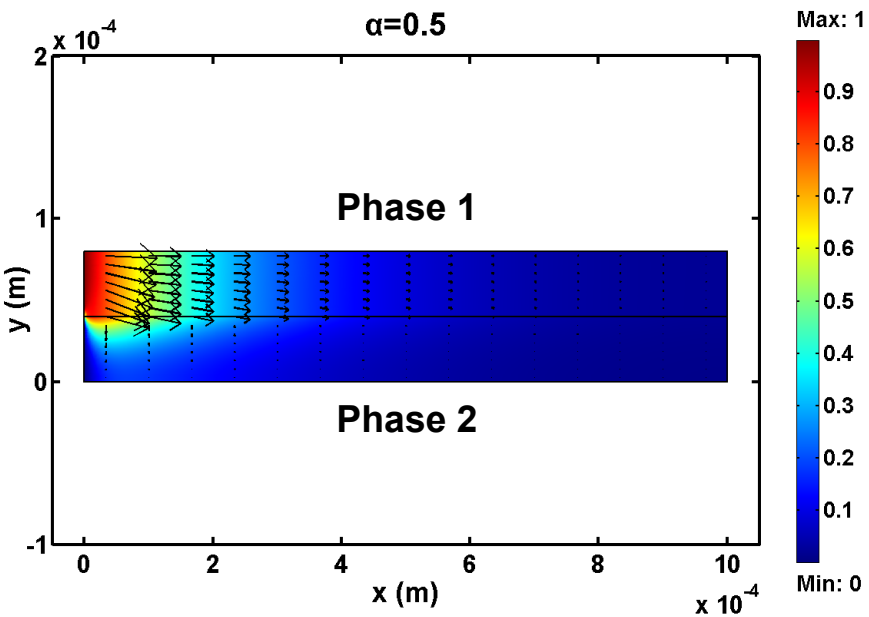
$$m_{12} = \frac{\mu_1}{\mu_2} = 16.5$$

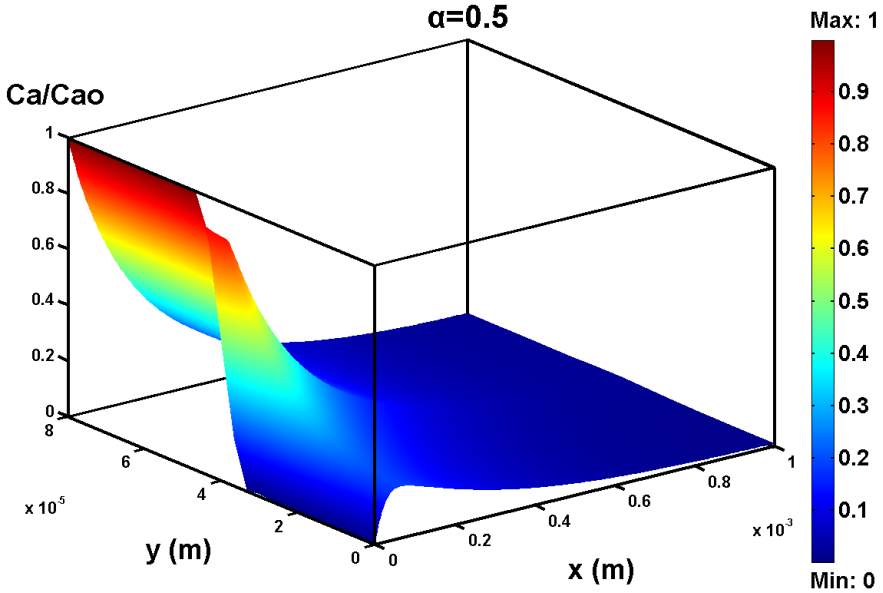




Concentration contours *(α =0.5; Q_2/Q_1=1.5; H=80μm)*

