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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.
  - Euler-Lagrange – Liquid modelled as a continuum and gas bubbles tracking in a Lagrangian way.
- 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

$$\frac{d\boldsymbol{x}_b}{dt} = \boldsymbol{u}_b$$

$$\rho_b V_b \frac{d\boldsymbol{u}_b}{dt} = \boldsymbol{F}_G + \boldsymbol{F}_P + \boldsymbol{F}_D + \boldsymbol{F}_L + \boldsymbol{F}_{AM}$$

- The forces acting on a bubble are modelled as
  - Gravity: $\boldsymbol{F}_G = (\rho_b - \rho_f) V_b \boldsymbol{g}$
  - Pressure: $\boldsymbol{F}_P = V_b \rho_f \frac{D\boldsymbol{u}_f}{Dt}$,

Bubble Dynamics cont'd

- Drag: $\boldsymbol{F}_D = -\frac{1}{2} C_D \rho_f A_b \left|\boldsymbol{u}_b - \boldsymbol{u}_f\right| \left(\boldsymbol{u}_b - \boldsymbol{u}_f\right)$
- Lift: $\boldsymbol{F}_L = -C_L \rho_f V_b \left(\boldsymbol{u}_b - \boldsymbol{u}_f\right) \times \nabla \times \boldsymbol{u}_f$
- Added mass: $\boldsymbol{F}_{AM} = -C_{VM} \rho_f V_b \left(\frac{d\boldsymbol{u}_b}{dt} - \frac{D\boldsymbol{u}_f}{Dt}\right)$

- 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 and C_{VM}) that need to be defined to close the equations.

Bubble Dynamics – Force closure models

- Drag coefficient closure models:

Drag closure A – Ishii and Zuber (1979)	Drag closure B – Liu et al (1993)
$C_D = \frac{2}{3}\sqrt{Eo}$	$C_D = \begin{cases} \frac{24}{Re}\left(1 + \frac{1}{6}Re^{2/3}\right) & Re \leq 1000 \\ 0.424 & Re > 1000 \end{cases}$

- Lift coefficient closure models:

Lift closure A	Lift closure B – Tomiyama (1998)
$C_L = 0.5$	$C_L = \begin{cases} min[0.288\tanh(0.121Re_b), f(Eo)] & Eo \leq 4 \\ f(Eo) & 4 < Eo \leq 10 \\ -0.27 & 10 < Eo \end{cases}$ $f = 0.00105Eo^3 - 0.0159Eo^2 - 0.0204Eo - 0.474$ The Eötvös number is defined as $Eo = \frac{g\lvert\rho_f - \rho_b\rvert d_b^2}{\sigma}$

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

Volume of Fluid

- Free surface interactions are modelled using VOF approach.
- Navier-Stokes equations:

$$\nabla \cdot \boldsymbol{u} = \boldsymbol{0}$$

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

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

- Fluids are tracked using a scalar field α.

$$\frac{\partial \alpha_q}{\partial t} + \nabla \cdot \left(\alpha_q \boldsymbol{u}\right) + \nabla \cdot \left[\alpha_q \left(1 - \alpha_q\right) \boldsymbol{v}_{\boldsymbol{qp}}\right] = 0$$

Volume of Fluid cont'd

- Smagorinsky sub-grid scale (SGS) model was used.
- The SGS viscosity is implemented as

