Direct numerical simulation of bubble train flow in a square mini-channel and evaluation of liquid phase residence time distribution

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*Multiphase Flows: Simulation, Experiment and Application
Rossendorf, 1. – 3. Juni 2005*
• Introduction and motivation

• Bubble train flow
  – Computational setup in DNS
  – Validation and simulation results

• Evaluation of residence time distribution
  – Procedure
  – Results of RTD for bubble train flow
  – Fitting by compartment model

• Conclusions and outlook
Introduction

Multi-fluid flow in narrow channels

- Monolithic reactors with catalytic walls
  - Chemical inert gas bubbles segment the liquid phase and enhance its mixing
• Micro bubble column of IMM*  
  – High values of interfacial area per unit volume  
    • Efficient mass transfer across interface  
      (e.g. absorption, liquid-liquid extraction)  
  – Defined interface geometry  
    • Concept of „numbering up“ instead of „scaling up“
Motivation

• Experimental investigation of these two-phase flows is difficult because of small dimensions and often yields integral data only

• Goal:
  – Perform direct numerical simulation of bubble train flow in a single channel to resolve local flow phenomena
  – Use DNS results to evaluate residence time distribution for liquid phase
In-house code TURBIT-VOF

• Volume-of fluid method for interface tracking
  – Interface is locally approximated by plane (PLIC method)

• Governing equations for two incompressible fluids
  – Single field momentum equation with surface tension term
  – Zero divergence condition for center-of-mass velocity
  – Advection equation for liquid volumetric fraction $f$

• Solution strategy
  – Projection method resulting in pressure Poisson equation
  – Explicit third order Runge-Kutta time integration scheme

• Discretization in space
  – Finite volume formulation for regular staggered grid
  – Second order central difference approximations
Flow characterization

- Elongated bubble which fill almost the entire channel cross section (Taylor bubbles)
- Bubbles have identical shape and move with same axial velocity
- The flow is fully described by a unit cell of length $L_{uc}$ consisting of a bubble and a liquid slug

$uc = \text{"unit cell"}$
Experiment of Thulasidas et al.*

- Square vertical channel
  - Channel cross section: 2 mm \( \times \) 2 mm (\( W^* = 2 \) mm)

- Air bubbles in silicon oil
  - Silicon oil of different viscosity
  - Wide range of capillary numbers \( Ca_B \equiv \mu_1^* U_B^* / \sigma^* \)

- Specification of flow rates of air and oil

- Length of unit cell, gas content in unit cell and axial pressure drop adjust accordingly

Numerical set up with TURBIT-VOF

• Consider one flow unit cell only (one bubble, one slug)
• Account for influence of trailing/leading unit cells by periodic boundary conditions in axial direction
• Flow is driven in vertical direction by specified axial pressure gradient and buoyancy
  – Gas and liquid flow rates adjust accordingly
• Length of flow unit cell, $L_{uc}$, is input parameter
  – Investigation of influence of $L_{uc}$
• Fluid properties

<table>
<thead>
<tr>
<th>( \rho_l )</th>
<th>( \rho_g )</th>
<th>( \mu_l )</th>
<th>( \mu_g )</th>
<th>( \sigma )</th>
</tr>
</thead>
<tbody>
<tr>
<td>957 kg/m(^3)</td>
<td>11.7 kg/m(^3)</td>
<td>0.048 Pa s</td>
<td>1.84 ( \times ) 10(^{-4}) Pa s</td>
<td>0.022 N/m</td>
</tr>
</tbody>
</table>

Factor 10 higher than \( \rho \) and \( \mu \) of air

• Initial bubble shapes (void fraction \( \varepsilon = 33\% \))

• Simulations are started from gas and liquid at rest
## Computational parameters

<table>
<thead>
<tr>
<th>Case</th>
<th>$L_{uc} / W$</th>
<th>Domain</th>
<th>Grid</th>
<th>Time steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>1</td>
<td>$1 \times 1 \times 1$</td>
<td>$48 \times 48 \times 48$</td>
<td>24,000</td>
</tr>
<tr>
<td>A2</td>
<td>1</td>
<td>$1 \times 1 \times 1$</td>
<td>$64 \times 64 \times 64$</td>
<td>60,000</td>
</tr>
<tr>
<td>B</td>
<td>1.25</td>
<td>$1 \times 1.25 \times 1$</td>
<td>$48 \times 60 \times 48$</td>
<td>24,000</td>
</tr>
<tr>
<td>C</td>
<td>1.5</td>
<td>$1 \times 1.5 \times 1$</td>
<td>$48 \times 72 \times 48$</td>
<td>26,000</td>
</tr>
<tr>
<td>D</td>
<td>1.75</td>
<td>$1 \times 1.75 \times 1$</td>
<td>$48 \times 84 \times 48$</td>
<td>26,000</td>
</tr>
<tr>
<td>E</td>
<td>2</td>
<td>$1 \times 2 \times 1$</td>
<td>$48 \times 96 \times 48$</td>
<td>28,000</td>
</tr>
</tbody>
</table>

Results on both grids show only slight differences
Bubble shape and trajectories of mass less particles for case A

- Bubble has axisymmetric shape
- One large vortex inside the bubble
- Small azimuthal flow inside bubble
Computed bubble shape and velocity field for different values of $L_{uc}$

Velocity field in vertical mid-plane
Right half: frame of reference moving with bubble
Left half: fixed frame of reference
### Comparison with experiment

