Computational modelling of slug flow in a capillary millireactor

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Outline

- Introduction
- Single Phase Modelling
- Two Phase Modelling
- Conclusions and Path Forward

Introduction

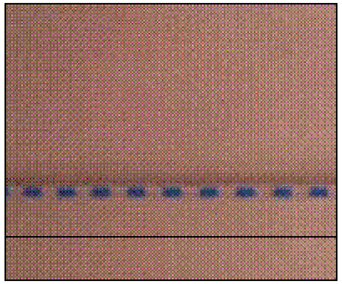
Why the small scales attract Chemical Engineers?

- An important method of process intensification
- Chemical processing advantage is due to increased heat and mass transfer
- Better mass transfer leads to reduced process volume and higher reaction rate
- Precise control of high intensity and hazardous reactions
- Scale up is possible by replication

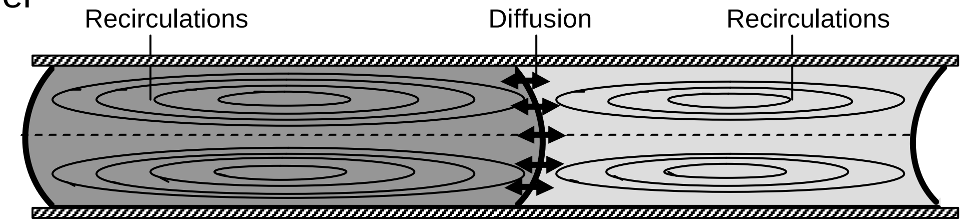
Introduction

Slug Flow

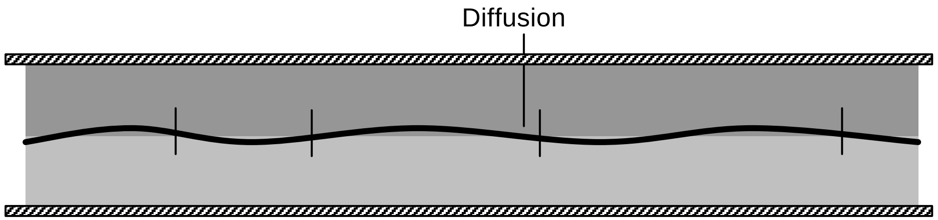
- Uniform slug size



- Enhanced mass transfer



Slug Flow



Parallel Flow

- High throughputs creating smaller slug size
- Easy post reaction separation by gravity

Objective

"To obtain the fundamental understanding of hydrodynamics to design an appropriate reactor concept exhibiting best possible conversion and selectivity for a given liquid-liquid reaction by experimentation and computational techniques"

Problems and Important Parameters

Problems

? Experimental slug flow stability

? Hydrodynamics

? Selectivity problem

? Internal circulations

? Presence of film

Important Parameters

- Pressure drop
- Flow patterns
- Circulation time
- Slug dimensions (Length and Diameter)
- Mass transfer coefficient
- Film thickness

Single Phase CFD

Problem Details and Solver

- Operating conditions of Dummann et al. (2003)* and our laboratory experiments
- Retrieved the geometries from experimental snapshots
- Finite Element Package, FEATFLOW was used

$$u_t - \nu \Delta u + u \bullet \nabla u + \nabla p = f$$

$$\nabla \bullet u = 0 \qquad in \quad \Omega \times [0, T]$$

Assumptions

- Front and back interface of the slug is same
- Incompressible flow

* Dummann et al., The capillary microreactor: the new concept of intensification of heat and mass transfer in liquid-liquid reactions, *Catalysis Today, 79-80, 433-439, 2003.*

