Large-eddy simulation of bubbly turbulent flows based on an Euler-Lagrange approach for a huge number of microbubbles

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Objectives

Continuous Phase

Dispersed Phase

Channel Flow Simulations

Conclusions & Outlook
1 Objectives

2 Continuous Phase

3 Dispersed Phase

4 Channel Flow Simulations

5 Conclusions & Outlook
Objectives
Accurate simulation of turbulent bubbly flows at high volume loadings

Objectives
1. Objectives
2. Continuous Phase
3. Dispersed Phase
4. Channel Flow Simulations
5. Conclusions & Outlook
LESOCC
Large Eddy Simulation On Curvilinear Coordinates

• Navier–Stokes solver (incompressible fluid)

• 3–D finite-volume approach
  – Curvilinear body–fitted coordinate system
  – Non–staggered (cell–centered) grid arrangement
  – Block–structured grids

• Spatial discretization
  – Viscous fluxes: central differences $O(\Delta x^2)$
  – Convective fluxes: five different schemes, central diff. $O(\Delta x^2)$, CDS–2

Numerical Method: LESOCC I
LESOCC
Large Eddy Simulation On Curvilinear Coordinates

- Temporal discretization
  - Predictor step (momentum eqns.): low-storage Runge–Kutta scheme, $\mathcal{O}(\Delta t^2)$
  - Corrector step (pressure–correction equation): SIP solver (ILU)

- Pressure–velocity coupling: Momentum interpolation of Rhie & Chow (1983)

- Various subgrid-scale and wall models

- High–performance computing techniques
  - Vectorized and parallelized
Outline

1. Objectives
2. Continuous Phase
3. Dispersed Phase
4. Channel Flow Simulations
5. Conclusions & Outlook
Assumptions

- Lagrangian frame of reference for the dispersed phase
- High volume fraction possible $\Rightarrow$ two- and four-way coupling
- Low density ratio of the bubbles: $\rho_b / \rho_f \ll 1$

Governing Equations for the Dispersed Phase
Assumptions

- Lagrangian frame of reference for the dispersed phase
- High volume fraction possible \( \Rightarrow \) two- and four-way coupling
- Low density ratio of the bubbles: \( \rho_b / \rho_f \ll 1 \)

Newton’s second law:

\[
\frac{d\mathbf{u}_b}{dt} = \frac{1}{m_b} \sum_i \mathbf{F}_i \\
\frac{d\mathbf{x}_b}{dt} = \mathbf{u}_b \\
\frac{d\omega_b}{dt} = \frac{1}{l_b} \mathbf{T}
\]
Assumptions

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Newton’s second law:

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General procedure:

Interpolation of $\mathbf{u}_f$ to bubble location
Assumptions

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General procedure:

Interpolation of $\mathbf{u}_f$ to bubble location

4th order Runge-Kutta scheme

Analytic solution

Governing Equations for the Dispersed Phase
All forces needed!

- Drag

\[ \mathbf{F}_D = \frac{1}{8} C_D \rho_f \pi d_b^2 |\mathbf{u}_f - \mathbf{u}_b| (\mathbf{u}_f - \mathbf{u}_b) \]

- Spherical bubble:

\[ C_{D,s} = \begin{cases} 
\frac{16}{Re_b} & \text{clean} \\
\frac{24}{Re_b} & \text{contam.} \\
\end{cases} \left[ 1 + 2 \left( 1 + \frac{16}{Re_b} + \frac{3.315}{\sqrt{Re_b}} \right) \right] + 0.15 Re_b^{0.687} \]

- Ellipsoidal bubble:

\[ C_{D,e} = 4E_0 / (E_0 + 9.5) \]

⇒ Combine:

\[ C_D = \sqrt{C_{D,s}^2 + C_{D,e}^2} \]

Except the Basset history force

Forces on Bubbles
Test: single rising bubble in a resting fluid

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<tr>
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<td>Sim., clean</td>
<td>Sim., contam.</td>
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<td>Terminal rise velocity [m/s]</td>
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<td>$d_b$ [mm]</td>
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Forces on Bubbles
All forces needed!

