# Microreactor Engineering

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## Two-Phase-Flow Microchannel Reactors I

In Affiliation With:

**MBI**

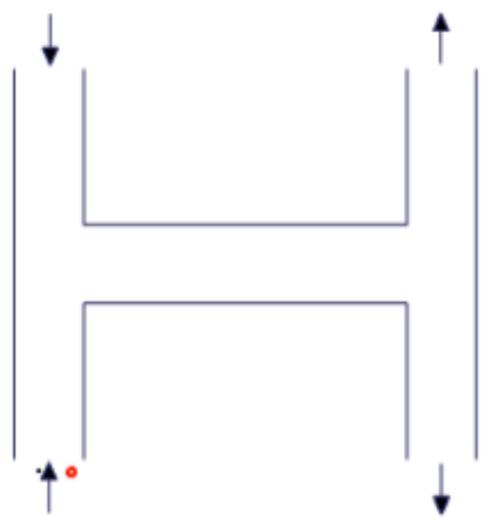
Microproducts Breakthrough Institute

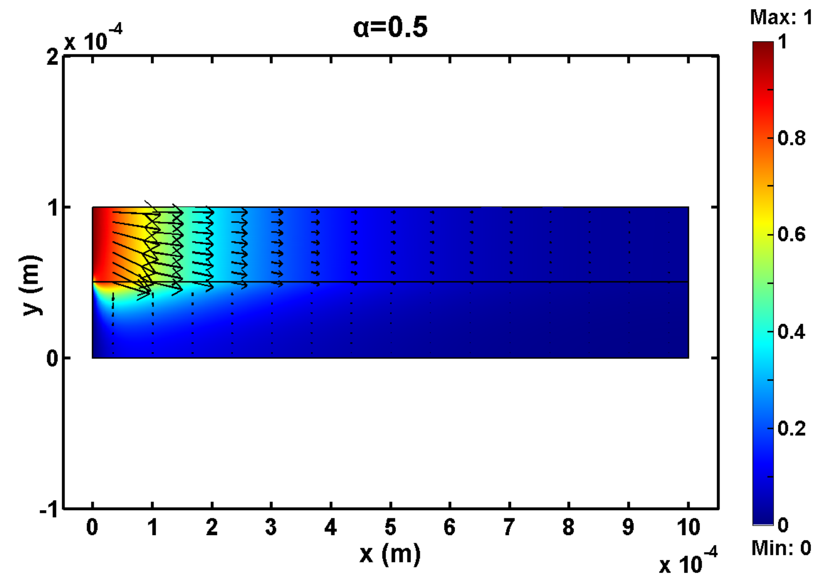
**PTT - LOA**

PTT - Laboratories Of America

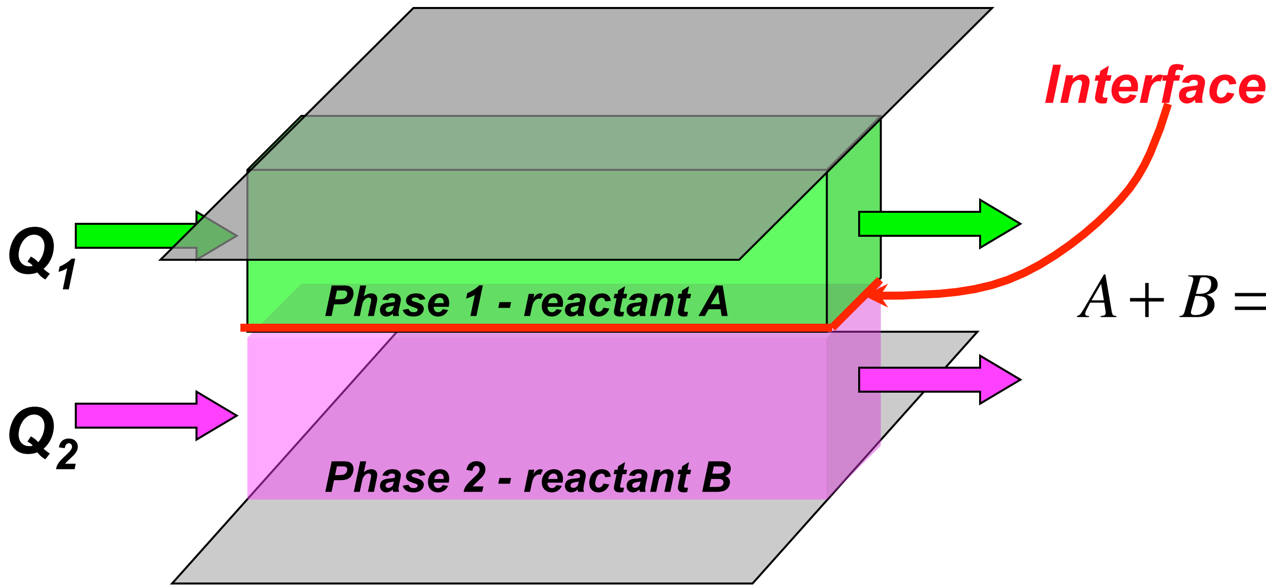
# Problem Statement

- Investigate phenomena pertinent to convection, diffusion, and reaction in two-phase immiscible microreaction systems.
- Develop two-dimensional velocity and diffusion-reaction models for the flow of two immiscible phases to predict conversion in microreactors.





