3D-Euler-Euler modeling of adiabatic poly-disperse bubbly flows based on particle-center-averaging method

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Last but not least, I am very grateful for the support and love of my family, especially my parents.
Abstract

An inconsistency exists in bubble force models used in the standard Euler-Euler simulations. The bubble force models are typically developed by assuming that the forces act on the bubbles’ centers of mass. However, in the standard Euler-Euler model, each bubble force is a function of the local gas volume fraction because the phase-averaging method is used. This inconsistency can lead to gas over-concentration in the center or near the wall of a channel when the bubble diameter is larger than the computational cell size. Besides, a mesh-independent solution may not exist in such cases. In addition, the bubble deformation is not fully considered in the standard Euler-Euler model. In this thesis, a particle-center-averaging method is used to represent the bubble forces as forces that act on the bubbles’ centers of mass. A particle-center-averaged Euler-Euler approach for bubbly flow simulations is developed by combining the particle-center-averaged Euler-Euler framework with a Gaussian convolution method. The convolution method is used to convert the phase-averaged and the particle-center-averaged quantities. The remediation of the inconsistency in the standard Euler-Euler model by the particle-center-averaging method is demonstrated using a simplified two-dimensional test case.

Bubbly flows in different vertical pipes are used to validate the particle-center-averaged Euler-Euler approach. The bubbly flow simulation results for the particle-center-averaged Euler-Euler model and the standard Euler-Euler model are compared with experimental data. For monodisperse simulations, the particle-center-averaging method alleviates the over-predictions of the gas volume fraction peaks for wall-peaking cases and for finely dispersed flow case. Whereas, no improvement is found in the simulated gas volume fraction for center-peaking cases because the over-prediction caused by the inconsistency has been smoothed by the turbulent dispersion. Moreover, the axial gas and liquid velocities simulated with both Euler-Euler models are similar, which proves that the closure models for bubble forces and turbulence are correctly applied in the particle-center-averaged Euler-Euler model. For fixed polydisperse simulations, the particle-center-averaging method can also alleviate the over-prediction of the gas volume fraction peak in the center or near the wall of a pipe. The axial gas velocities simulated with both Euler-Euler models are about the same. Comparisons are also made for the simulation results of bubbly flows in a cylindrical bubble column and the experimental data. The gas volume fractions and the axial gas velocities simulated with both Euler-Euler models almost coincide with each other, which indicates that the sink and source terms for the continuity equations and the degassing boundary are set correctly in the particle-center-averaged Euler-Euler model.

An oblate ellipsoidal bubble shape is considered in the particle-center-averaged Euler-Euler simulations by an anisotropic diffusion. The influence of bubble shape on the simulation results of bubbly pipe flows is investigated. The results show that considering the oblate ellipsoidal bubble shape in simulations can further alleviate the over-predictions of the gas volume fraction peaks for wall peaking cases, but it has little influence on the gas volume fractions of center-peaking cases and the axial gas velocities.
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### Nomenclature