$$\nu_{SGS} = c_k \sqrt{k_{SGS}} \Delta$$

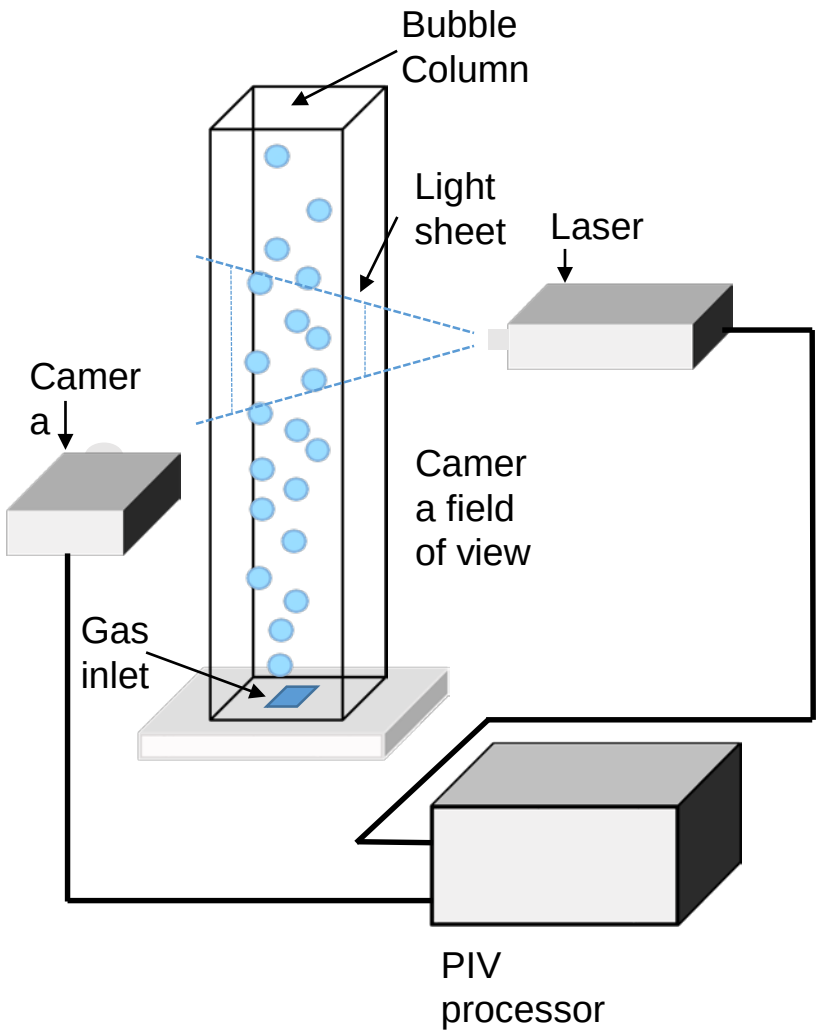
  - k_{SGS} is given by

$$k_{SGS} = \frac{c_k \Delta^2}{c_\epsilon} \left\| \widetilde{\boldsymbol{D}} \right\|^2$$

  - Δ is a top-hat filter with a filter width estimated as the cubic root of the cell volume
  - $\widetilde{\boldsymbol{D}}$ 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.