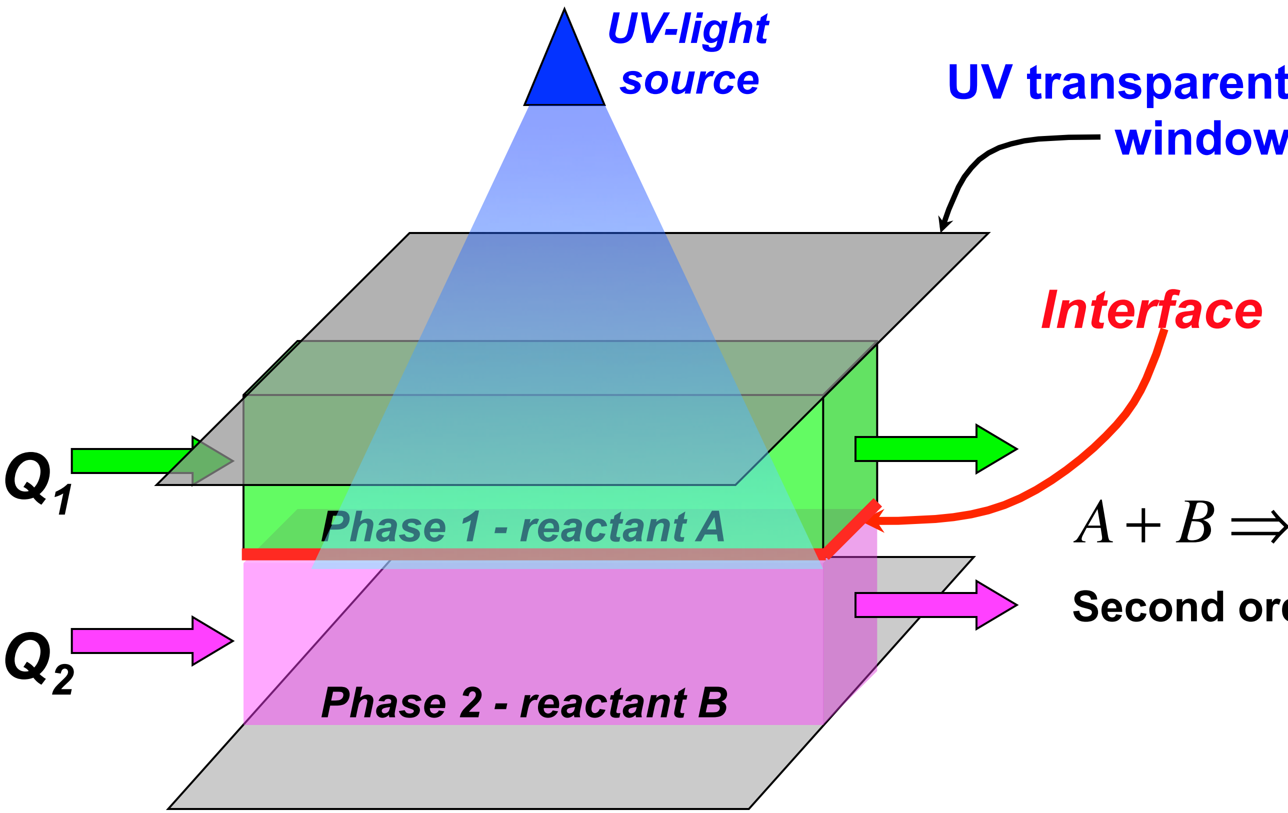
# Problem Statement




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

- Second order chemical reaction;
- Two reactants enter micro-channel separately with different flow rates $Q_1$ and $Q_2$;
- Two reactants have different properties ($D, \rho, \mu, \sigma$)