Wall Film

- Film thickness (Bretherton law),

$$h = 1.34 R Ca^{2/3}$$

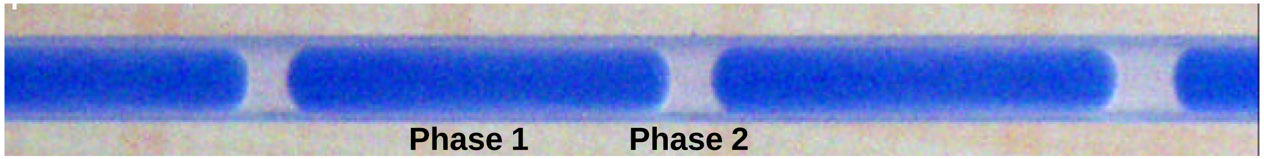
- The slug velocity and average flow velocity

$$V_s = \frac{2}{1 + (R_s / R)^2} V_{av}$$

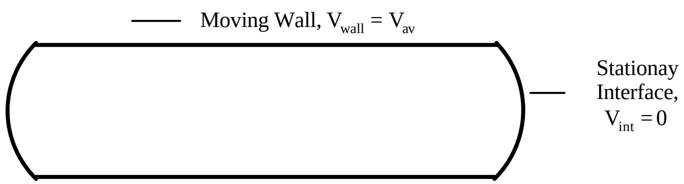
- No stagnant film

$$Q_{av} = Q_{film} + Q_{slug}$$

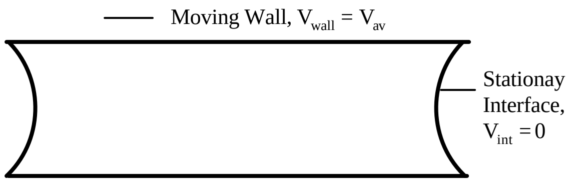
Boundary Conditions



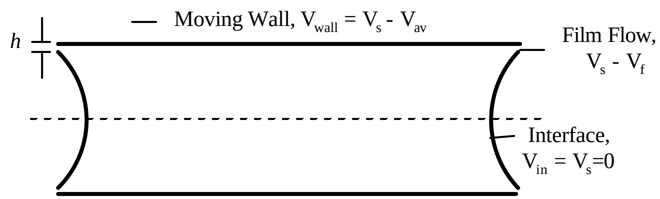
Phase 1



Phase 2

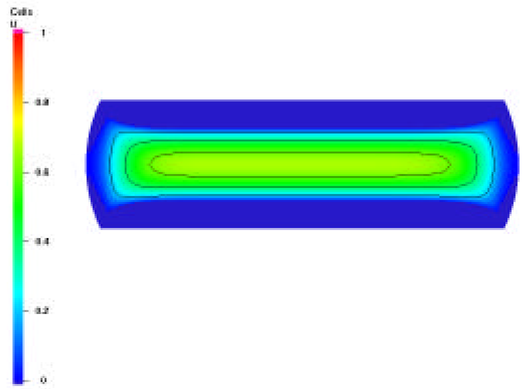