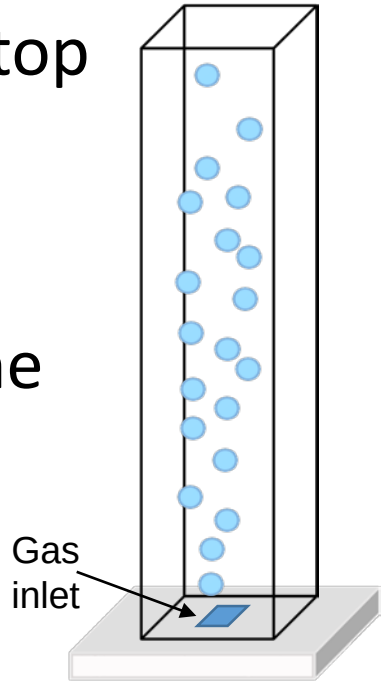


Numerical details

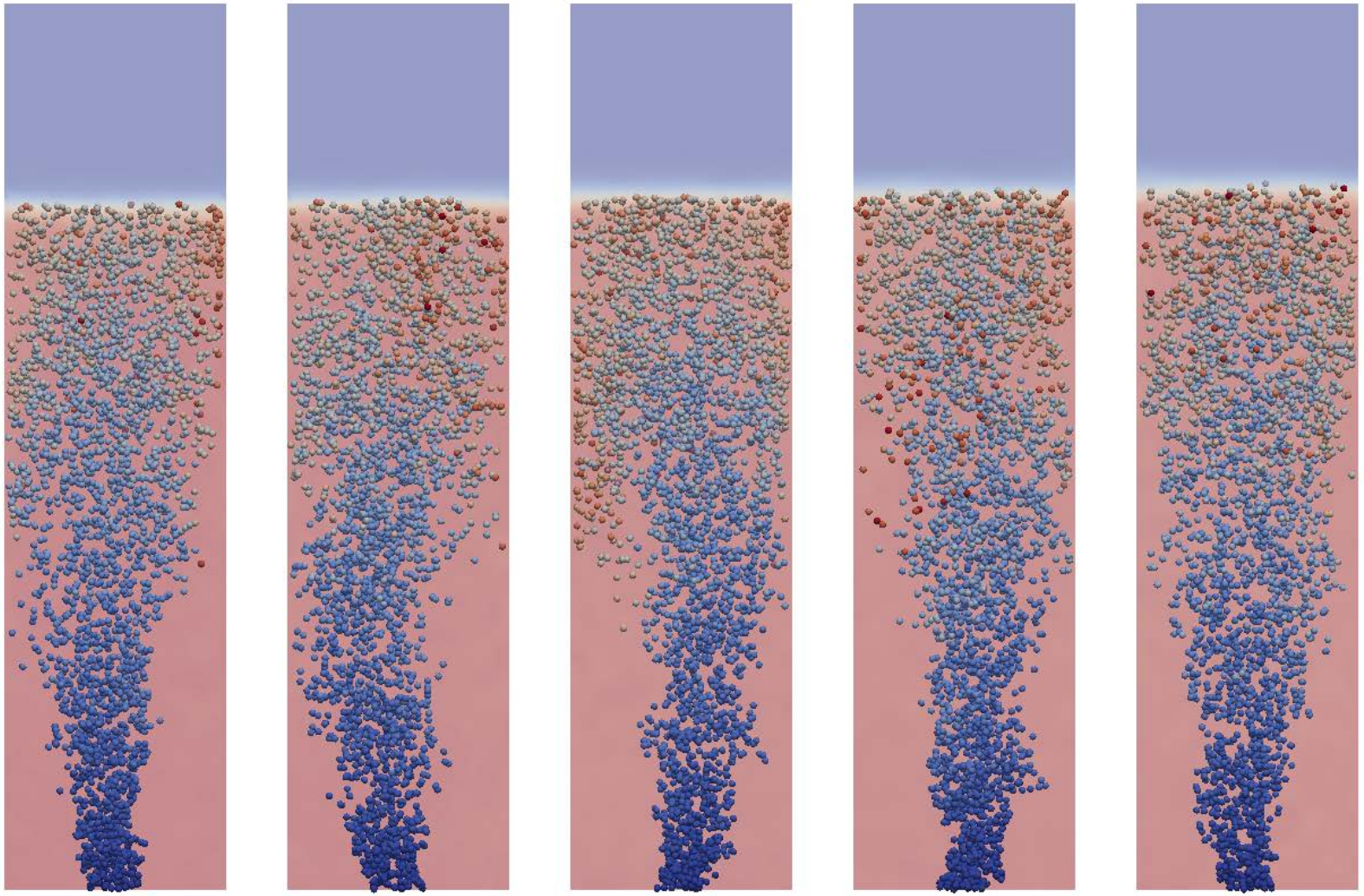
- Governing equations and solution algorithms were implemented as a solver using version 5.04 of the Caelus open source library (www.caelus-cml.com).
- Simulated computational domain had a height of 0.6 m.
  - height was chosen to be far enough away from the liquid surface as not to impact it.
- A patch 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.