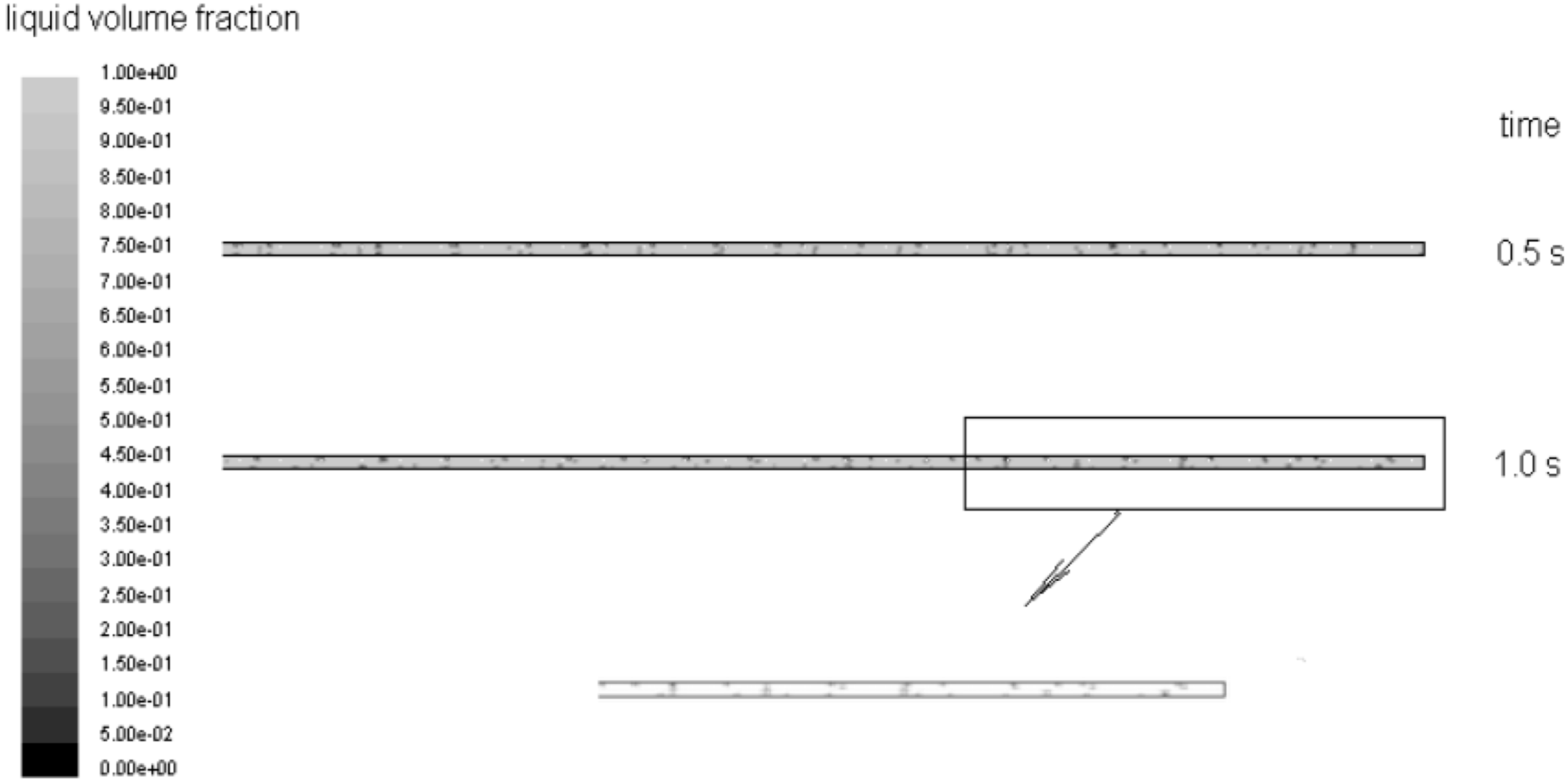
# Problem Statement




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

**Second order chemical reaction;**

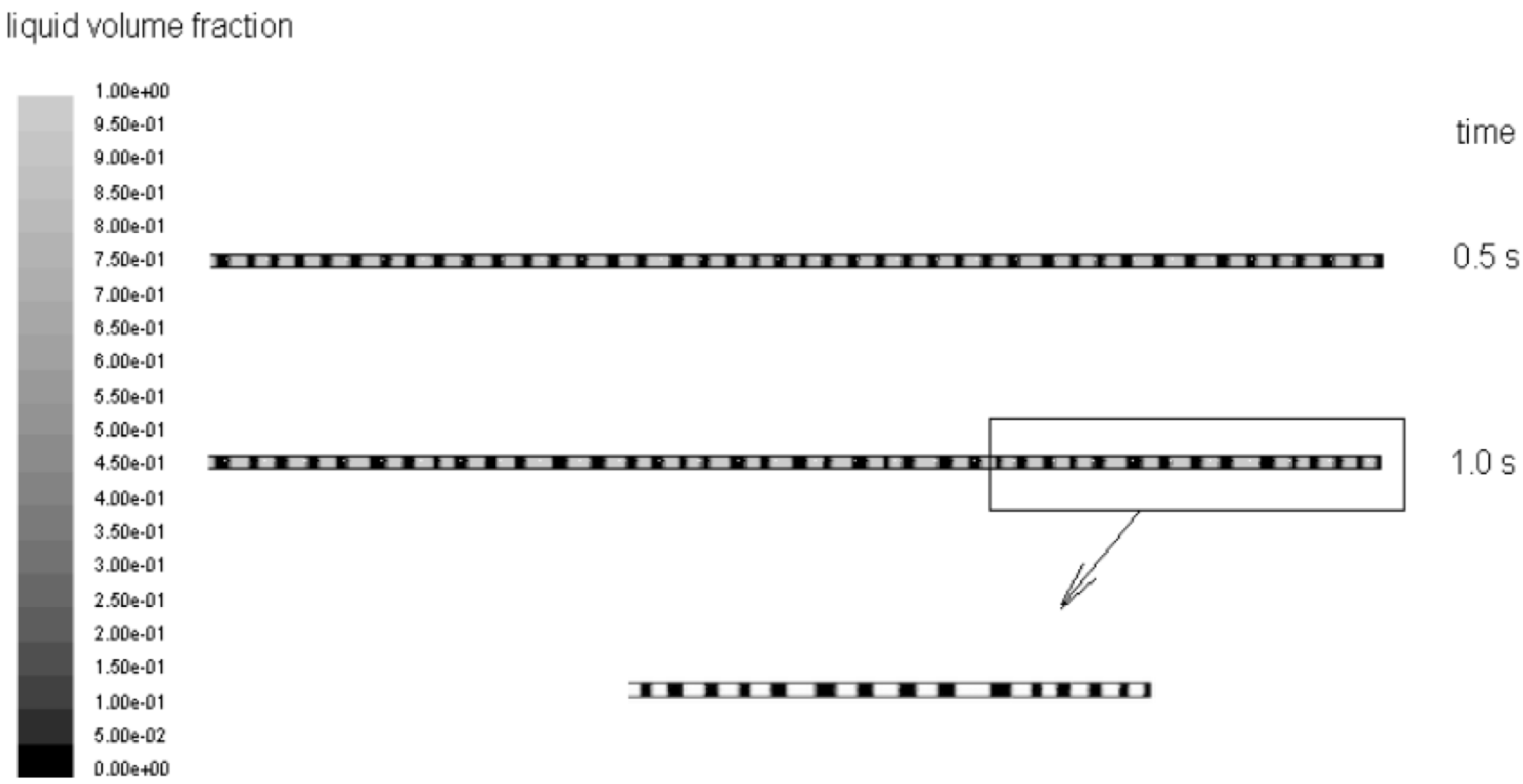
# Two-Phase Flow in Microchannels




Bubbly flow ($U_L$= 5.997 m/s, $U_G$ = 0.396 m/s)

