Euler-Lagrange Large Eddy Simulation of a Square Cross-sectioned Bubble Column

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Introduction

• Bubble columns are widely used in the chemical and biochemical process industries.

• Flows in bubble columns can be simulated using Euler-Euler or Euler-Lagrange approaches.
  – Euler-Euler – both phases described as a continuum.

• This work presents 3D transient simulations using Euler-Lagrange approach with LES.
Bubble Dynamics

• The motion of an individual bubble is computed from equations of motion in a Lagrangian frame.
  – Position and momentum equations are
  \[
  \frac{d}{dt} x_b = u_b
  \]
  \[
  \rho_b V_b \frac{d}{dt} u_b = F_G + F_P + F_D + F_L + F_{AM}
  \]

• The forces acting on a bubble are modelled as
  – Gravity: \( F_G = (\rho_b - \rho_f)V_b g \)
  – Pressure: \( F_P = V_b \rho_f \frac{Du_f}{Dt} \)
Bubble Dynamics cont’d

- Drag: \( F_D = -\frac{1}{2} C_D \rho_f A_b |u_b - u_f|(u_b - u_f) \)
- Lift: \( F_L = -C_L \rho_f V_b (u_b - u_f) \times \nabla \times u_f \)
- Added mass: \( F_{AM} = -C_{VM} \rho_f V_b \left( \frac{du_b}{dt} - \frac{Du_f}{Dt} \right) \)

• Other forces may be present, depending on the application.
• For this work, collision and momentum transfer (growth) were ignored.
• A stochastic discrete random walk model is used to determine the instantaneous fluid velocity.
• These forces contain empirical constants \( (C_D, C_L \text{ and } C_{VM}) \) that need to be defined to close the equations.
Bubble Dynamics – Force closure models

• Drag coefficient closure models:

|-----------------------------------------|-----------------------------------|
| $C_D = \frac{2}{3}\sqrt{Eo}$          | $C_D = \begin{cases} 
\frac{24}{Re} \left(1 + \frac{1}{6}Re^{2/3}\right) & Re \leq 1000 \\
0.424 & Re > 1000 
\end{cases}$ |

• Lift coefficient closure models:

<table>
<thead>
<tr>
<th>Lift closure A</th>
<th>Lift closure B – Tomiyama (1998)</th>
</tr>
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</table>
| $C_L = 0.5$    | $C_L = \begin{cases} 
\min[0.288 \tanh(0.121Re_b), \ f(Eo)] & Eo \leq 4 \\
\ f(Eo) & 4 < Eo \leq 10 \\
-0.27 & 10 < Eo 
\end{cases}$ |

\[ f = 0.00105Eo^3 - 0.0159Eo^2 - 0.0204Eo - 0.474 \]

The Eötvös number is defined as $Eo = \frac{g(\rho_f - \rho_b)d_b^2}{\sigma}$

• Virtual mass coefficient closure: $C_{VM} = 0.5$. 

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Volume of Fluid

• Free surface interactions are modelled using VOF approach.

• Navier-Stokes equations:

\[ \nabla \cdot \mathbf{u} = 0 \]

\[
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\rho_m \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot [\mu_{m,eff} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho_m \mathbf{g} + \mathbf{F}_\sigma + \mathbf{S}
\]

– Continuum Surface Force model of Brackbill et al (1992) used for surface tension force

• Fluids are tracked using a scalar field \( \alpha \).

\[
\frac{\partial \alpha_q}{\partial t} + \nabla \cdot (\alpha_q \mathbf{u}) + \nabla \cdot [\alpha_q (1 - \alpha_q) \mathbf{v}_{qp}] = 0
\]
Volume of Fluid cont’d