$$m_{12} = \frac{\mu_1}{\mu_2} = 3.7$$





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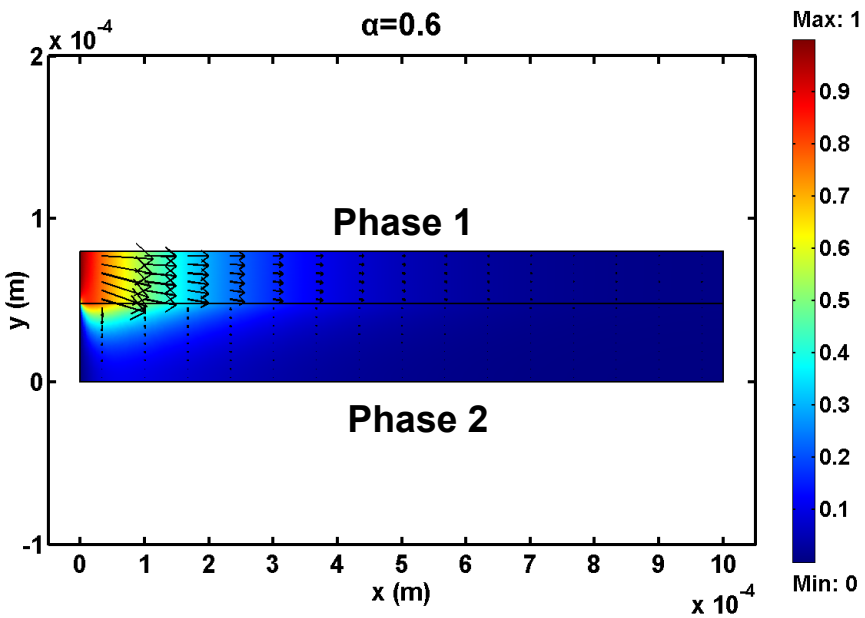