Du et al., *Two-Phase Flow in Mini Flow Channels* International Journal of Chemical Reactor Engineering, Vol[8] article A15 (2010)

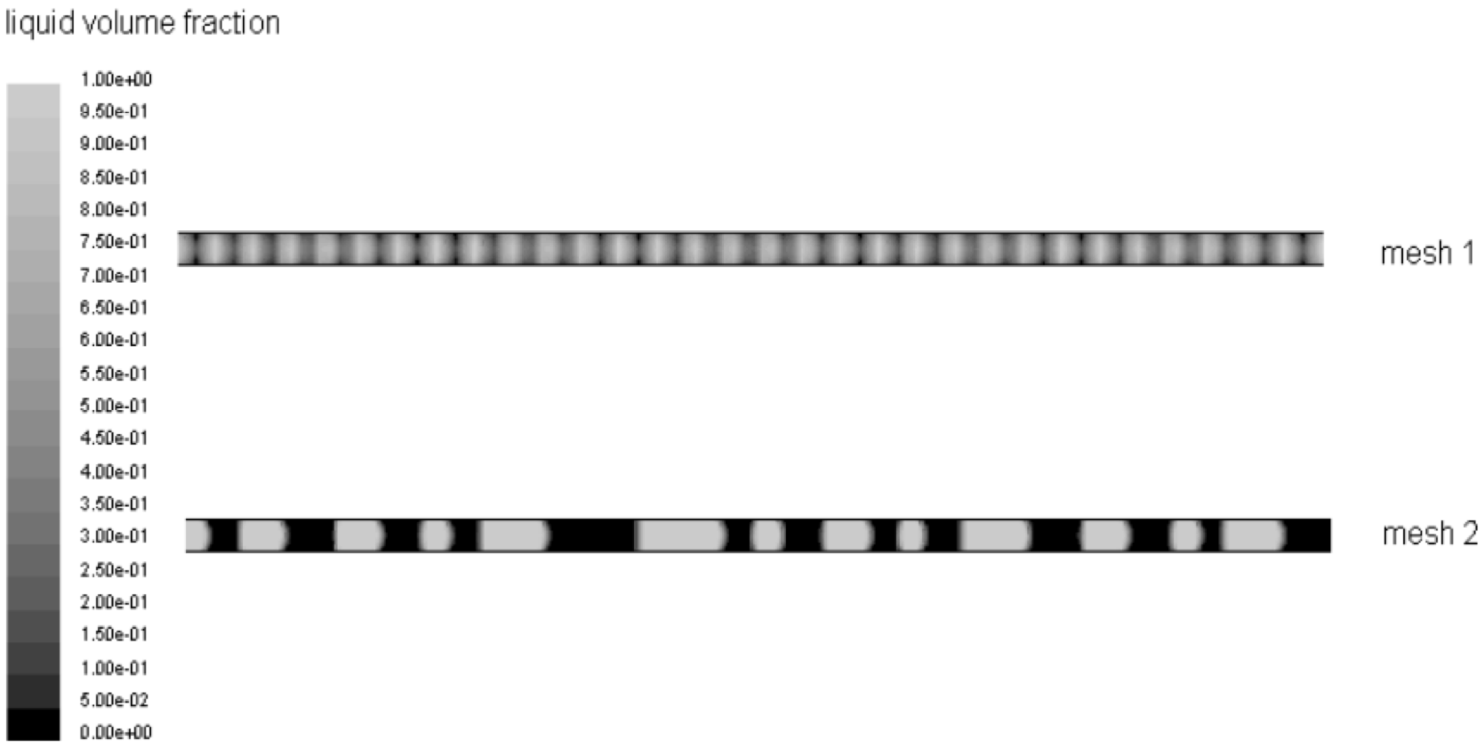
# Two-Phase Flow in Microchannels




Slug flow ($U_L$= 0.608 m/s, $U_G$ = 0.498 m/s)

Du et al., *Two-Phase Flow in Mini Flow Channels* International Journal of Chemical Reactor Engineering, Vol[8] article A15 (2010)