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<th>Unit</th>
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<tbody>
<tr>
<td>( a, a_N )</td>
<td>coefficient in algebraic equation</td>
<td>-</td>
</tr>
<tr>
<td>( A )</td>
<td>matrix of coefficients of discretized momentum equation</td>
<td>-</td>
</tr>
<tr>
<td>( (A_k)_D )</td>
<td>diagonal matrix decomposed from ( A ) for the phase ( k )</td>
<td>-</td>
</tr>
<tr>
<td>( C^N )</td>
<td>the set of all possible dynamic states for a system containing ( N ) indistinguishable bubbles</td>
<td>-</td>
</tr>
<tr>
<td>( C_{\text{diff}} )</td>
<td>diffusion coefficient</td>
<td>m(^2) s(^{-1})</td>
</tr>
<tr>
<td>( C )</td>
<td>coefficient of force</td>
<td>-</td>
</tr>
<tr>
<td>( C_0 )</td>
<td>Courant number</td>
<td>-</td>
</tr>
<tr>
<td>( d_B )</td>
<td>bubble diameter</td>
<td>m</td>
</tr>
<tr>
<td>( d_{B_i} )</td>
<td>representative bubble diameter of bubble velocity group ( i )</td>
<td>m</td>
</tr>
<tr>
<td>( d_{B_j} )</td>
<td>representative bubble diameter of bubble size group ( j )</td>
<td>m</td>
</tr>
<tr>
<td>( d_H )</td>
<td>horizontal (major) axis of an oblate ellipsoidal bubble</td>
<td>m</td>
</tr>
<tr>
<td>( d_V )</td>
<td>vertical (minor) axis of an oblate ellipsoidal bubble</td>
<td>m</td>
</tr>
<tr>
<td>( D )</td>
<td>pipe diameter</td>
<td>m</td>
</tr>
<tr>
<td>( D_{ij}(i,j=x,y,z) )</td>
<td>diffusion tensor component</td>
<td>m(^2) s(^{-1})</td>
</tr>
<tr>
<td>( D_{s} )</td>
<td>diffusion tensor for a spherical bubble</td>
<td>m(^2) s(^{-1})</td>
</tr>
<tr>
<td>( E )</td>
<td>error used to measure the difference between expected and solved gas volume fraction</td>
<td>-</td>
</tr>
<tr>
<td>( E_0 )</td>
<td>Eötvös number</td>
<td>-</td>
</tr>
<tr>
<td>( f )</td>
<td>force per unit control volume</td>
<td>kg m(^{-2}) s(^{-2})</td>
</tr>
<tr>
<td>( f_{D,\text{correction}} )</td>
<td>correction term for drag force</td>
<td>kg m(^{-2}) s(^{-2})</td>
</tr>
<tr>
<td>( f_{\text{VM,correction}} )</td>
<td>correction term for virtual mass force</td>
<td>kg m(^{-2}) s(^{-2})</td>
</tr>
<tr>
<td>( F_B )</td>
<td>resultant force for a single bubble</td>
<td>kg m s(^{-2})</td>
</tr>
<tr>
<td>( F_1, F_2 )</td>
<td>blending function</td>
<td>-</td>
</tr>
<tr>
<td>( f_j )</td>
<td>volume fraction of the bubble size group ( j )</td>
<td>-</td>
</tr>
<tr>
<td>( f_i )</td>
<td>volumetric flow rate fraction of the bubble velocity group ( i )</td>
<td>-</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>$g$</td>
<td>acceleration of gravity</td>
<td>m s$^{-2}$</td>
</tr>
<tr>
<td>$h$</td>
<td>position vector to the point of zero potential</td>
<td>m</td>
</tr>
<tr>
<td>$I$</td>
<td>turbulence intensity</td>
<td>-</td>
</tr>
<tr>
<td>$J$</td>
<td>unit tensor</td>
<td>-</td>
</tr>
<tr>
<td>$k$</td>
<td>superficial velocity</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$L$</td>
<td>turbulent kinetic energy</td>
<td>m$^2$ s$^{-2}$</td>
</tr>
<tr>
<td>$M$</td>
<td>distance between the bubble’s center-of-mass and the wall</td>
<td>m</td>
</tr>
<tr>
<td>$m_B$</td>
<td>number of computational cells covered by a bubble</td>
<td>-</td>
</tr>
<tr>
<td>$N$</td>
<td>bubble mass</td>
<td>kg</td>
</tr>
<tr>
<td>$N_{\text{cell}}$</td>
<td>the number of computational cells</td>
<td>-</td>
</tr>
<tr>
<td>$N_{\text{g}}$</td>
<td>the number of bubble velocity groups</td>
<td>-</td>
</tr>
<tr>
<td>$n$</td>
<td>number density of bubble centers</td>
<td>m$^{-3}$</td>
</tr>
<tr>
<td>$n_w$</td>
<td>unit wall-normal vector pointing into the fluid</td>
<td>-</td>
</tr>
<tr>
<td>$n_s$</td>
<td>unit normal vector directed outward from bubble surface</td>
<td>-</td>
</tr>
<tr>
<td>$P_k$</td>
<td>production term for turbulent kinetic energy</td>
<td>kg m s$^{-3}$</td>
</tr>
<tr>
<td>$P(N; t)$</td>
<td>probability density function of a dynamic state at time $t$</td>
<td>-</td>
</tr>
<tr>
<td>$P(x, u^b, t)$</td>
<td>one-bubble probability density function</td>
<td>m$^{-4}$ s</td>
</tr>
<tr>
<td>$P(x, t)$</td>
<td>probability</td>
<td>-</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>$p_{\text{rgh}}$</td>
<td>pseudo pressure ($=p - \rho_mgh$)</td>
<td>Pa</td>
</tr>
<tr>
<td>$q_{\text{v,d}}$</td>
<td>gas volumetric flow rate in each inlet patch</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>$r$</td>
<td>radial coordinate</td>
<td>m</td>
</tr>
<tr>
<td>$R$</td>
<td>radius of a pipe or a cylindrical bubble column</td>
<td>m</td>
</tr>
<tr>
<td>$R_s$</td>
<td>radius of a diffusion sphere</td>
<td>m</td>
</tr>
<tr>
<td>$R_c$</td>
<td>radius of a diffusion circle</td>
<td>m</td>
</tr>
<tr>
<td>$R_P$</td>
<td>source in algebraic equation</td>
<td>-</td>
</tr>
<tr>
<td>$R$</td>
<td>source vector</td>
<td>-</td>
</tr>
<tr>
<td>$Re$</td>
<td>bulk Reynolds number ($=2\rho_c</td>
<td>u_c</td>
</tr>
<tr>
<td>$Re_B$</td>
<td>bubble Reynolds number ($=\rho_c</td>
<td>u_d - u_c</td>
</tr>
<tr>
<td>$S$</td>