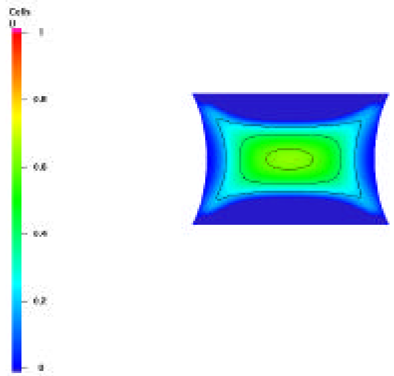
Without Film

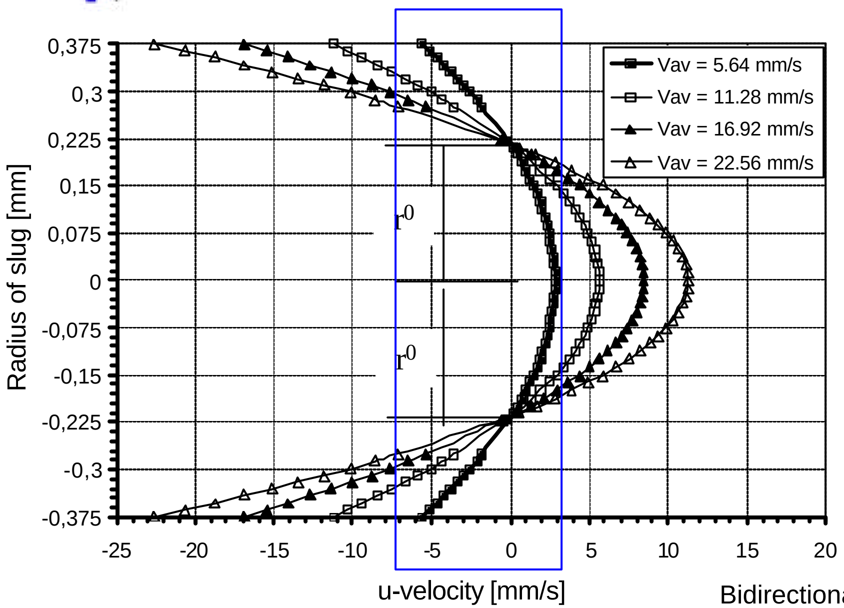


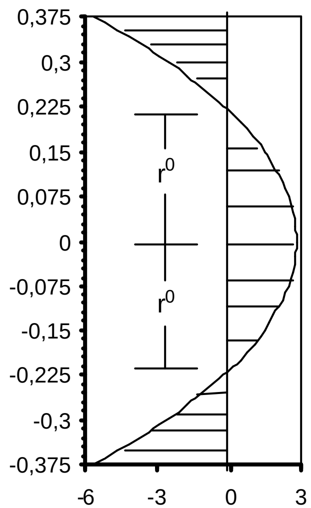
With Film

Velocity (x-directional) Profile









Parabolic (Poiseuille) Profile

Bidirectional velocity profile (phase 1, L = 2.379 mm, D = 0.75 mm)

Internal Circulations

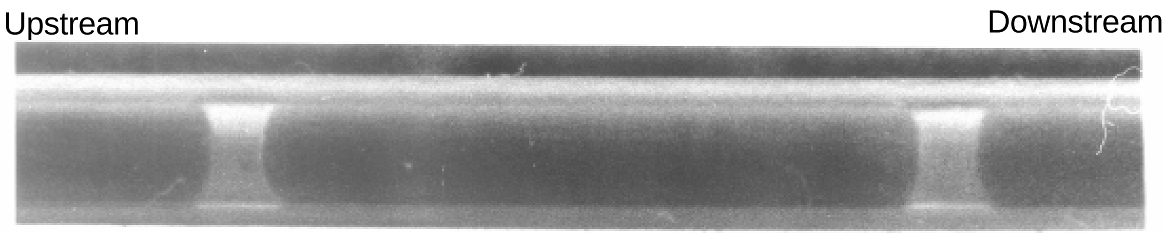


Fig: Liquid-liquid slug flow through capillary millireactor

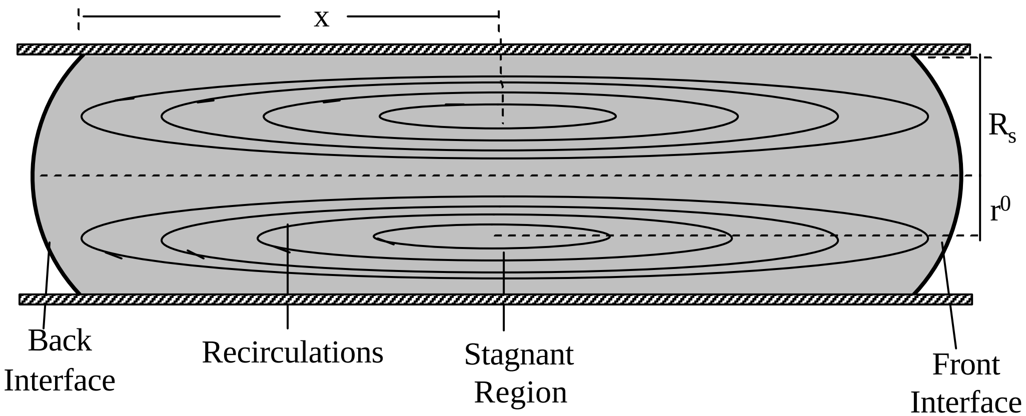


Fig: Phase 1 (Without Film)