- Buoyancy + Gravity
  \[ F_B + F_G = gV_b (\rho_b - \rho_f) \]

- Pressure gradient
  \[ F_{PG} = \rho_f V_b \frac{Du_f}{Dt} \]

- Added-mass
  \[ F_{AM} = \frac{1}{2} \rho_f V_b \left( \frac{Du_f}{Dt} - \frac{Du_b}{Dt} \right) \]

\(^1\)Except the Basset history force
All forces needed!

- **Lift**

\[ \mathbf{F}_L = C_L \rho_b V_b (\mathbf{u}_f - \mathbf{u}_b) \times \text{rot} \mathbf{u}_f \]

- \( \text{Re}_b \ll 1: \)

\[ C_{L,s} = \frac{6}{\pi^2} \left( \text{Re}_b \text{Sr} \right)^{-\frac{1}{2}} \frac{2.255}{\left(1 + 0.2\frac{\text{Re}_b}{\text{Sr}}\right)^{\frac{3}{2}}} \]

- \( \text{Re}_b \gg 1: \)

\[ C_{L,l} = \frac{1}{2} \frac{1 + 16/\text{Re}_b}{1 + 29/\text{Re}_b} \]

\( \Rightarrow \) **Combine:**

\[ C_D = \sqrt{C_{L,s}^2 + C_{L,l}^2} \]

\(^1\text{Except the Basset history force}\)
Challenge for LES:

- Fluid solver provides filtered fluid velocity $\bar{u}_f$
- Full velocity needed: $u_f = \bar{u}_f + u'_f$

Subgrid-scale Model for the Dispersed Phase
**Challenge for LES:**

- Fluid solver provides filtered fluid velocity $\overline{u}_f$
- Full velocity needed: $u_f = \overline{u}_f + u'_f$

**Subgrid-scale model of Pozorski and Apte (2009)**

\[
du'_s = -G u'_s \, dt + \sqrt{2\sigma_{SGS}^2} \, B \, dW
\]

Langevin eq. $\rightarrow u'_f$ at bubble position

- Randomness
- Temporal coupling
  - Crossing trajectory effect
  - Continuity effect
- Directional coupling

\[\leftarrow\text{Stochastic diff. term}\]
\[\leftarrow\text{Drift term}\]
\[\leftarrow\text{Matrix form}\]
Subgrid-scale model of Pozorski and Apte (2009)

\[
du'_s = -G u'_s \, dt + \sqrt{2\sigma^2_{SGS}} \, B \, dW
\]

- Turbulent kinetic energy: \( k_{SGS} = \frac{1}{2} (\bar{u}_f - \bar{u}_f)^2 \)
- Estimated fluctuations: \( \sigma_{SGS} = \sqrt{\frac{2}{3} k_{SGS}} \)
- Fluctuation length scale: \( \Delta_{SGS} \)
  - \( \Delta_{\text{filter}} \) (Pozorski and Apte, 2009)
  - Here: \( \Delta_{\text{filter}} f_{\text{van Driest}} \)
- Fluctuation time scale: \( \tau'_L = C \frac{\Delta_{SGS}}{\sigma_{SGS}} \)
- Crossing trajectory & continuity effect \( \leftarrow \) Csanady (1963)
- Matrix \( G \Rightarrow B = \sqrt{G} \)

\[
G_{ij} = \frac{1}{\tau'_{L,\perp}} \delta_{ij} + \left( \frac{1}{\tau'_{L,\parallel}} - \frac{1}{\tau'_{L,\perp}} \right) r_i r_j, \quad r_i = \frac{u_{rel,i}}{|u_{rel}|}
\]
C-Space vs. P-Space Tracking

- **P-space is curvilinear**
  - Point location not trivial
  - Time-consuming search algorithms required