• Smagorinsky sub-grid scale (SGS) model was used.
• The SGS viscosity is implemented as
  \[ \nu_{SGS} = c_k \sqrt{k_{SGS} \Delta} \]
  – \( k_{SGS} \) is given by
  \[ k_{SGS} = \frac{c_k \Delta^2}{c_\epsilon \|\widetilde{D}\|^2} \]
  – \( \Delta \) is a top-hat filter with a filter width estimated as the cubic root of the cell volume
  – \( \widetilde{D} \) the filtered rate of strain tensor.
Experiments

- Dean et al (2000) performed measurements in a 3D rectangular bubble column filled with water.
- Column had square cross section 0.15m x 0.15 m and height of 1 m.
- Column is filled with distilled water to a height of 0.45m.
- Air is introduced through a perforated plate at the bottom of the column with a superficial velocity of 5 mm/s.
• Governing equations and solution algorithms were implemented as a solver using version 5.04 of the Caelus open source library (www.caelus-cml.com).

• Simulated computational domain had a height of 0.6 m.  
  – height was chosen to be far enough away from the liquid surface as not to impact it.

• A patch with size 0.0375 m × 0.0375 m was created at the bottom of the column to facilitate injection of bubbles. The mesh consisted of hexahedral cells with a distribution 32 × 32 × 128, giving a cell edge length of 4.6 mm.
• **Boundary conditions:**
  – no-slip on the side walls, free slip condition on gas inlet and top of column.
  – zero gradient condition for pressure and gas phase volume fraction on all boundaries.
  – Injection of the bubbles occurred through a small patch at the base of the column with a velocity of 0.08 m/s.

• **Fluid properties:**
  – Density and kinematic viscosity:
    • Gas - 1.2 kg/m³ and 1.48×10⁻⁵ m²/s.
    • Water - 1000 kg/m³ and 1×10⁻⁶ m²/s.
Results

50 s 75 s 100 s 125 s 150 s
Results – Effect of force closure models

- Combinations of the drag and lift interfacial closure models were tested.

- Effect of
  - Drag: compare set A with C and B with D.
  - Lift: compare set A with B and C with D.

- Results presented
  - Time averaged liquid vertical velocity.
  - Time averaged vertical and horizontal velocity fluctuations.

<table>
<thead>
<tr>
<th>Closure Set</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Closure models</td>
<td>Drag A / Lift A</td>
<td>Drag A / Lift B</td>
<td>Drag B / Lift A</td>
<td>Drag B / Lift B</td>
</tr>
</tbody>
</table>
• Drag – at low and high regions, Drag closure A gives better results.

• Lift – increasing lift coefficient spreads bubble plume and reduces vertical velocity. Either set A or D best.
• Overall shape of profiles predicted, however, magnitude is under predicted.
• Profile shape is more sensitive to drag coefficient than lift.
• Closure set A does a better job at predicting the fluctuating liquid velocities.
• Using closure model A – investigate effect of changing $c_k$ in SGS model.

• $c_k = 0.047$ gives the most consistency with experimental data.
• Fluctuations in the horizontal direction are lower than in the vertical direction → the flow is anisotropic.

• Horizontal velocity fluctuation less sensitive to changes in $c_k$ than vertical velocity fluctuations.

• $c_k = 0.047$ results agree well with experimental data.
Conclusions

• Numerical simulations of the gas-liquid two-phase flow in a square-section bubble column were conducted with the open source software Caelus 5.04.

• A VOF-Lagrange approach with gravity, drag, lift, pressure and added mass forces was used.

• Simulation results were compared with the experiments of Deen et al.

• Ishii and Zuber drag model with a constant lift coefficient $C_L = 0.5$ gave the best match to the experimental mean and fluctuating liquid velocity.
Conclusions

• Horizontal liquid velocity fluctuations showed no dependency on the SGS model parameter $c_K$.
• Vertical fluctuations decreased with increasing $c_K$.
• Simulation results were shown to be in reasonable agreement with the experimental data.
Acknowledgements

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Questions

• Applied CCM
  – Specialise in the application, development, support and training of OpenFOAM®-based software
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