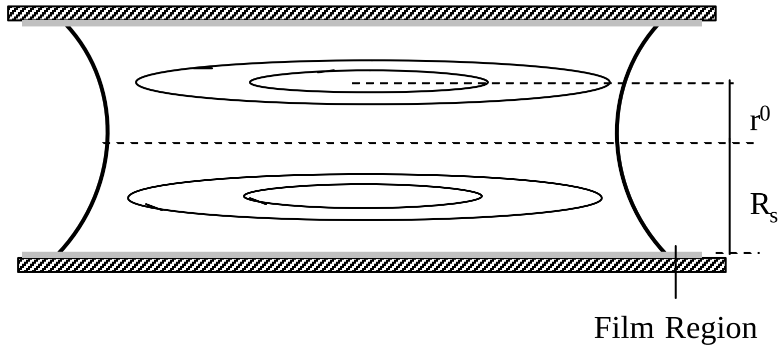


Fig: Phase 2 (With Film)

Internal Circulations

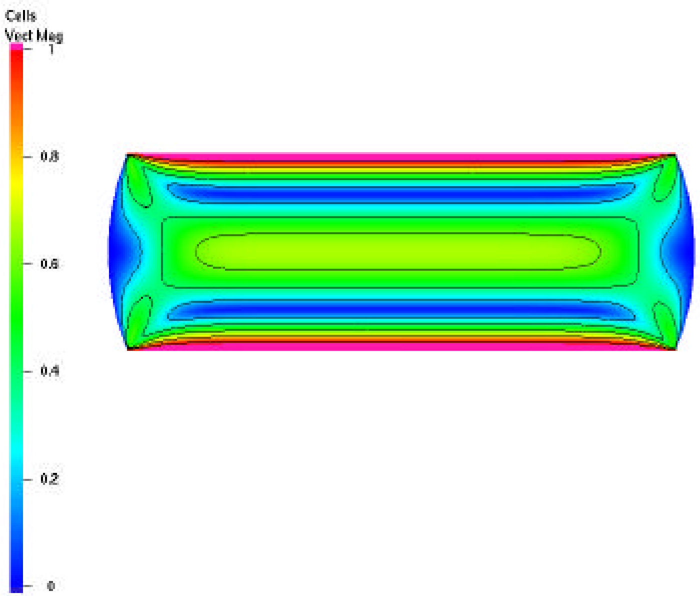


Fig: Phase 1

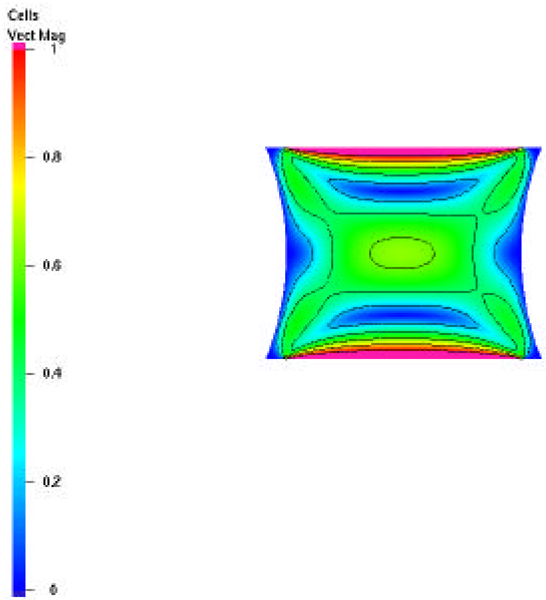


Fig: Phase 2

Recirculation Time

- Important parameter for
  - Mass Transfer
  - Mixing
- Time Required for liquid particles to move from one end of the slug to the other end
- Recirculation Time = Volume/Volumetric throughputs

Without film

$$t_{nofilm} = \frac{l\left(r^0\right)^2}{2\frac{l}{V_{av}}\int_0^{r^0} U(r)\, r\, dr}$$

With film

$$t_{film} = \frac{l\left(r^0\right)^2}{2\frac{l}{V_s}\int_{r^0}^{r} U(r)\, r\, dr}$$