- **C-space is orthonormal**
  - Point location trivial
  - No search algorithms required
P-space is curvilinear
Point location not trivial
⇒ Time-consuming search algorithms required

C-Space vs. P-Space Tracking
P-space is curvilinear
Point location not trivial
⇒ Time-consuming search algorithms required

C-space is orthonormal
Point location trivial
⇒ No search algorithms required

C-Space vs. P-Space Tracking
1 Objectives
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DNS:
Channel downflow of Molin et al. (2012)

Present Simulation:

Flow
- \( \text{Re}_\tau = \frac{u_\tau \delta}{\nu} = 150, \delta = 20 \text{ mm} \)
- Fixed pressure gradient
- Grid: \( 256 \times 128 \times 256 \) CV
- Periodic BC stream- and spanwise
- No-slip BC at smooth wall
- Two-way coupled

Bubbles
- \( N_b = 21,940 \)
- \( d_b = 220 \mu\text{m} \)
- \( \Phi_{V,\text{tot}} = 1 \cdot 10^{-4} \)
- Surfactant contaminated
- Bubble SGS model not activated

Setup of the Test Case
Comparison with the Reference Case
Comparison with the Reference Case
Comparison with the Reference Case

- Slight overestimation of the velocities in the channel center
- Fluctuations slightly underpredicted

- Bubbles follow fluid motion
- Close agreement for volume fraction

⇒ Close overall agreement between present sim. and reference data
DNS: Channel downflow of Molin et al. (2012)

Present Simulation:

Flow
- $\text{Re}_\tau = \frac{u_\tau \delta}{\nu} = 150$, $\delta = 20\text{ mm}$
- Fixed pressure gradient
- Grid: $256 \times 128 \times 256$ CV
- Periodic BC stream- and spanwise
- No-slip BC at smooth wall
- Two-way coupled

Bubbles
- $N_b = 21,940/43,880/87,760$
- $d_b = 220\mu\text{m}$
- $\Phi_{V,\text{tot}} = 1 \cdot 10^{-4}/2 \cdot 10^{-4}/4 \cdot 10^{-4}$
- Surfactant contaminated
- Bubble SGS model not activated

Increased Volume Fraction
Fluid

\[ \langle u_f \rangle / u_\tau \]

\[ y^+ \]

\[ \Phi V_{,tot} = 1 \cdot 10^{-4} \]
\[ \Phi V_{,tot} = 2 \cdot 10^{-4} \]
\[ \Phi V_{,tot} = 4 \cdot 10^{-4} \]

Bubbles

\[ \langle u_b \rangle / u_\tau \]

\[ y^+ \]

\[ \Phi V_{,tot} = 1 \cdot 10^{-4} \]
\[ \Phi V_{,tot} = 2 \cdot 10^{-4} \]
\[ \Phi V_{,tot} = 4 \cdot 10^{-4} \]

- \( \Phi V_{,tot} = 2 \times 10^{-4} \): strongly reduced fluid velocity
- \( \Phi V_{,tot} = 4 \times 10^{-4} \): reversed flow \( \rightarrow \) upflow

\( \Rightarrow \) Strong impact of momentum added by two-way coupling

Increased Volume Fraction
Higher volume fraction

- Fluctuations strongly reduced
- Bubble and fluid fluctuations equal
  → Fluid fluctuations driven by the bubbles

⇒ Laminarization
Fluid

\[ \frac{\langle v'_f v'_f \rangle}{u^2} \tau \frac{y}{\delta} \]

\[ \Phi_{V,tot} = 1 \cdot 10^{-4} \]
\[ \Phi_{V,tot} = 2 \cdot 10^{-4} \]
\[ \Phi_{V,tot} = 4 \cdot 10^{-4} \]