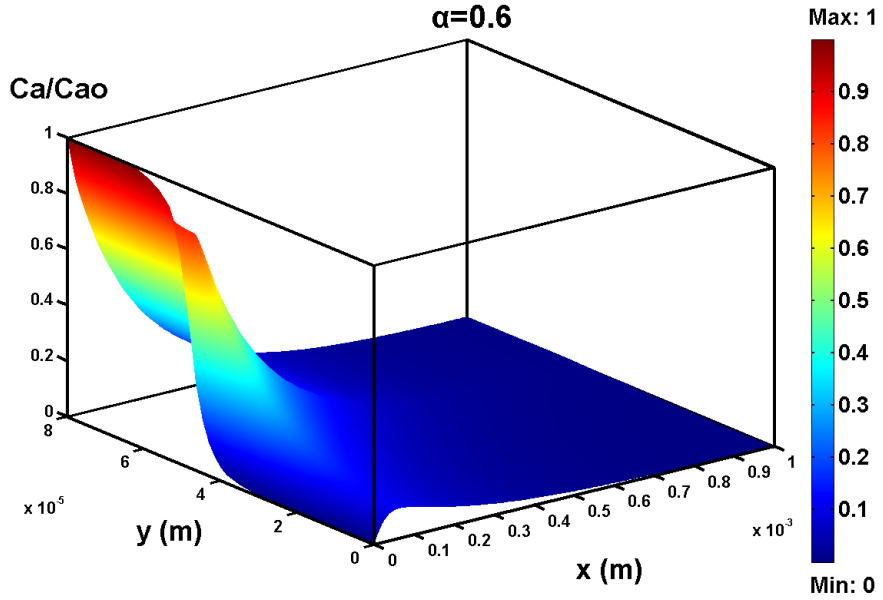
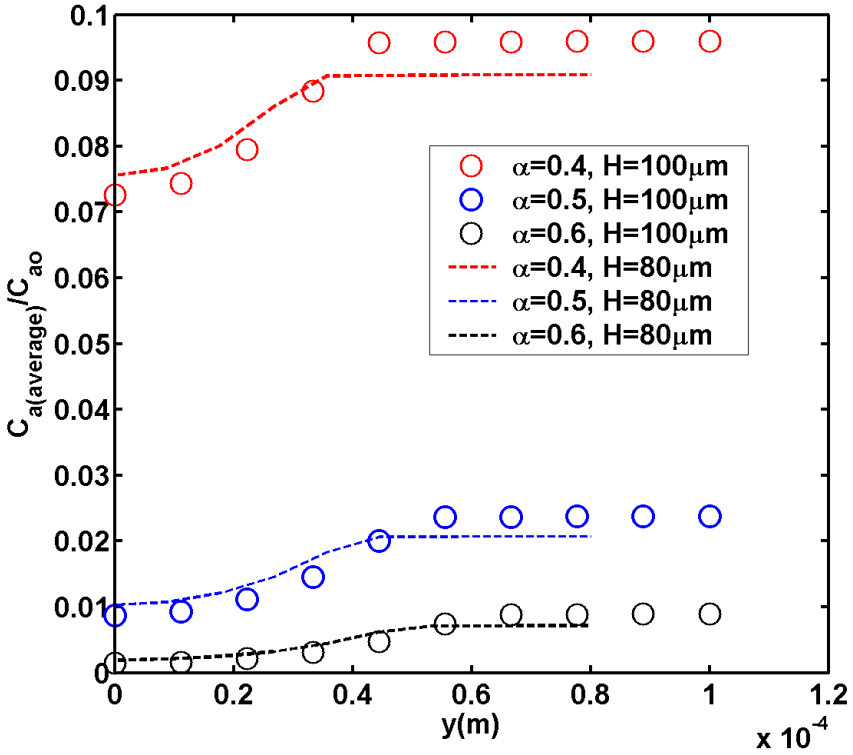
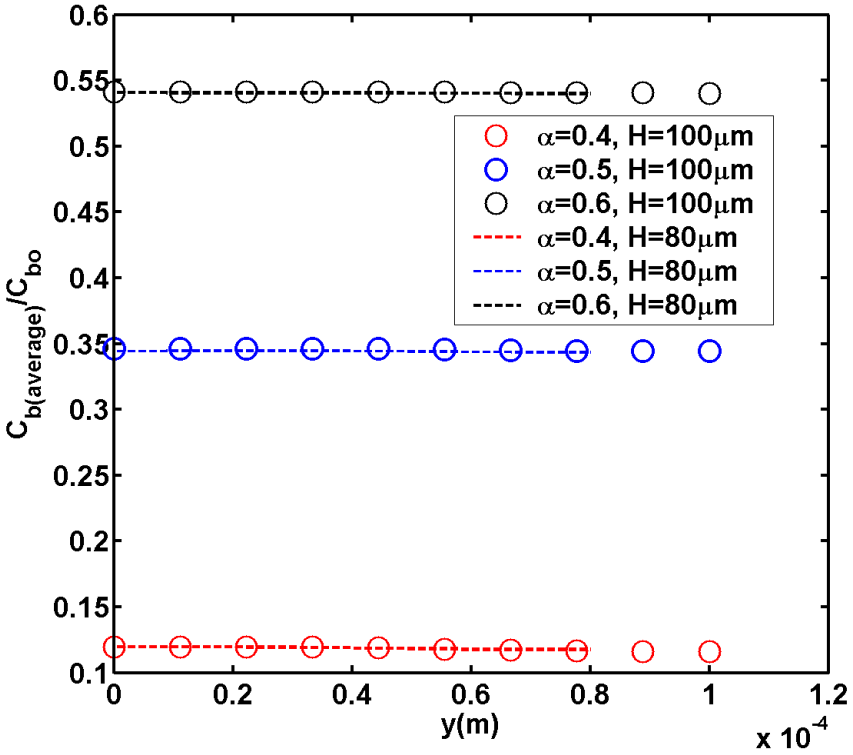
$$m_{12} = \frac{\mu_1}{\mu_2} = 0.47$$