<td>source or sink</td>
<td>-</td>
</tr>
<tr>
<td>$S_{\text{d,other}}$</td>
<td>mass source or sink for the disperse phase in the domain excluding the mass sink for the degassing boundary</td>
<td>kg m$^{-3}$ s$^{-1}$</td>
</tr>
<tr>
<td>$S_E$</td>
<td>explicit volume source term</td>
<td>-</td>
</tr>
<tr>
<td>$S_I$</td>
<td>coefficient of the implicit volume source term</td>
<td>-</td>
</tr>
<tr>
<td>$S_B$</td>
<td>surface area of a bubble</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$S_P$</td>
<td>surface of the cell $P$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$S_I$</td>
<td>cell surface area vector with its magnitude equal to the cell surface area</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$S$</td>
<td>viscous stress tensor</td>
<td>kg m$^{-1}$ s$^{-2}$</td>
</tr>
<tr>
<td>$T$</td>
<td>Reynolds stress tensor</td>
<td>kg m$^{-1}$ s$^{-2}$</td>
</tr>
<tr>
<td>$t$</td>
<td>physical time</td>
<td>s</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>time step</td>
<td>s</td>
</tr>
<tr>
<td>$u$</td>
<td>axial velocity component</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$u$</td>
<td>velocity vector</td>
<td>m s$^{-1}$</td>
</tr>
</tbody>
</table>
## Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_{PCAM}$</td>
<td>mixture velocity vector ($=\beta_d u_d + \alpha_c u_c$)</td>
<td>m s(^{-1})</td>
</tr>
<tr>
<td>$V_e$</td>
<td>volume of diffusion ellipsoid</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$V_s$</td>
<td>volume of a diffusion sphere</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$V_b$</td>
<td>bubble volume</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$V_{Bi}$</td>
<td>representative volume of the bubble velocity group $i$</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$V_{cell}$</td>
<td>cell volume</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$V_{total}$</td>
<td>total volume of the layer of cells nearest to degassing boundary</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$V_p$</td>
<td>cell volume</td>
<td>m(^3)</td>
</tr>
<tr>
<td>$\chi$</td>
<td>phase indicator function</td>
<td>-</td>
</tr>
<tr>
<td>$x, y, z$</td>
<td>spatial coordinates</td>
<td>m</td>
</tr>
<tr>
<td>$X_{cell}$</td>
<td>coordinate of bubble center location</td>
<td>m</td>
</tr>
<tr>
<td>$y$</td>
<td>coordinate vector of bubble center location</td>
<td>m</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>gradient operator</td>
<td>-</td>
</tr>
<tr>
<td>$\nabla_f$</td>
<td>gradient operator for the direction perpendicular to cell face</td>
<td>-</td>
</tr>
<tr>
<td>$\nabla_v$</td>
<td>divergence operator</td>
<td>-</td>
</tr>
<tr>
<td>$\cdot$</td>
<td>phase-averaged</td>
<td>-</td>
</tr>
<tr>
<td>$\cdot_b$</td>
<td>basic averaged</td>
<td>-</td>
</tr>
<tr>
<td>$\cdot_{cs}$</td>
<td>cross-section averaged value</td>
<td>-</td>
</tr>
<tr>
<td>$&lt;, &gt;$</td>
<td>particle-center-averaged</td>
<td>-</td>
</tr>
<tr>
<td>$\sim$</td>
<td>dimensionless</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>phase volume fraction</td>
<td>-</td>
</tr>
<tr>
<td>$\alpha_{d,j}$</td>
<td>gas volume fraction in the computational cell $j$</td>
<td>-</td>
</tr>
<tr>
<td>$\beta$</td>
<td>gas volume fraction assigning all bubble volume to bubble center</td>
<td>-</td>
</tr>
<tr>
<td>$r$</td>
<td>diffusivity</td>
<td>-</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Dirac delta function</td>
<td>-</td>
</tr>
<tr>
<td>$\Delta_c$</td>
<td>computational cell spacing</td>
<td>m</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>turbulent eddy dissipation rate</td>
<td>-</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>damping factor</td>
<td>-</td>
</tr>
<tr>
<td>$\mu$</td>
<td>dynamic viscosity</td>
<td>kg m(^{-1}) s(^{-1})</td>
</tr>
<tr>
<td>$\mu_{turb}$</td>
<td>turbulent dynamic viscosity</td>
<td>kg m(^{-1}) s(^{-1})</td>
</tr>
<tr>
<td>$\nu_{turb}$</td>
<td>turbulent eddy viscosity</td>
<td>m(^2) s(^{-1})</td>
</tr>
<tr>
<td>$\rho$</td>
<td>density</td>
<td>kg m(^{-3})</td>
</tr>
<tr>
<td>$\rho_m$</td>
<td>mixture density ($=\alpha_d \rho_d + \alpha_c \rho_c$)</td>
<td>kg m(^{-3})</td>
</tr>
<tr>
<td>$\Delta \rho$</td>
<td>density difference between both phases ($=\rho_c - \rho_d$)</td>
<td>kg m(^{-3})</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>surface tension coefficient</td>
<td>kg s(^{-2})</td>
</tr>
<tr>
<td>$\sigma_{ac}$</td>
<td>Schmidt number</td>
<td>-</td>
</tr>
<tr>
<td>$\sigma_s$</td>
<td>stress tensor</td>
<td>kg m(^{-1}) s(^{-2})</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>surface stress tensor originating from non-uniform</td>
<td>kg m(^{-1}) s(^{-2})</td>
</tr>
<tr>
<td>$\tau$</td>
<td>distribution of pressure force on the surface of a bubble</td>
<td>s</td>
</tr>
<tr>
<td>$\tau_{opt_e}$</td>
<td>optimized diffusion pseudo-time for an ellipsoidal bubble</td>
<td>s</td>
</tr>
</tbody>
</table>
# Nomenclature

## Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_{\text{opt}}$</td>
<td>optimized diffusion pseudo-time for a spherical bubble</td>
<td>s</td>
</tr>
<tr>
<td>$\tau_{\text{Turb}}$</td>
<td>life-time of a large-scale eddy</td>
<td>s</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>quantity</td>
<td>-</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>column vector for $\Phi$</td>
<td>-</td>
</tr>
<tr>
<td>$\chi$</td>
<td>aspect ratio of bubble diameter ($=d_H/d_V$)</td>
<td>-</td>
</tr>
<tr>
<td>$\omega$</td>
<td>turbulent eddy frequency</td>
<td>s$^{-1}$</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>fluid domain</td>
<td>m$^3$</td>
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## Subscripts

<table>
<thead>
<tr>
<th>Subscript</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>c</td>
<td>continuous phase</td>
</tr>
<tr>
<td>collision</td>
<td>collision stress</td>
</tr>
<tr>
<td>d</td>
<td>disperse phase</td>
</tr>
<tr>
<td>di</td>
<td>disperse phase of velocity group $i$</td>
</tr>
<tr>
<td>D</td>
<td>drag force</td>
</tr>
<tr>
<td>f</td>
<td>surface center of the cell</td>
</tr>
<tr>
<td>in</td>
<td>inlet</td>
</tr>
<tr>
<td>k</td>
<td>phases (d for disperse phase; c for continuous phase)</td>
</tr>
<tr>
<td>L</td>
<td>shear-lift force</td>
</tr>
<tr>
<td>N</td>
<td>center of a cell which is a neighboring cell of the cell with its center at $P$</td>
</tr>
<tr>
<td>opt</td>
<td>optimized</td>
</tr>
<tr>
<td>$P$</td>
<td>the center of a cell</td>
</tr>
<tr>
<td>r</td>
<td>radial direction</td>
</tr>
<tr>
<td>VM</td>
<td>virtual mass force</td>
</tr>
<tr>
<td>WL</td>
<td>wall-lift force</td>
</tr>
<tr>
<td>x</td>
<td>$x$ axis direction</td>
</tr>
<tr>
<td>y</td>
<td>$y$ axis direction</td>
</tr>
<tr>
<td>z</td>
<td>$z$ axis direction</td>
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### Superscripts