Recirculation Time

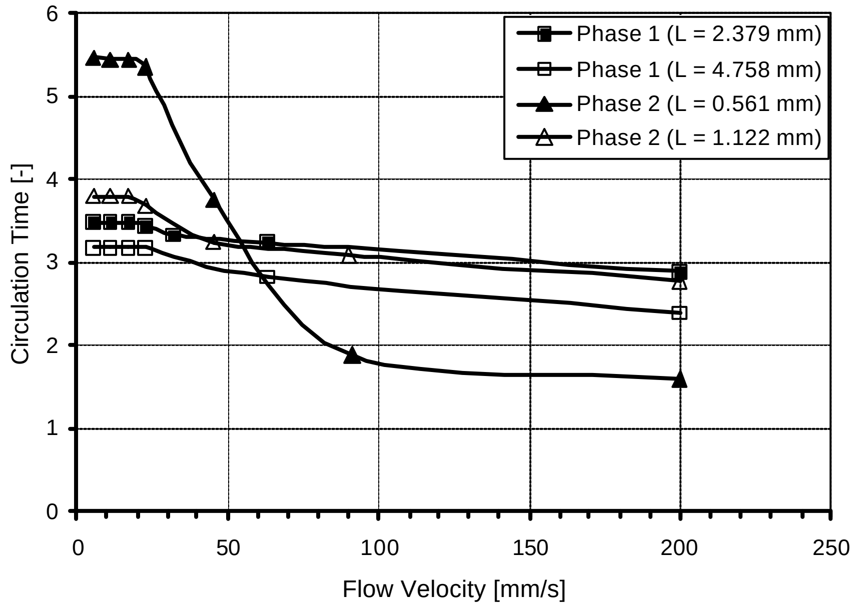
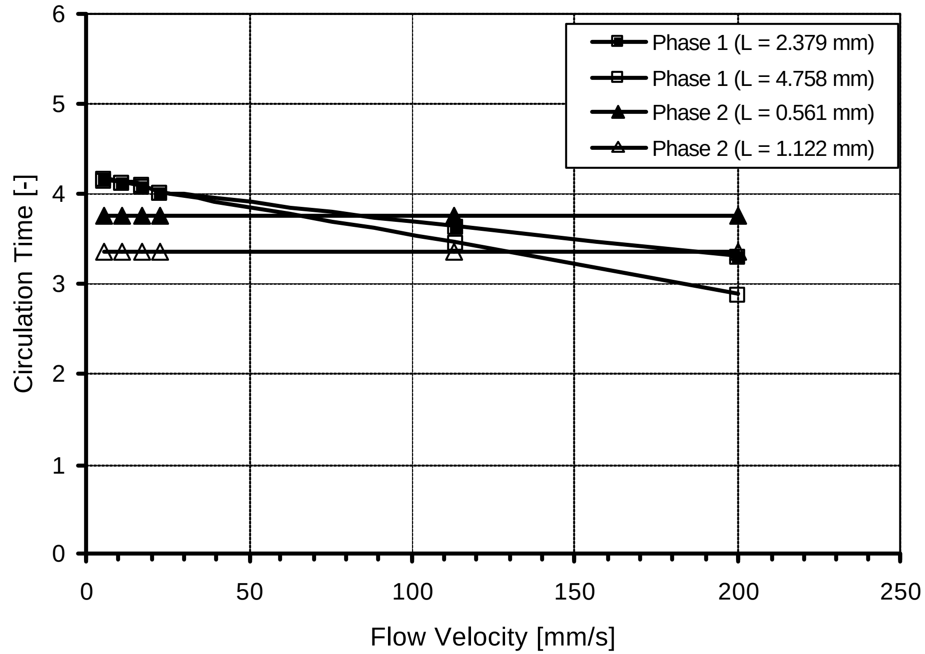