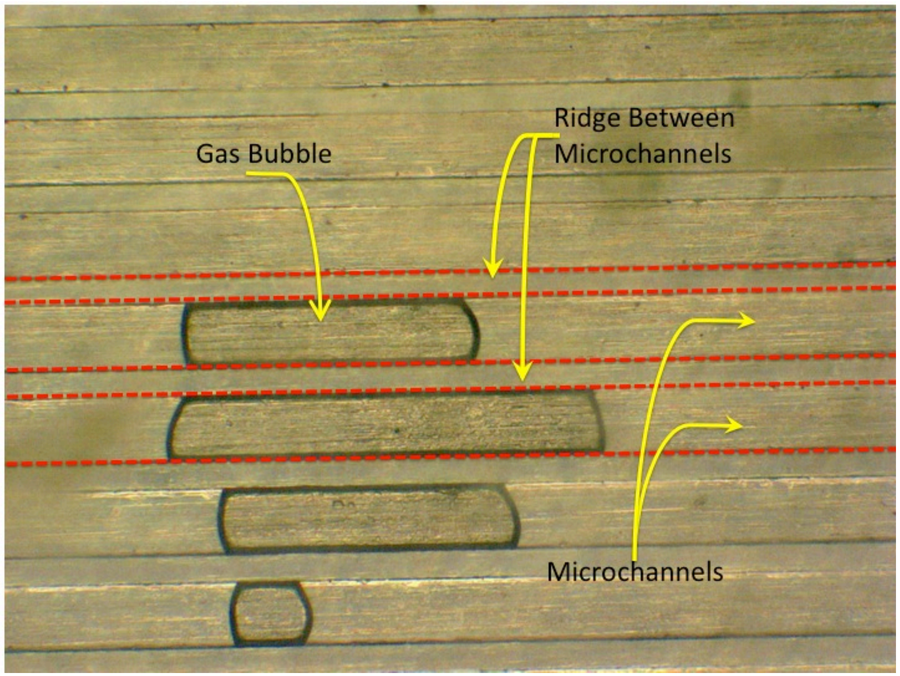
# Two-Phase Flow in Microchannels

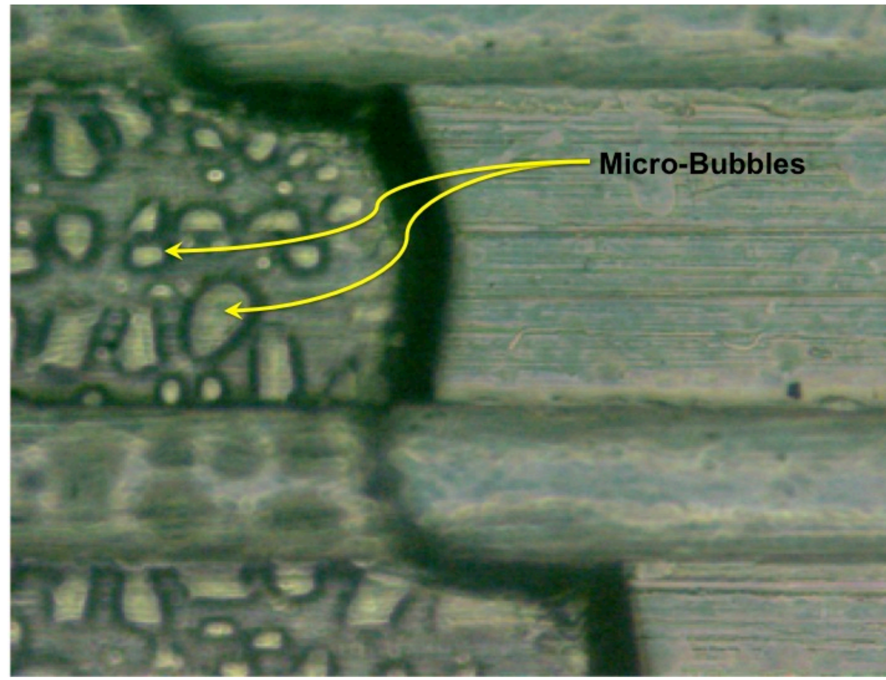



Simulated results at different mesh resolutions for straight channel (t=1.0 s)
Mesh 1: 9600 meshes, (0.1 mm x 0.5 mm), Mesh 2: 24000 meshes, (0.1 mm x 0.2 mm)

Du et al., *Two-Phase Flow in Mini Flow Channels* International Journal of Chemical Reactor Engineering, Vol[8] article A15 (2010)

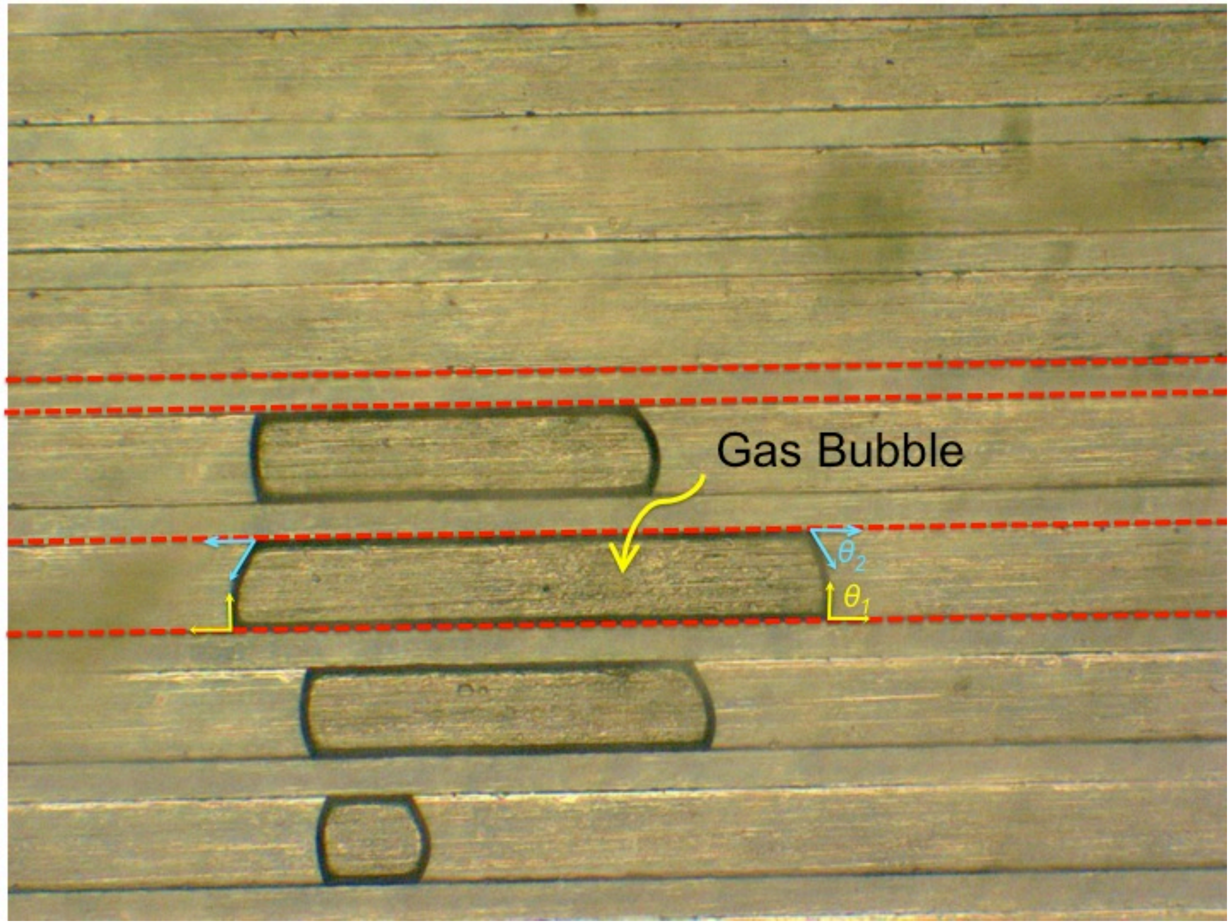
# Micro/Meso size Bubbles in Microchannels