<table>
<thead>
<tr>
<th>Superscript</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>axial</td>
<td>axial direction</td>
</tr>
<tr>
<td>D</td>
<td>drag force</td>
</tr>
<tr>
<td>exp</td>
<td>expected</td>
</tr>
<tr>
<td>inner</td>
<td>each side of the inner square</td>
</tr>
<tr>
<td>k</td>
<td>turbulent kinetic energy</td>
</tr>
<tr>
<td>L</td>
<td>shear-lift force</td>
</tr>
<tr>
<td>m</td>
<td>mass</td>
</tr>
<tr>
<td>max</td>
<td>maximum</td>
</tr>
<tr>
<td>n</td>
<td>new value</td>
</tr>
<tr>
<td>o</td>
<td>old value</td>
</tr>
<tr>
<td>outer</td>
<td>the side between the inner square and the outer circle</td>
</tr>
<tr>
<td>sol</td>
<td>solved</td>
</tr>
<tr>
<td>total</td>
<td>total number</td>
</tr>
<tr>
<td>TD</td>
<td>turbulent dispersion force</td>
</tr>
<tr>
<td>VM</td>
<td>virtual mass force</td>
</tr>
<tr>
<td>WC</td>
<td>wall-contact force</td>
</tr>
<tr>
<td>WL</td>
<td>wall-lift force</td>
</tr>
<tr>
<td>ε</td>
<td>turbulent eddy dissipation rate</td>
</tr>
<tr>
<td>ω</td>
<td>turbulent eddy frequency</td>
</tr>
<tr>
<td>*</td>
<td>predicted quantity</td>
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</tbody>
</table>

### Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNS</td>
<td>direct numerical simulation</td>
</tr>
<tr>
<td>E-E</td>
<td>Euler-Euler model</td>
</tr>
<tr>
<td>FEP</td>
<td>fluorinated ethylene-propylene resin</td>
</tr>
<tr>
<td>HZDR</td>
<td>Helmholtz-Zentrum Dresden-Rossendorf</td>
</tr>
<tr>
<td>LDV</td>
<td>laser Doppler velocimetry system</td>
</tr>
<tr>
<td>MUSIG</td>
<td>multiple size group</td>
</tr>
<tr>
<td>MULES</td>
<td>multidimensional limiting of fluxes</td>
</tr>
<tr>
<td>MTLoop</td>
<td>measurement test loop</td>
</tr>
<tr>
<td>OpenFOAM</td>
<td>open source field operation and manipulation</td>
</tr>
<tr>
<td>PCAM</td>
<td>particle-center-averaging method</td>
</tr>
<tr>
<td>PISO</td>
<td>pressure implicit with splitting of operator</td>
</tr>
</tbody>
</table>
1 Introduction

1.1 Challenges of the standard Euler-Euler model for simulation of disperse two-phase flow

Gas-liquid bubbly flows widely exist in our daily life. They occur in a kettle with boiling water or in a beer mug after the beer is poured into the mug. They are also frequently encountered in chemical engineering, energy production, oil and gas industries, and biotechnology. For example, they appear in a boiling water reactor core and the steam generators of a pressurized water reactor. In such flows, the gas and liquid are called phases. The dispersed gas phase is separated by the continuous liquid phase. Exploring the flow mechanisms of the two-phase flows can ensure safety and improve the efficiency of industrial facilities, but many of the flow mechanisms are still not well understood due to their high complexity. In general, experimental study and numerical simulation are two available ways to explore the flow mechanisms. Experimental investigations on bubbly flows face the difficulty in measuring the velocities and the distributions of the two phases. They are usually costly and time-consuming. In comparison, numerical simulation provides a more accessible way to study such flows. In the past years, with the development of computer technology, Euler-Euler model, Euler-Lagrange model and direct numerical simulation (DNS) became three major ways in bubbly flow simulations. Among these simulation methods, the Euler-Euler model, which is also called Eulerian two-fluid model, shows advantages for simulating bubbly flows up to industrial dimensions with an affordable computational cost. In the Euler-Euler model, two sets of conservation equations of mass, momentum, and energy are established for the continuous and the disperse phase. In the equations, some terms representing the interfacial interactions between the continuous and the disperse phase exist. These terms couple the two phases through jump conditions. The Euler-Euler model is widely used to simulate two-phase flows in steam generators, bubble columns, and the core of nuclear reactors (Zhao et al., 2021; Kumar et al., 2018; Rzehak et al., 2017; Hovi et al., 2016).
1.1.1 Inconsistency in bubble force models