Bubbles

\[ \frac{\langle v'_b v'_b \rangle}{u^2} \tau \frac{y}{\delta} \]

\[ \Phi_{V,tot} = 1 \cdot 10^{-4} \]
\[ \Phi_{V,tot} = 2 \cdot 10^{-4} \]
\[ \Phi_{V,tot} = 4 \cdot 10^{-4} \]

Increased Volume Fraction
\[ \langle \Phi V \rangle / \Phi V_{\text{tot}} \]

\[ y^+ \]

- \( \Phi_{V,\text{tot}} = 2 \times 10^{-4} \): bubbles pushed towards channel center
  
  \( \rightarrow \) Stronger lift due to higher \( u_{rel} \)

- \( \Phi_{V,\text{tot}} = 4 \times 10^{-4} \):
  - Peak at \( y^+ \approx 7 \)

Video: \( \Phi_{\text{tot}} = 1 \cdot 10^{-4} \)

Video: \( \Phi_{\text{tot}} = 4 \cdot 10^{-4} \)

Increased Volume Fraction
DNS:
Channel downflow of Molin et al. (2012)

Present Simulation:

Flow
- \( \text{Re}_\tau = u_\tau \delta / \nu = 150, \delta = 20 \text{ mm} \)
- Fixed pressure gradient
- Grid: 256 × 128 × 256 CV
- Periodic BC stream- and spanwise
- No-slip BC at smooth wall
- Two-way coupled

Bubbles
- \( N_b = 21,940/87,760 \)
- \( d_b = 220 \mu m/d_b = 138.6 \mu m \)
- \( \Phi_{V,\text{tot}} = 1 \cdot 10^{-4} \)
- Surfactant contaminated
- Bubble SGS model not activated

Increased Bubble Number
Increased Bubble Number
DNS: Channel downflow of Molin et al. (2012)

Present Simulation:

Flow
- \( \text{Re}_\tau = \frac{u_\tau \delta}{\nu} = 150, \ \delta = 20 \text{ mm} \)
- Fixed pressure gradient
- Grid: \( 128 \times 128 \times 128 \) CV
- Periodic BC stream- and spanwise
- No-slip BC at smooth wall
- Two-way coupled

Bubbles
- \( N_b = 21,940 \)
- \( d_b = 220 \mu \text{m} \)
- \( \Phi_{V,\text{total}} = 1 \cdot 10^{-4} \)
- Surfactant contaminated
- Particle SGS model of Pozorski & Apte (2009) activated

Influence of the Particle Subgrid-Scale Model
Without SGS-model
Langevin SGS-model

- Similar results for wall-normal and spanwise directions
Influence of the Particle Subgrid-Scale Model
- Correct level of turbulent kinetic energy added

Influence of the Particle Subgrid-Scale Model
- Correct level of turbulent kinetic energy added
- $k_{\text{SGS}}^{\text{seen}} > k_{\text{SGS}}$
- Bubbles tend to accumulate in regions of high fluctuations/turbulent kinetic energy

Influence of the Particle Subgrid-Scale Model
Conclusions

- LESOCC successfully extended towards tracking of bubbles
  → Very good agreement to DNS results
- Increased volume fraction
  - Decreases/reverts fluid velocity
  - Laminarizes the flow
- Increased bubble number with marginal effect
- Subgrid-scale model for the dispersed phase
  → Small influence for bubbles

Outlook

- Extend present investigations
- Higher Re flows
- Include coalescence & break-up of bubbles
Thank you for your attention!
Rhie, C.M. and Chow, W.L.; 1983
*A numerical study of the turbulent flow past an isolated airfoil with trailing edge separation* AIAA Journal, 21.

*Bubbles, drops and particles.* New York: Academic Press

Duineveld, P.C.; 1995
*The rise velocity and shape of bubbles in pure water at high Reynolds number.* J. Fluid. Mech.