Alana Warner Tuhy, *M.Sc. Thesis*, Oregon State University 2009

# Meso-size Bubbles in Microchannels




Alana Warner Tuhy, *M.Sc. Thesis*, Oregon State University 2009

# Problem Consideration

**The two fluids may have substantially different properties, which may create variety of reaction (process) cases:**

**Viscosity ratio $m_{12}=\mu_1/\mu_2$ influences velocity distribution and fluid residence time distribution in micro channels;**

**Diffusion coefficients of reactants *A and B* determine the scope & form of the governing differential equation, and location of the reaction zone;**

**Different fluid densities may influence the orientation of micro devices with respect to gravity;**

**Large surface tension may cause flow maldistribution.**

# Problem Consideration

There are additional elements of consideration that are important in 'constructing' governing model equations for reaction processes in microreactors:

**Reaction kinetics;**

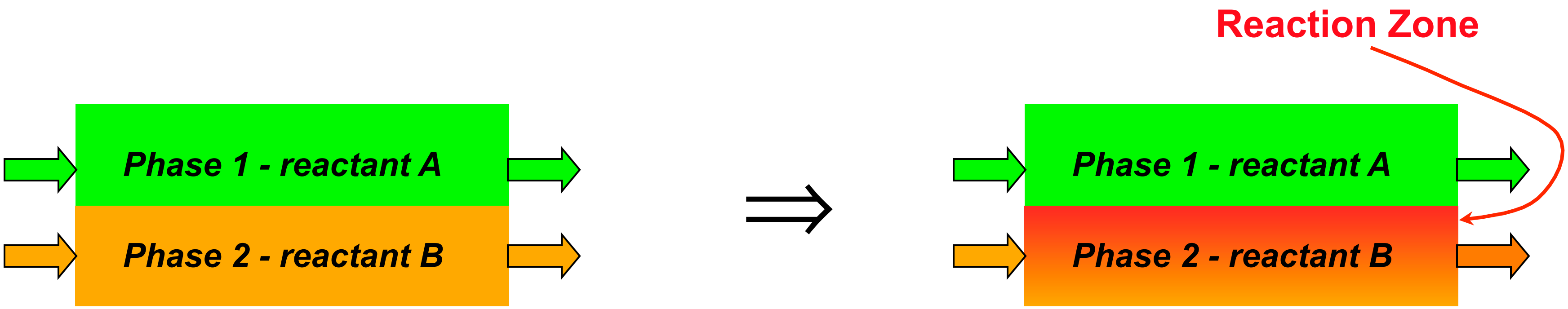
**Thermodynamic equilibrium;**

**Phase changes;**

# Problem Consideration

**Let us first consider different reaction situations that arise from different reactant diffusivities in the two phases (predominantly immiscible) in the micro channel reactor;**

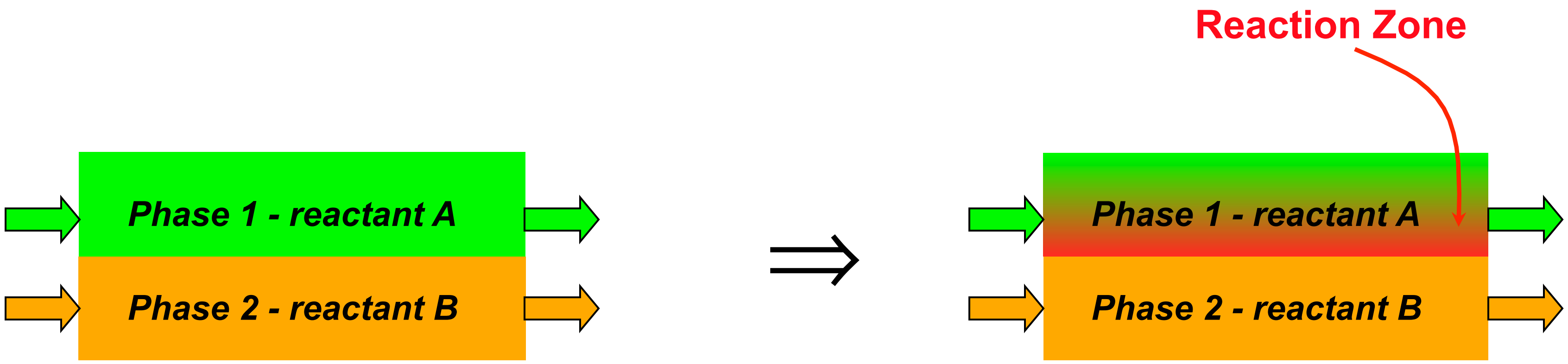
$$A + B \Rightarrow R \qquad -r_A = kC_AC_B$$