Numerical details cont'd

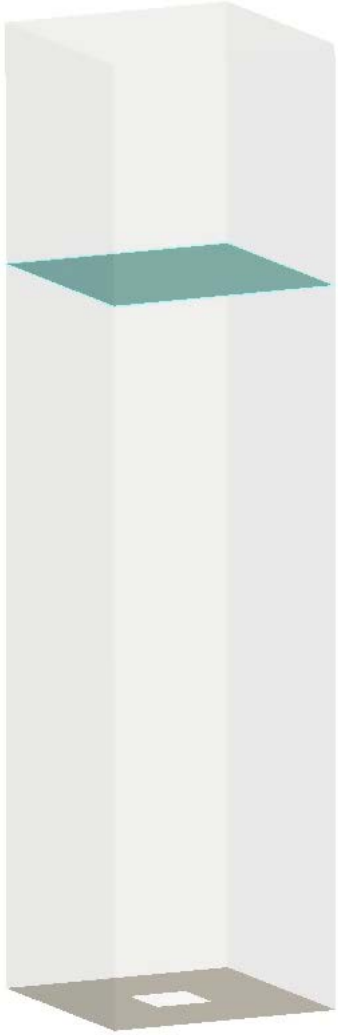
- Boundary conditions:
  - no-slip on the side walls, free slip condition on gas inlet and top of column.
  - zero gradient condition for pressure and gas phase volume fraction on all boundaries.
  - Injection of the bubbles occurred through a small patch at the base of the column with a velocity of 0.08 m/s.
- Fluid properties:
  - Density and kinematic viscosity:
    - Gas - 1.2 kg/m^3 and 1.48×10^{-5} m^2/s.
    - Water - 1000 kg/m^3 and 1×10^{-6} m^2/s.
  - Bubble size – 4 mm matching Dean et al (2001).



Results



50 s 75 s 100 s 125 s 150 s



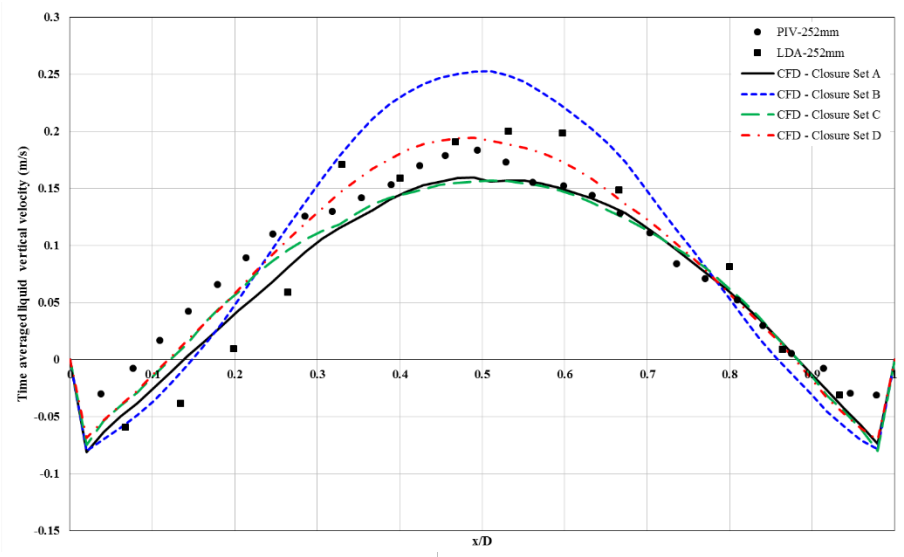
Results – Effect of force closure models