Pozorski, J. and Apte, S.V.; 2009
Csanady, G.T.; 1963
_Turbulent diffusion of heavy particles in the atmosphere._

Molin, D. and Marchioli, C. and Soldati, A.; 2012
_Turbulence modulation and microbubble dynamics in vertical channel flow._
Int. J. Multiphase Flow, 42.
Backup
Subgrid-scale model of Pozorski and Apte (2009)

\[ d\mathbf{u}'_s = -G \mathbf{u}'_s \, dt + \sqrt{2\sigma^2_{\text{SGS}}} \mathbf{B} \, d\mathbf{W} \]

- Turbulent kinetic energy: \( k_{\text{SGS}} = \frac{1}{2} (\bar{u}_f - \bar{u}_f)^2 \)
- Estimated fluctuations: \( \sigma_{\text{SGS}} = \sqrt{\frac{2}{3} k_{\text{SGS}}} \)
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\[ d\mathbf{u}'_s = -G\mathbf{u}'_s \, dt + \sqrt{2\sigma^2_{SGS}} \mathbf{B} \, d\mathbf{W} \]

- Crossing trajectory & continuity effect ← Csanady (1963)
  - Parallel to direction of relative motion
  \[ \tau'_{L,\parallel} = \frac{\tau'_{L}}{\sqrt{1 + \mathbf{u}_{rel}^2/\sigma^2_{rel}}} \]
  - Perpendicular to direction of relative motion
  \[ \tau'_{L,\perp} = \frac{\tau'_{L}}{\sqrt{1 + 4\mathbf{u}_{rel}^2/\sigma^2_{rel}}} \]
Subgrid-scale model of Pozorski and Apte (2009)

\[ du'_s = -G u'_s \, dt + \sqrt{2\sigma^2_{SGS}} \, B \, dW \]

- **Matrix G**

\[ G_{ij} = \frac{1}{\tau'_L,\perp} \delta_{ij} + \left( \frac{1}{\tau'_L,\parallel} - \frac{1}{\tau'_L,\perp} \right) r_i \, r_j \]

- **Matrix B = \sqrt{G}**

\[ B_{ij} = \frac{1}{\sqrt{\tau'_L,\perp}} \delta_{ij} + \left( \frac{1}{\sqrt{\tau'_L,\parallel}} - \frac{1}{\sqrt{\tau'_L,\perp}} \right) r_i \, r_j \]

- **Direction of relative motion** \( r_i = u_{rel,i} / |u_{rel}| \)
Present Simulation:

Flow
- \( \text{Re}_\tau = u_\tau \delta / \nu = 644, \delta = 20 \text{ mm} \)
- Grid: \( 128 \times 128 \times 128 \) CV
- Periodic BC stream- and spanwise
- No-slip BC at smooth wall
- Four-way coupled

Particles
- \( N_p = 6 \cdot 10^6 \)
- \( d_b = 4 \mu m \)
- \( \Phi_{V,\text{tot}} = 6.78 \cdot 10^{-7} \)
- \( \eta = 1.23 \cdot 10^{-3} \)
- SGS model of Pozorski & Apte (2009)
Subgrid-Scale Model for Solid Particles
Subgrid-Scale Model for Solid Particles
The subgrid-scale model for solid particles is illustrated with graphs showing the fluctuation and mean square of the velocity. The graphs depict the scaled velocity fluctuations $\langle u'_s \rangle / u_{bulk}$ and $\langle v'_s \rangle / u_{bulk}$, as well as the mean square of the velocity fluctuations $\langle u'_s u'_s \rangle / u_{bulk}^2$ and $\langle v'_s v'_s \rangle / u_{bulk}^2$, all scaled by $y/\delta$ and $10^{-3}$. Additionally, the subgrid-scale kinetic energy $k_{SGS}$ is shown, scaled by $u_{bulk}^2 y/\delta$ and $10^{-3}$.

$k_{SGS}$ is related to the filter size and the friction velocity as follows:

- $k_{SGS} \propto \Delta_{filter}$
- $k_{SGS} \propto \Delta_{filter} f_{wd}$
- $k_{SGS} \propto C_S \Delta_{filter} f_{wd}$