In the Euler-Euler simulations of gas-liquid bubbly flows, the interface between the gas and the liquid is not resolved and the momentum interactions between the gas and the liquid depend on the closure models for the bubble forces. However, there is an inconsistency between the development and the usage of the bubble force models. These force models are usually developed by mechanistic modeling or DNS simulations (Shi et al., 2020; Lucas et al., 2007). They can also be correlations obtained from experimental data (Hessenkemper et al., 2021; Tomiyama et al., 2002; Hosokawa et al., 2002). The force developed by these methods is usually a resultant force for a single bubble that acts on the bubble’s center-of-mass. For example, a typical way to develop the bubble force model from experimental data is: First, the trajectory of the bubbles’ centers of mass is recorded by a high-speed camera in the experiment. The centroid of all pixels that belong to a bubble’s projection is regarded as the bubble’s center-of-mass (Zaruba et al., 2007). Second, an equation of bubble motion is used to calculate the trajectory of the bubbles’ centers of mass (Tomiyama et al., 2002; Hosokawa et al., 2002). The equation includes an assumed bubble force formulation with an unknown coefficient. At last, the coefficient is determined by making the calculated trajectories fit the measurement trajectories.

In comparison, in the standard Euler-Euler model, since the phase-averaging method is used to derive the averaged field equations, each bubble force turns to be a function of the local gas volume fraction. This transformation is achieved by (Ishii and Hibiki, 2011)

\[
\bar{f}_d = \alpha_d \bar{F}_B / \bar{V}_B, \tag{1.1}
\]

where \( \bar{f}_d \) is the force per unit control volume for the disperse phase used in the averaged momentum equation of the disperse phase, \( \alpha \) is the volume fraction, \( \bar{F}_B \) is the resultant force for a single bubble that acts on the bubble’s center-of-mass, and \( \bar{V}_B \) is the bubble volume. Here and in the following, an overbar ("\( \bar{\} \)") indicates the phase-averaged quantity, and the subscript \( d \) denotes a quantity for the disperse phase.

In Eq. (1.1), \( \alpha_d \) is defined by

\[
\alpha_d = \overline{X_d^b}, \tag{1.2}
\]

where \( X \) is the phase indicator function. The value of \( X_d \) is 1 when the disperse phase exists, otherwise, it is 0. The overbar and the superscript \( b \) here indicate the basic averaged quantity. Usually, the basic averaging method can be time-averaging, volume-averaging, or ensemble-averaging. The phase-averaging method is usually used to average the field equations together with a basic averaging method. If it is used together with the ensemble-averaging method, it is called ensemble phase-averaging. In general, the variable \( \alpha_d \) is interpreted as gas volume fraction, which is only exact when the volume-averaging is used as the basic averaging method. Whereas, if the basic averaging method is the time-averaging, \( \alpha_d \) should be interpreted as the time fraction for the occurrence of the disperse phase (Ishii and Hibiki, 2011). Moreover, if the basic averaging method is the ensemble-averaging, \( \alpha_d \)
1.1 Challenges of the standard Euler-Euler model for simulation of disperse two-phase flow

(a) Force is a function of local gas volume fraction

(b) Force acts on bubble center

Figure 1.1 Influence of bubble force treatments.

\( \alpha_d \) is the expected value of the ratio between the volume of the disperse phase and the total volume, in the limit that the total volume approaches zero (Drew and Passman, 1998). Physically, \( \alpha_d \) should be interpreted as the possibility of finding the disperse phase. In the following, \( \alpha_d \) is generally called gas volume fraction.

In bubbly flow simulations, if the bubble diameter is smaller than the computational cell size, the inconsistency between the development and the usage of the bubble force models should not cause any problems. However, to obtain more detailed information in the flow field, the cell size can be smaller than the bubble diameter in the simulations. This situation is allowed in the Euler-Euler model when the time-averaging or the ensemble-averaging is used as the basic averaging method. In this situation, the inconsistency in the bubble force models can lead to nonphysical gas over-concentration in the center or near the wall of a channel. This phenomenon can be found in the two-phase flow simulation results with the standard Euler-Euler model in Lehnigk (2020) and Tomiyama et al. (2006, 2003). The reason for the gas over-concentration in the channel center is shown in Fig. 1.1 (a). As each bubble force in the standard Euler-Euler model is a function of the local gas volume fraction, a radial bubble force appears on the cells that contain a non-zero gas volume fraction. Even if the bubble center is located on the centerline of the channel, where the resultant radial force of the bubble should be zero, the radial bubble force still exists in some cells. Under the effects of the force, more and more gas is concentrated in the channel center. A similar phenomenon can happen near the wall as well.
1.1.2 Bubble dimension and deformation