Fig: Recirculation time without film

Fig: Recirculation time with film



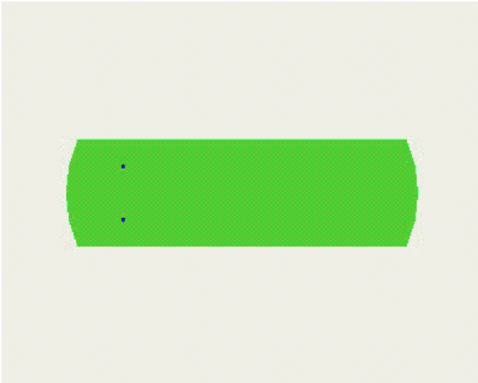
Particle Tracing

- Method of visualization
- Converts Eulerian description of a flow into Langragian description with selected particle
- In-house developed algorithm, GMVPT
- The new position of the particle from initial position is

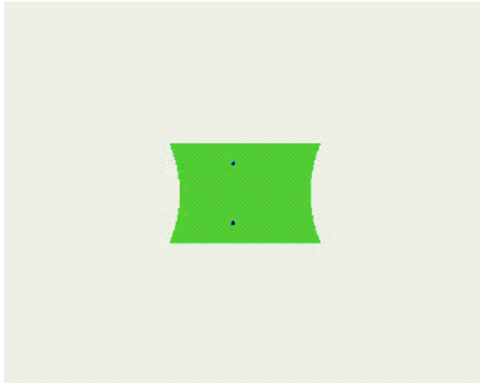
$$\tilde{Z} = Z + \Delta t . u_P$$

- Inserted tracers with constant frequency to simulate the constant stream of particle

Particle Tracing

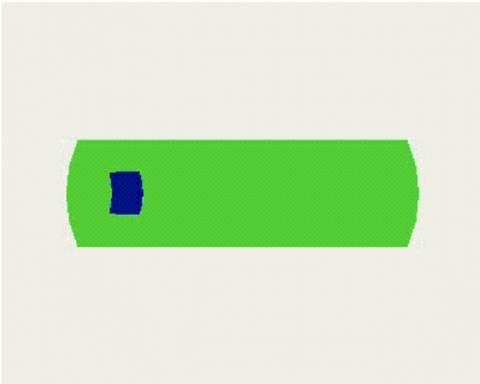


2 particles

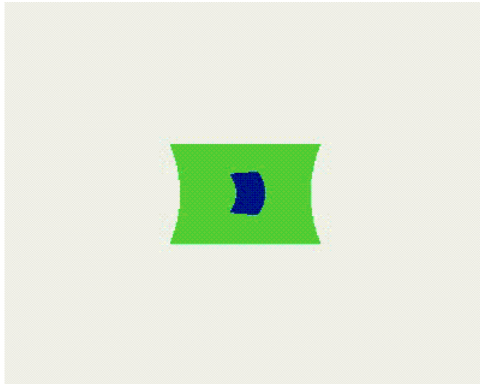


Phase 1	Phase 2
L = 2.379 mm	L = 1.12 mm
D = 0.75 mm	D = 0.75 mm
r = 0.2 mm	r = 0.25 mm
Vav = 5.64 mm/s	Vav = 5.64 mm/s

Particle Tracing



10, 000 Particles



Phase 1	Phase 2
L = 2.379 mm	L = 1.12 mm
D = 0.75 mm	D = 0.75 mm
Vav = 5.64 mm/s	Vav = 11.28 mm/s

Two Phase CFD (VOF)

- VOF is implicit volume tracking technique applied to fixed mesh
- Single set of momentum equation is shared by the fluids
- The different fluids are marked either by massless particles or by an indicator function
- Generally applied where the topology of interface is of interest
- Stratified flows, free surface flows, motion of large bubbles in liquid, etc.