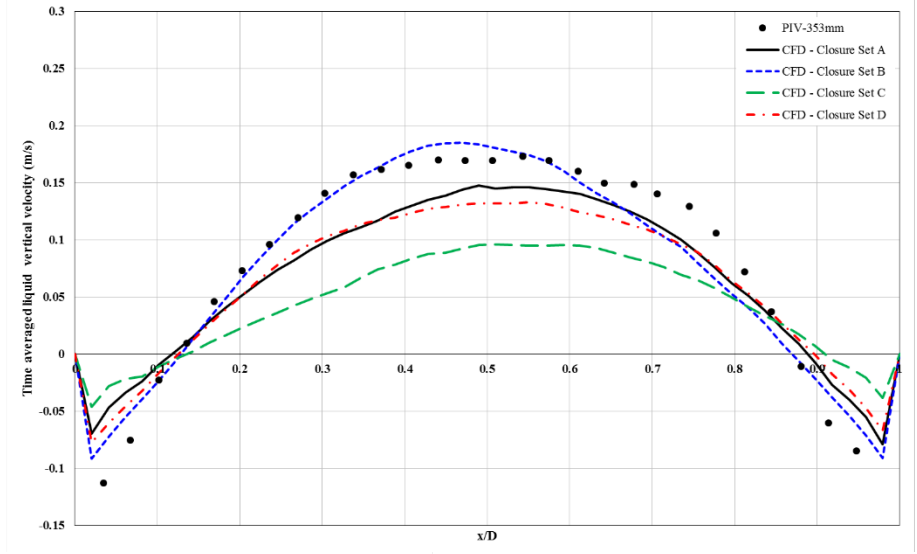
- Combinations of the drag and lift interfacial closure models were tested.

Closure Set	A	B	C	D
Closure models	Drag A / Lift A	Drag A / Lift B	Drag B / Lift A	Drag B / Lift B

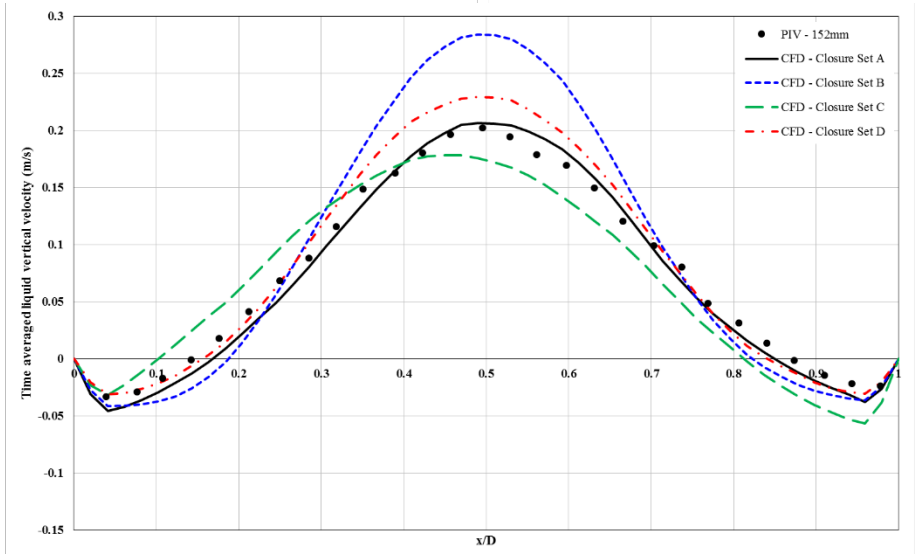
- Effect of
  - Drag: compare set A with C and B with D.
  - Lift: compare set A with B and C with D.
- Results presented
  - Time averaged liquid vertical velocity.
  - Time averaged vertical and horizontal velocity fluctuations.