In reality, a bubble takes up some space in the fluid domain. In a clean air-water system, a bubble that has an equivalent diameter smaller than 1.3 mm can keep a spherical shape due to the surface tension effects (Jeong and Park, 2015). If the equivalent diameter of a bubble is larger than 1.3 mm, the bubble shape may change to be an ellipsoid or a spherical cap, depending on the bubble Reynolds number and the bubble size (Grace et al., 1976). Bubble dimension and deformation influence the distribution of the gas volume fraction. As the gas-liquid interface is not resolved in the standard Euler-Euler model, the effects of the bubble dimension and deformation are considered by the bubble force models. For example, the shear-lift force coefficient of Tomiyama et al. (2002) depends on the modified Eötvös number, which is related to the bubble deformation. Nevertheless, in bubbly flow simulations with the standard Euler-Euler model, the peak of the gas volume fraction can still be located on the wall. The closest distance between the peak and the wall should be around one bubble radius (Lubchenko et al., 2018). This indicates that the bubble dimension and deformation are not fully considered in the standard Euler-Euler model.

1.2 State of the art

1.2.1 Recovery of bubble force consistency

To recover the consistency of the bubble force models used in the standard Euler-Euler simulations, the force models should be employed in the same way as they are developed (Fig. 1.1 (b)). Therefore, in the disperse phase momentum equation, each bubble should be represented by a mass point so that the bubble forces can act on the bubbles’ centers of mass and influence the center-of-mass velocities.

A way to achieve this goal is that in the averaging process, each bubble is regarded as a whole and its properties are attached to its center. Such an averaging method has been proposed by some researchers before. Based on the volume-averaging method, Anderson and Jackson (1967) and Jackson (1997) proposed to introduce a particle phase average to average the quantities in which the particle should be regarded as a whole, such as the center-of-mass velocity. Similarly, in the 1990s, based on the ensemble-averaging method, Zhang and Prosperetti (1997, 1994a,b) and Prosperetti (1998) suggested using a particle averaging method to average the quantities for the disperse phase in which the global particle attributes are averaged directly. The basic idea of the particle phase average and the particle averaging method are the same. In this thesis, these two averaging methods are represented by the specific term “particle-center-averaging method (PCAM)”. When the PCAM is employed for the disperse phase, the disperse phase field equations are related to the particle number density. Whereas, the PCAM should not be used for the continuous phase since the liquid should not be regarded as a whole. The previous studies agreed that
the phase-averaging method should be used for the continuous phase. The detailed theory for the Euler-Euler framework based on PCAM, including the averaging methods and the averaged field equations, can be found in the previous studies. However, the treatment for the condition that the particle diameter is larger than the cell size was not mentioned. Afterward, Moraga et al. (2006) applied the Euler-Euler model based on PCAM to simulate wall-bounded bubbly flows. They interpreted the Euler-Euler model based on PCAM in a way that is similar to the standard Euler-Euler model. For example, similar to the phase indicator function, they introduced a bubble center-indicator function. Whereas, in their simulations, the influence of the disperse phase on the flow of the continuous phase was neglected.

Similar to the idea of PCAM, Lucas et al. (2007, 2001) developed a one-dimensional Euler-Euler solver that treats each bubble as a mass point. The bubbles’ centers of mass location are solved by the bubble force balance. The gas volume fraction is obtained by the convolution of the bubbles’ centers of mass location and the bubble dimension. A three-dimensional solver is needed to study bubbly flows comprehensively, but it has not been developed so far. Tomiyama et al. (2006, 2003) also proposed an Euler-Euler model assigning all the bubble volume to its center. A bubble number density is introduced in the solution. The gas volume fraction is solved by post-processing the solution of the bubble number density. The Euler-Euler model was applied to simulate the bubbly flows in a vertical pipe and a 4 × 4 rod bundle, and the simulation results agree well with the experimental data (Hayashi et al., 2014; Hosokawa and Tomiyama, 2009). However, the disperse phase momentum equation they used is not related to bubble number density and the turbulent dispersion force in the equation is still a function of the gas volume fraction. Therefore, the correction made by Tomiyama et al. (2006, 2003) to recover the consistency of the bubble force models is not comprehensive.

Overall, an Euler-Euler model for three-dimensional simulations recovering the consistency of the bubble force model and fully considering the bubble dimension and deformation has not been developed so far. Using the Euler-Euler framework based on PCAM has the potential to recover the consistency of the bubble force models. However, employing the Euler-Euler framework based on PCAM in bubbly flow simulations requires a way to convert the particle-center-averaged and the phase-averaged quantities for the condition that the bubble diameter is larger than the cell size.