VOF Model

Each fluid is governed by incompressible Navier-Stokes equation

$$\left(\frac{\partial v}{\partial t} + v \cdot \nabla v\right) - \nabla \cdot (2m_i S) + \nabla p = r_i g$$

$$\nabla \cdot v = 0 \qquad in\ \Omega_i,\ i = 1,2$$

$$S = \frac{1}{2}\left(\nabla v + [\nabla v]^T\right)$$

The indicator function is given by $\frac{\partial j}{\partial t} + v.\nabla j = 0$

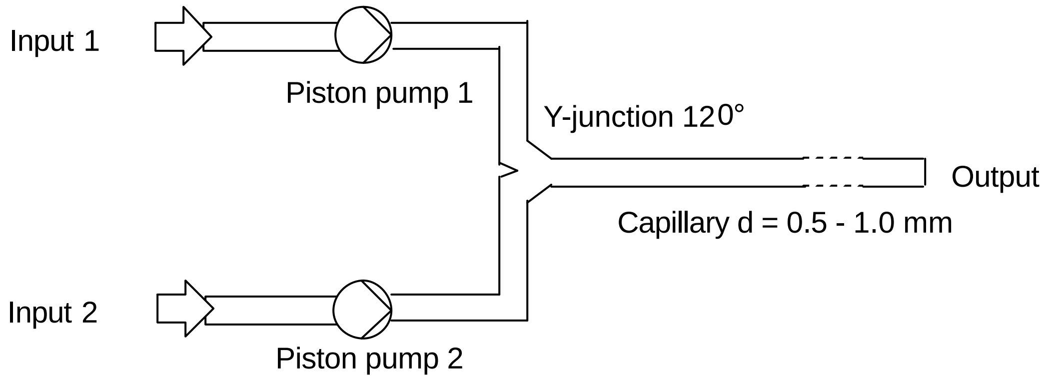
Assumption:

- No surface tension implemented
- No mass transfer between two liquids
- Isothermal condition

In-house developed open source code, FEATFLOW

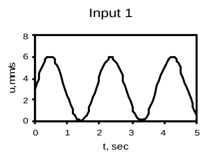
Slug Flow

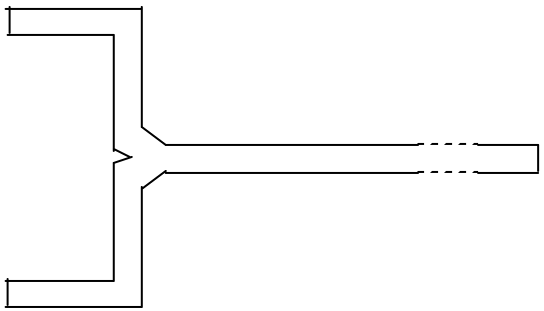
- Physical Experiments



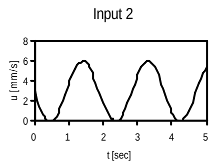
- Numerical Experiments

Input 1 $u_1 = u_1^0 + e_1 \sin\left(\frac{t}{t}\right)$



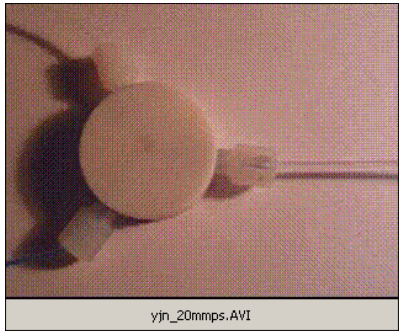


Input 2 $u_2 = u_2^0 + e_2 \sin\left(-\frac{t}{t}\right)$

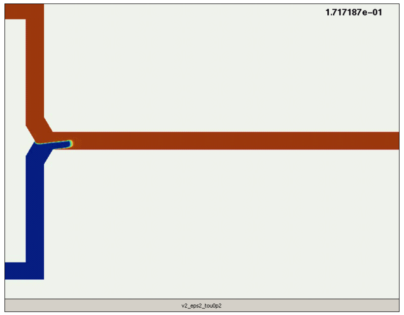


Two-phase Results

- Y-Junction Flow
  Experimental



- Y-Junction Flow
  CFD Simulation



Conclusion

- Bidirectional velocity profile was observed in each slug (L>D)
- Circulation time decreases with increase in flow velocity
- Film has no significant effect on circulation time
- Particle tracing shows well qualitative prediction of internal circulations
- VOF-CFD methodology can capture slug flow

Path Forward

- Experiments for internal circulations

  PIV measurements
- Use surface tension in VOF methodology
- Study of hydrodynamic parameters

  Experimentation

  CFD simulation
- Study mass transfer and mixing