Results – Effect of closure model cont'd



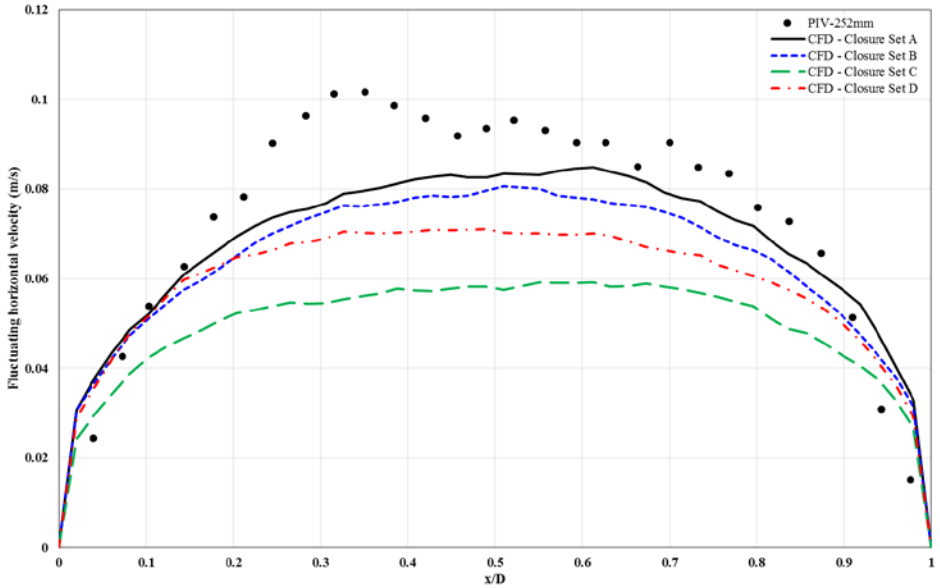


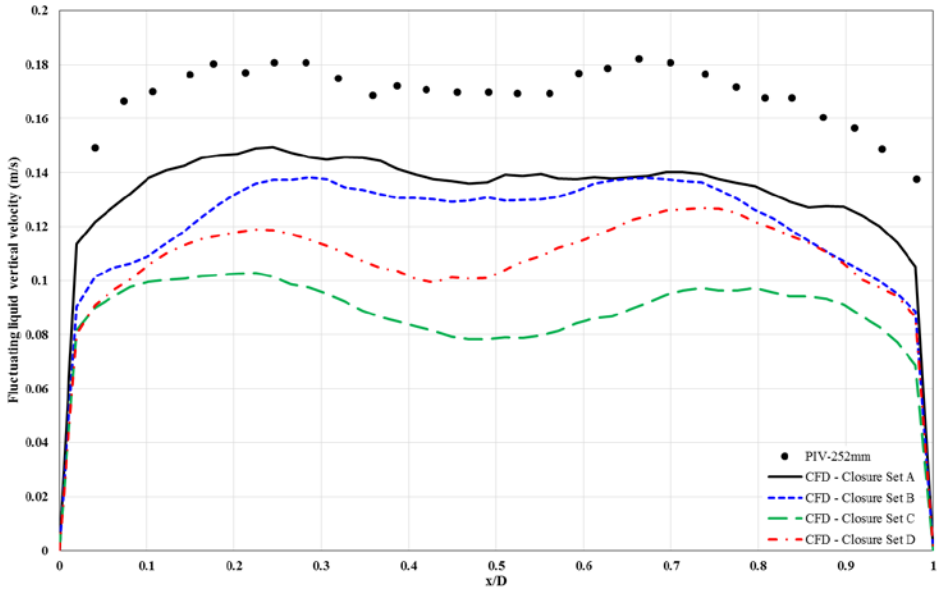
- Drag – at low and high regions, Drag closure A gives better results.



- Lift – increasing lift coefficient spreads bubble plume and reduces vertical velocity. Either set A or D best.

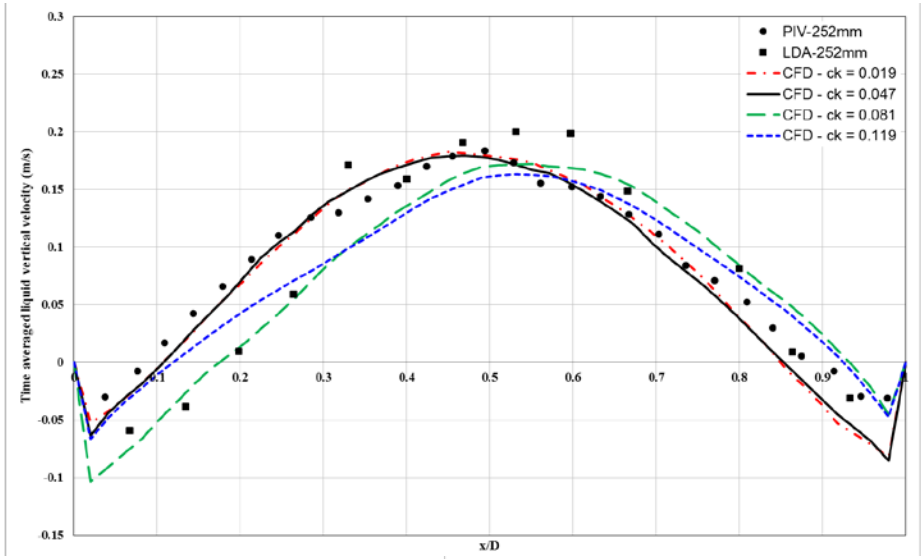
Results – Effect of closure model cont'd

