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

Parallel Flow
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
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

\[ u_t - νΔu + u \cdot \nabla u + \nabla p = f \]
\[ \nabla \cdot u = 0 \quad \text{in} \quad Ω \times [0, T] \]

Assumptions

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

Wall Film

- Film thickness (Bretherton law),
  \[ h = 1.34 R C a^{2/3} \]

- 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
- Moving Wall, $V_{wall} = V_{w}$
- Stationary Interface, $V_{int} = 0$

Phase 2
- Moving Wall, $V_{wall} = V_{s} - V_{av}$
- Film Flow, $V_{f} - V_{w}$
- Interface, $V_{in} = V_{f}$ = 0

Without Film

With Film
Velocity (x-directional) Profile

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

Parabolic (Poiseuille) Profile
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 and 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:
\[
\tau_{\text{nofilm}} = \frac{l \left( r^0 \right)^2}{2 \frac{l}{V_{\text{av}}} \int_{0}^{r^0} U(r) r \, dr}
\]

With film:
\[
\tau_{\text{film}} = \frac{l \left( r^0 \right)^2}{2 \frac{l}{V_{\text{s}}} \int_{r^0}^{r} U(r) r \, dr}
\]
Recirculation Time

Fig: Recirculation time with film

Fig: Recirculation time without 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

$$\tilde{Z} = Z + \Delta t \cdot v_p$$

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

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

Phase 2
L = 1.12 mm
D = 0.75 mm
r = 0.25 mm
Vav = 5.64 mm/s
**Particle Tracing**

<table>
<thead>
<tr>
<th>Phase 1</th>
<th>Phase 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>L = 2.379 mm</td>
<td>L = 1.12 mm</td>
</tr>
<tr>
<td>D = 0.75 mm</td>
<td>D = 0.75 mm</td>
</tr>
<tr>
<td>Vav = 5.64 mm/s</td>
<td>Vav = 11.28 mm/s</td>
</tr>
</tbody>
</table>

10,000 Particles
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

\[
\left( \frac{\partial v}{\partial t} + v \cdot \nabla v \right) - \nabla \cdot (2 \mu_i S) + \nabla p = \rho_i g \\
\nabla \cdot v = 0 \quad \text{in } \Omega_i, \ i = 1, 2
\]

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

The indicator function is given by

\[
\frac{\partial \phi}{\partial t} + v \cdot \nabla \phi = 0
\]

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

\[
\text{Input 1 } \quad u_1 = u_1^0 + \varepsilon_1 \sin \left( \frac{t}{\tau} \right)
\]

\[
\text{Input 2 } \quad u_2 = u_2^0 + \varepsilon_2 \sin \left( -\frac{t}{\tau} \right)
\]
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