**Reactant *A* diffuses into Phase 2, but**
**Reactant *B* does not diffuse into Phase 1.**

# Problem Consideration

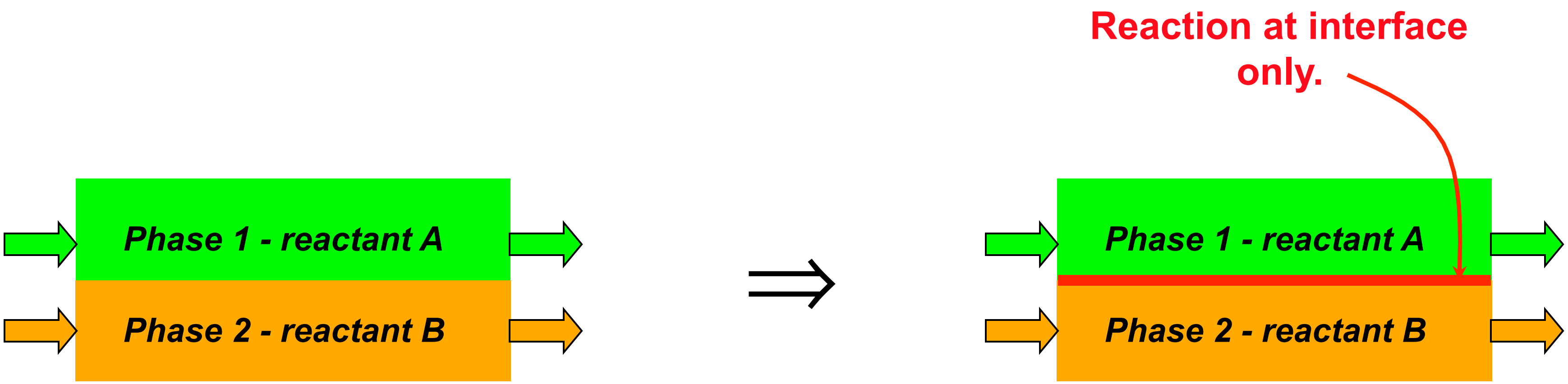
$$A + B \Rightarrow R \qquad -r_A = kC_A C_B$$




**Reactant *B* diffuses into Phase 1, but**
**Reactant *A* does not diffuse into Phase 2.**

# Problem Consideration

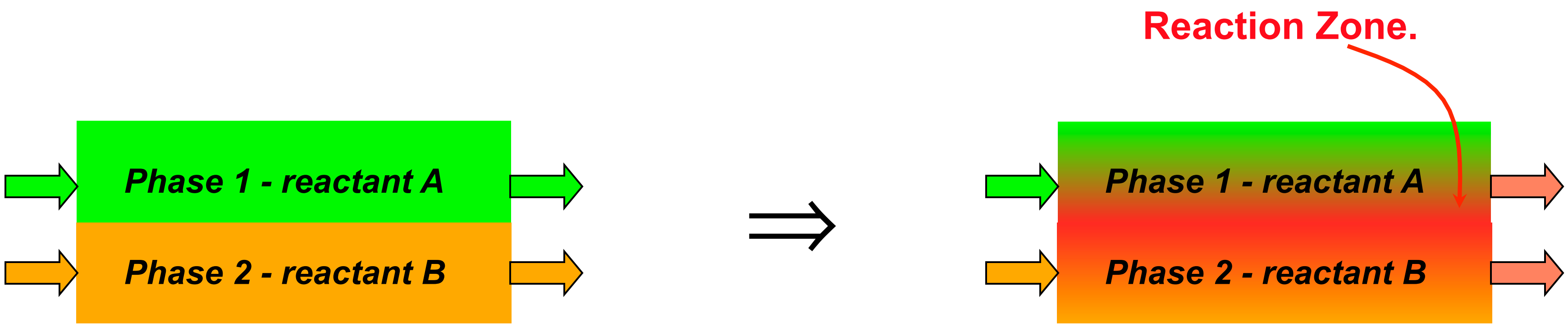
$$A + B \Rightarrow R \qquad -r_A = kC_AC_B$$




**Reactant *B* does not diffuse into Phase 1, and Reactant *A* does not diffuse into Phase 2.**

# 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.**

# Velocity Profile (two-dimensional, steady-state)

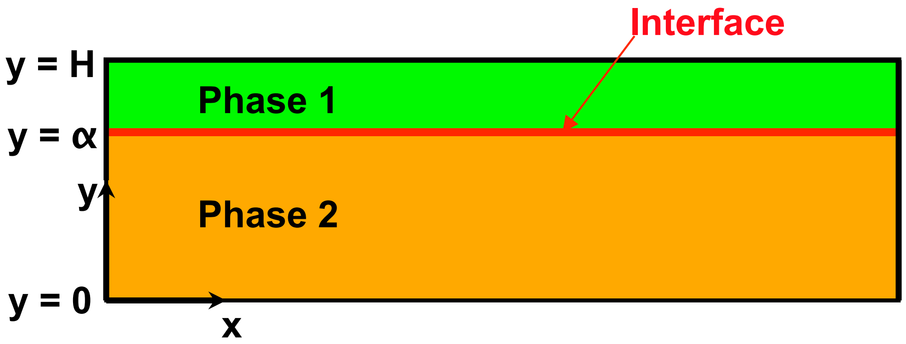
## 1. Convection Equations

Navier-Stokes Equations

$$\frac{\partial^2 u_1}{\partial y^2} = \frac{1}{\mu_1}\frac{dP}{dx}$$

$$\frac{\partial^2 u_2}{\partial y^2} = \frac{1}{\mu_2}\frac{dP}{dx} = \frac{m_{12}}{\mu_1}\frac{dP}{dx}$$