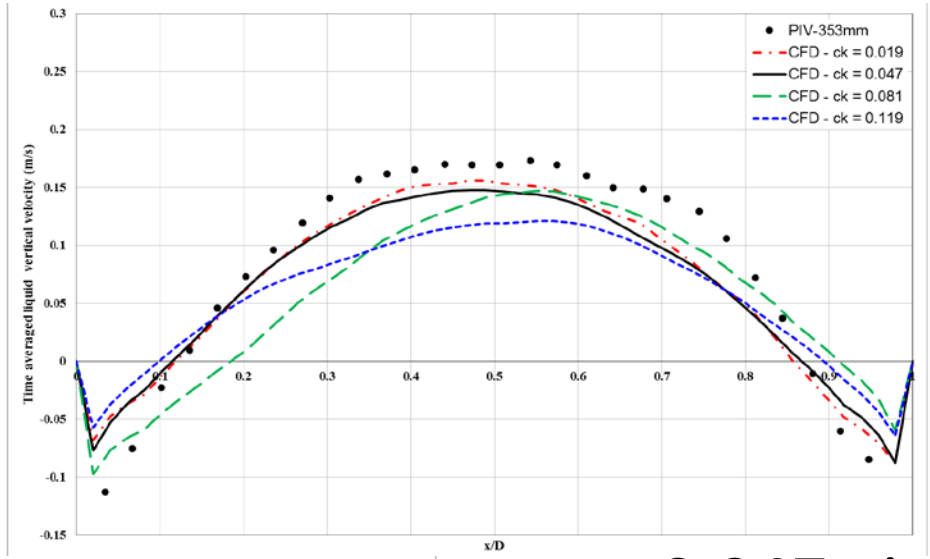




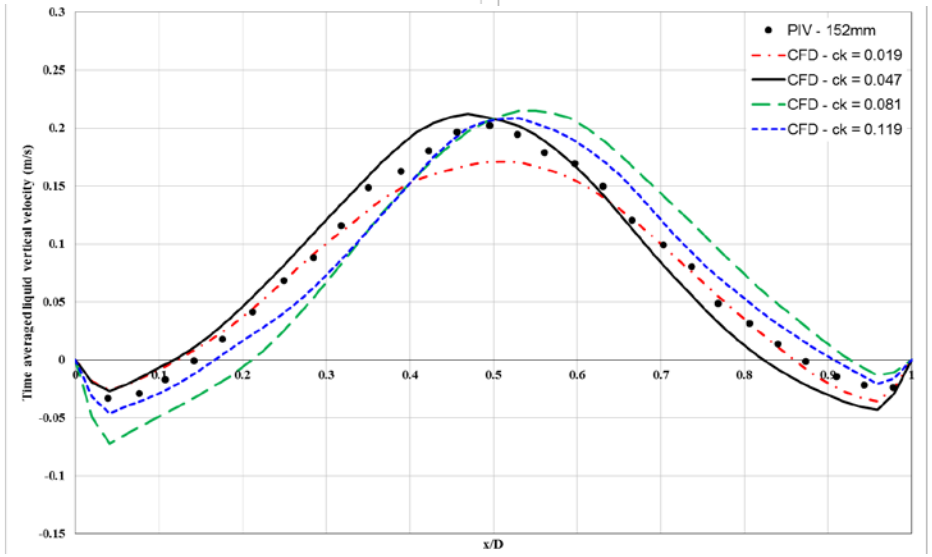
- Overall shape of profiles predicted, however, magnitude is under predicted.
- Profile shape is more sensitive to drag coefficient than lift.
- Closure set A does a better job at predicting the fluctuating liquid velocities.