Non-dimensional bubble diameter  | Relative velocity  | Non-dimensional $U_B$

<table>
<thead>
<tr>
<th>Case</th>
<th>$L_{uc} / W$</th>
<th>$Ca_B$</th>
<th>$D_B / W$</th>
<th>$(U_B-J_{total})/U_B$</th>
<th>$U_B/J_{total}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1</td>
<td>0.204</td>
<td>0.81</td>
<td>1.80</td>
<td>0.445</td>
</tr>
<tr>
<td>B</td>
<td>1.25</td>
<td>0.207</td>
<td>0.84</td>
<td>1.75</td>
<td>0.430</td>
</tr>
<tr>
<td>C</td>
<td>1.5</td>
<td>0.215</td>
<td>0.85</td>
<td>1.75</td>
<td>0.430</td>
</tr>
<tr>
<td>D</td>
<td>1.75</td>
<td>0.238</td>
<td>0.85</td>
<td>1.78</td>
<td>0.438</td>
</tr>
<tr>
<td>E</td>
<td>2</td>
<td>0.253</td>
<td>0.85</td>
<td>1.80</td>
<td>0.445</td>
</tr>
</tbody>
</table>

Experimental data* correlated in terms of capillary number $Ca_B \equiv \mu U_B / \sigma$

|     | 0.2 – 0.25 | 0.82 – 0.86 | 1.68 – 1.84 | 0.435 – 0.475 |

Residence time distribution

- The residence time distribution (RTD) is an important measure for characterization of any chemical reactor
  - The RTD influences yield and selectivity
- Common experimental method to determine RTD
  - Add tracer at reactor inlet as a pulse and measure the tracer concentration at the outlet
Examples for RTD

- **Problems for micro reactors**
  - Reaction volume is usually much smaller than the volume of inlet and the volume necessary to measure tracer at outlet

- **Alternative**: Determine RTD from DNS data
**Procedure to evaluate RTD from DNS data**

- Use previously computed DNS results for fully developed flow at a certain instant in time
- Introduce virtual particles in mesh cells entirely filled with liquid
  - particle distance = $1 / n_{ppul}$
  - $n_{ppul}$ = number of particles per unit length
- Track particles in fixed frame of reference
  - Problem: Velocity field in fixed frame of reference is **unsteady**
  - But: **steady** velocity field in frame of reference moving with bubble
  - Determine fluid velocity at the instantaneous particle position from its relative position to the virtually with velocity $U_B$ moving bubble
- Store time the particle needs to travel an axial distance of $L_{uc}$
- Normalize histogram for all particles to obtain RTD
Influence of $n_{ppul}$ for BTF Case A

Bubble breakthrough time $t_B = \frac{L_{uc}}{U_B}$

Exponential decay
Compartment model

Plug flow reactor and stirred vessel in series

\[
E_{\text{VRTD}} = \begin{cases} 
0 & \text{for } t < \frac{L_{\text{uc}}}{U_B} \\
\frac{U_L}{L_{\text{uc}}} \exp \left( - \frac{U_L}{L_{\text{uc}}} \cdot t + \frac{U_L}{U_B} \right) & \text{for } t \geq \frac{L_{\text{uc}}}{U_B}
\end{cases}
\]

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E_{\text{VRTD}} = \begin{cases} 
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\end{cases}
\]
Compartment model for case A

\[
E_{\text{VRTD}} = \begin{cases} 
0 & \text{for } t < \frac{L_{ac}}{U_B} \\
\frac{U_L}{L_{sc}} \exp \left( - \frac{U_L}{L_{sc}} \cdot t + \frac{U_L}{U_B} \right) & \text{for } t \geq \frac{L_{ac}}{U_B}
\end{cases}
\]

\[
E_{\text{VRTD}} = \begin{cases} 
0 & \text{for } t < \frac{L_{ac}}{U_B} \\
\frac{J_L}{L_{sc}} \exp \left( - \frac{J_L}{L_{sc}} \cdot t + \frac{J_L}{U_B} \right) & \text{for } t \geq \frac{L_{ac}}{U_B}
\end{cases}
\]

Case A: \( n_{\text{pul}} = 96 \); Eq. (16); Eq. (17)
Compartment model for case B

Case B: \( n_{\text{ppul}} = 96 \); Eq. (16); Eq. (17)
Compartment model for case C

Case C: $n_{ppul} = 96$; Eq. (16); Eq. (17)
Compartment model for case D

Case D: \( n_{ppul} = 64 \); Eq. (16); Eq. (17)
Compartment model for case E

Case E: \( n_{ppul} = 64 \);  
- Eq. (16);  
- Eq. (17)
Conclusions

• Direct numerical simulation of bubble train flow (BTF)
  – Square vertical mini-channel of width $W = 2$ mm
  – Co-current vertical flow of air bubbles in silicon oil
  – Good agreement with experimental data from literature

• Original procedure to evaluate the liquid phase RTD
  – Introduction of mass-less particles into volume of liquid phase
  – Tracking of particles and detecting time to travel distance $L_{uc}$
  – Evaluated RTD is well described by compartment model with plug flow reactor and stirred vessel in series

• Outlook
  – Determine RTD for traveling distance $n_{uc} \cdot L_{uc}$ ($n_{uc} = 2, 3, ...$)
  – Obtain RTD for arbitrary $n_{uc}$ by convolution of RTD for $n_{uc} = 1$ (?)