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




### *Boundary Conditions*

$$@ \quad y = H; \quad u_1 = 0 \quad (no-slip\ \ condition)$$

$$@ \quad y = 0; \quad u_2 = 0 \quad (no-slip\ \ condition)$$

$$@ \quad y = \alpha; \quad u_1 = u_2$$

$$@ \quad y = \alpha; \quad \frac{\partial u_1}{\partial y} = \frac{1}{m_{12}}\frac{\partial u_2}{\partial y}$$

# Velocity Profile (two-dimensional, steady-state)

**Introduce Non-dimensional variables**

$$y' = \frac{y}{H} \qquad u_1' = \frac{u_1}{\left(\frac{1}{\mu_1}\left(\frac{dP}{dx}\right)H^2\right)} \qquad u_2' = \frac{u_2}{\left(\frac{1}{\mu_1}\left(\frac{dP}{dx}\right)H^2\right)}$$

**Non-dimensional equations**

$$\frac{\partial^2 u_1'}{\partial y'^2} = 1 \qquad (\alpha \le y' \le 1)$$

$$\frac{\partial^2 u_2'}{\partial y'^2} = m_{12} \qquad (0 \le y' < \alpha)$$

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

**Non-dimensional boundary conditions**

$$@\ y' = 1, \quad u_1' = 0 \quad (no - slip\ condtion)$$

$$@\ y' = 0, \quad u_2' = 0 \quad (no - slip\ condtion)$$

$$@\ y' = \alpha, \quad u_1' = u_2'$$

$$@\ y' = \alpha, \quad \frac{\partial u_1'}{\partial y'} = \frac{1}{m_{12}} \frac{\partial u_2'}{\partial y'}$$

# Velocity Profile (two-dimensional, steady-state)

**Non-dimensional velocity profile equations**

$$u_1' = -\left(\frac{y'^2}{2} + C_1 y' + C_2\right) \qquad (\alpha \le y' \le 1)$$

$$u_2' = -\left(m_{12}\frac{y'^2}{2} + m_{12} C_1 y'\right) \qquad (0 \le y' < \alpha)$$

$$C_1 = \frac{\frac{1}{2}\left(m_{12}\alpha^2 - \alpha^2 + 1\right)}{\left(\alpha - 1 - m_{12}\alpha\right)}$$

$$C_2 = -\left(\frac{1}{2} + C_1\right)$$

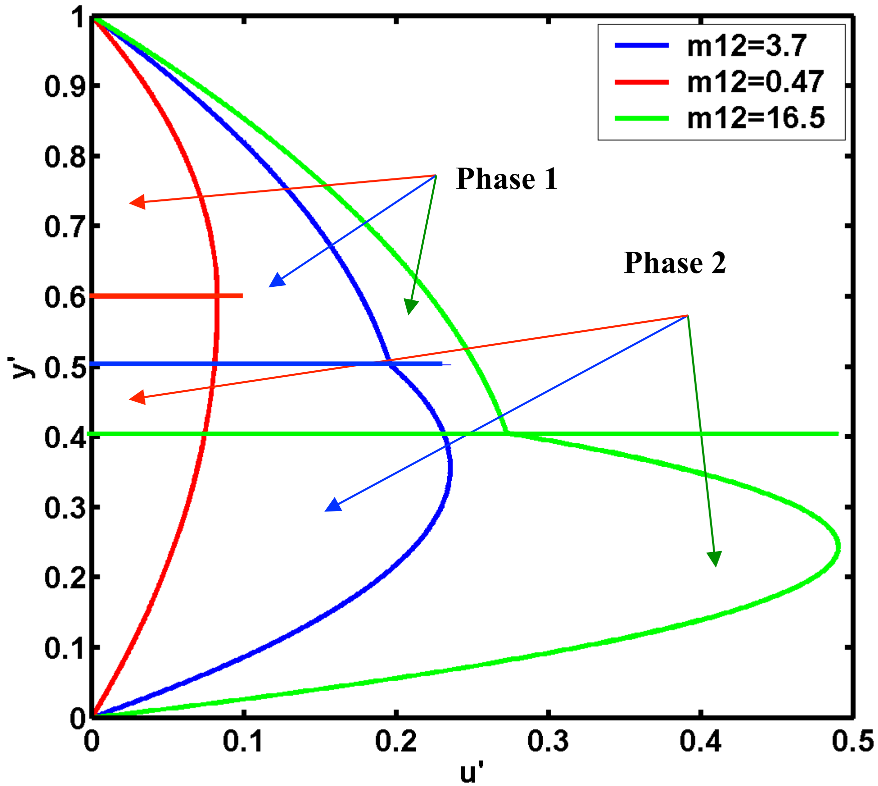
**Non-dimensional volume flow rate equations**

$$Q_1 = \int_\alpha^1 u_1' dy' = -\left[\frac{1}{6}\left(1-\alpha^3\right) + \frac{C_1}{2}\left(1-\alpha^2\right) + C_2(1-\alpha)\right]$$

$$Q_2 = \int_0^\alpha u_2' dy' = -m_{12}\left(\frac{\alpha^3}{6} + C_1\frac{\alpha^2}{2}\right)$$

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

# Velocity Profile




**Fully developed velocity profiles**

**Interface locations of two phase flow**

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

People. Ideas. Innovation.

*Thank you for your attention!*

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