Results – Sensitivity to SGS model



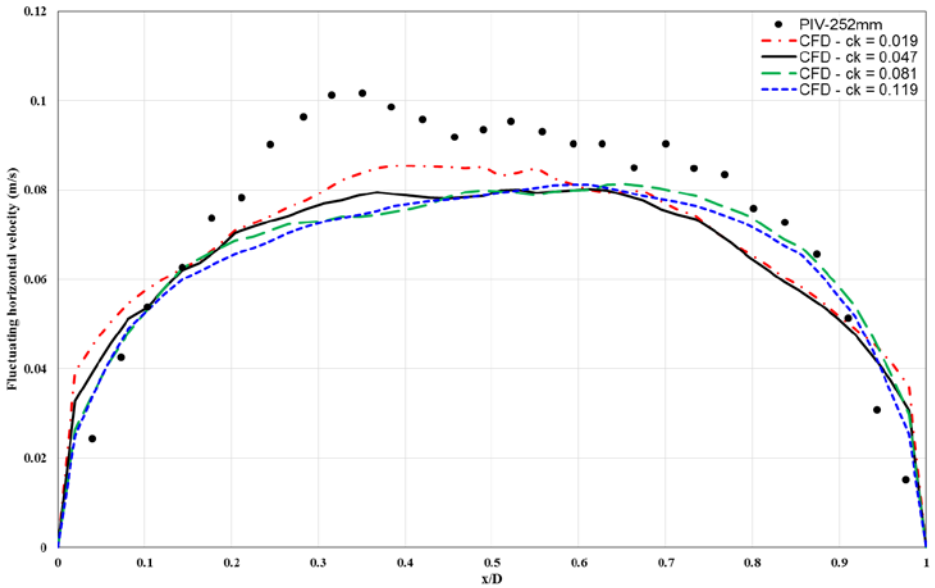


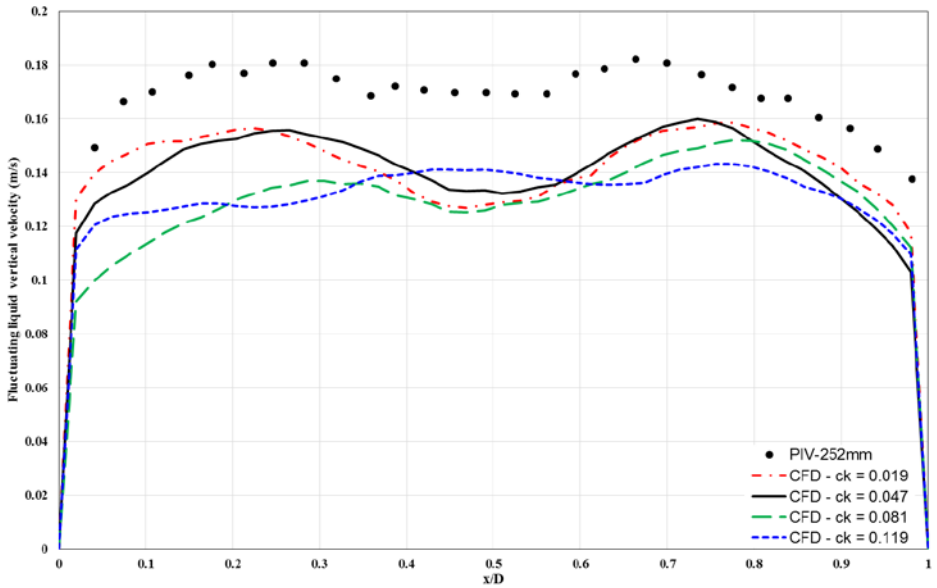
- Using closure model A – investigate effect of changing c_k in SGS model.



- c_k = 0.047 gives the most consistency with experimental data.

Results – Sensitivity to SGS model cont'd





- 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
  - Creators and maintainers of caelus
  - Locations: Australia and Canada
  - Contact: d.Stephens@appliedccm.com.au