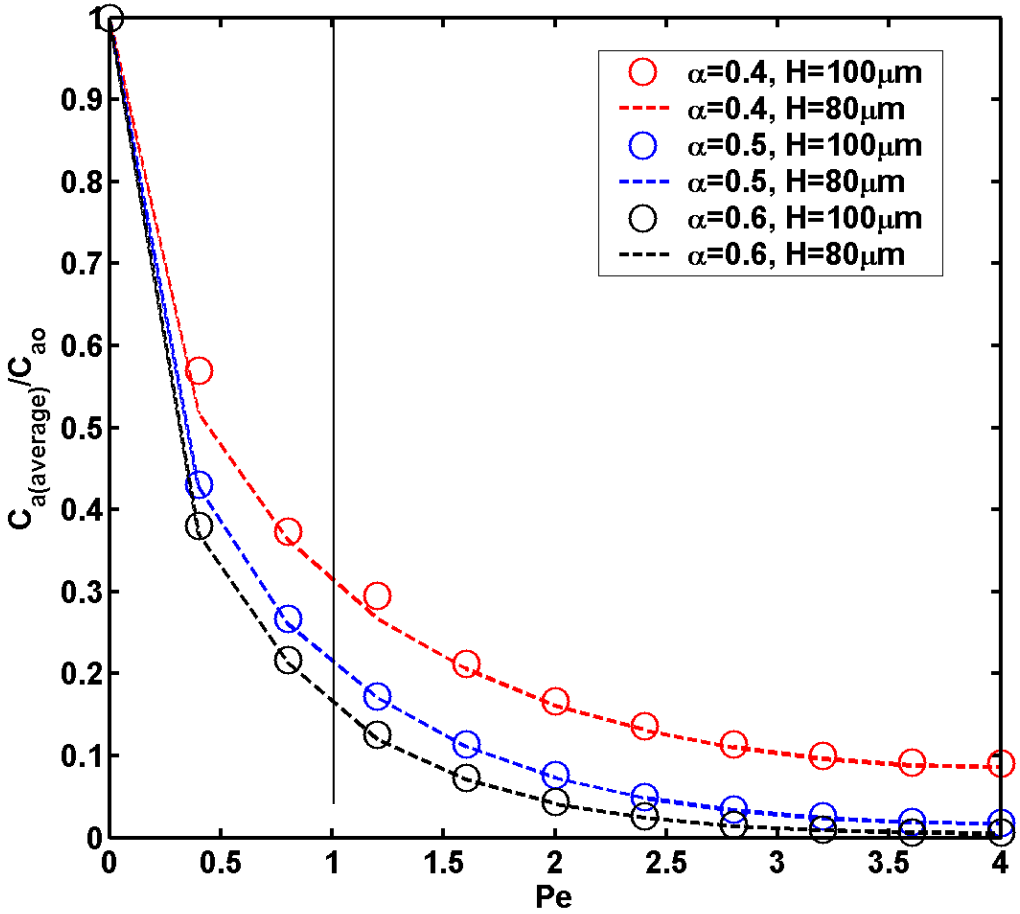


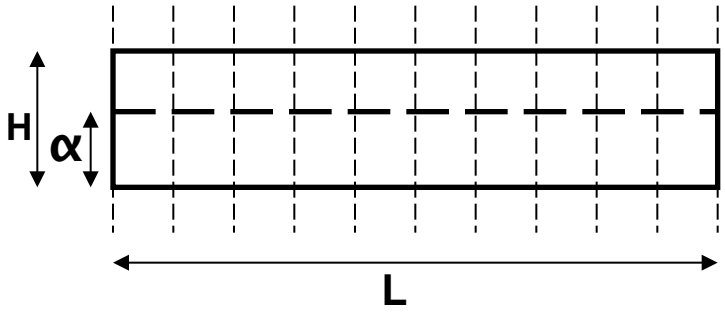
Concentration profile at exit





Peclet Number - Characteristic Times





$$Pe = \frac{uL}{D} = \left(\frac{L}{H}\right)^2 \frac{\tau_{D,H}}{\tau_H}$$

u = Mean velocity
L = Characteristic length
D = Diffusivity

Summary

- Two-dimensional exact solution of velocity profile for two phase flow was successfully derived.
- The interface locations are dependent on flow rate ratio and viscosity ratio between two phase flows.
- The flow rate ratio is more effective to locate interface than viscosity ratio.
- The case where $\alpha = 0.6$ and $H = 80\ \mu m$ is observed as the fastest reaction process rate for Reactant A compared to the other cases.
- Diffusion dominates transport when $Pe<1$, and large concentration gradients can be observed when $Pe>1$.

Recommendations

Three-dimensional models to predict more realistic micro-reaction;

Micro-reaction in flow developing region;

Optimize micro-channel geometry with respect to a defined objective function;

Validate the two-dimensional models by experiment.

Oregon State UNIVERSITY OSU College of Engineering

People. Ideas. Innovation.

Thank you for your attention!

Special thanks to Prof. In-Won Kim from Konkuk University (Korea)
in developing this material.