### 1.2.2 Quantity conversion and consideration of bubble dimensions

In the Euler-Euler model based on PCAM, two different methods are used to average the solution variables for the disperse and the continuous phase, namely the PCAM and the phase-averaging method, respectively. Hence, a way to relate the particle-center-averaged and the phase-averaged quantities is needed. Bubble dimension and deformation information is included in the quantity transformations. In previous studies, a bubble shape
factor or a matrix that represents the fraction of the bubble volume inside a computational cell was used to calculate the gas volume fraction from the bubble number density (Lucas et al., 2007; Tomiyama et al., 2006, 2003). The shape factor or the matrix is determined by the bubble diameter, the cell size, and the bubble shape. This way to calculate the gas volume fraction is equivalent to a convolution method with a kernel function, and the shape factor or the matrix works like a kernel function. In bubbly flow simulations with an Euler-Lagrange method, a convolution method is used to transfer Lagrangian quantities to the Eulerian fields and vice versa (Lau et al., 2014, 2011; Bokkers et al., 2006; Darmana et al., 2006). The kernel function used in the convolution represents the influence of the Lagrangian quantities defined at the bubbles’ centers of mass on the Eulerian quantities in a certain influence region around the bubbles’ centers of mass and vice versa (Lau et al., 2014).

However, some difficulties exist in using the convolution method directly. On the one hand, it is complicated to deal with the kernel function near curved boundaries or corners of a domain where the boundaries meet non-orthogonally (Sun and Xiao, 2015a). On the other hand, the computational cost for employing the convolution method in three-dimensional bubbly flow simulations is high. In contrast, a diffusion-based coarse-graining algorithm proposed by Sun and Xiao (2015a) is theoretically equivalent to a convolution method with a Gaussian kernel function and it gives similar results as the convolution method by selecting a suitable diffusion pseudo-time. More importantly, this method requires less computational resources. Hence, in this thesis, the diffusion-based method is used to realize the Gaussian convolution method to convert the particle-center-averaged and the phase-averaged quantities.

For the quantity conversion with the diffusion-based method, bubble deformation can be considered by using anisotropic diffusion. To determine the diffusion tensor for the anisotropic diffusion, the theory of a diffusion tensor imaging method is employed. The method was used in the biomedical field to provide diffusion information in an anisotropic medium and its theory was well-developed (Kingsley, 2006; Basser, 1995). The relation between the diffusion tensor and the diffusion shape was explained in Basser (1995).

1.2.3 Numerical treatment of bubble forces

For an Euler-Euler solver which solves the field equations with a segregated solution procedure and an iterative method, some bubble forces are treated semi-implicitly to ensure the stability and the convergence of the solution (Rusche, 2002). In the Euler-Euler model based on PCAM, the bubble force of the disperse phase is the resultant force that acts on the bubbles’ centers of mass, while the force of the continuous phase is a function of the local gas volume fraction. To keep the forces consistent, a transform between the force of the disperse phase and the force of the continuous phase is required. Whereas, the semi-implicit numerical treatment of the bubble forces increases the difficulty for the transform.
1.3 Goal and outline of the thesis

First, this thesis aims to recover the consistency of the bubble force models for bubbly flow simulations. To realize this, a particle-center-averaged Euler-Euler approach is developed by combining the particle-center-averaged Eulerian framework and a Gaussian convolution method. Second, this thesis aims to reveal the nonphysical results caused by the inconsistency and illustrate the ability of the approach in improving the results. In this process, comparisons are made between the simulation results and measurement data for bubbly flows in different geometries. Third, this thesis aims to consider the bubble deformation in simulations and investigate its effects on the simulation results. The novelties of this work come from the following aspects: First, it forms a particle-center-averaged Euler-Euler approach for bubbly flow simulation. The approach makes it possible to use the PCAM in bubbly flow simulations where the bubble diameter can be larger than the cell size. The bubble dimension is fully considered in the approach. Second, a wall contact force for an oblate ellipsoidal bubble is developed to avoid the bubbles’ centers of mass coming nonphysically close to the wall. Third, correction terms for the drag and the virtual mass force of the continuous phase are proposed to keep the simulations stable and the forces between the disperse phase and the continuous phase consistent. Fourth, an anisotropic diffusion method is introduced to consider bubble deformation in the Euler-Euler simulations.

The remaining part of this thesis is organized as follows. Chapter 2 introduces the theoretical and the numerical methods of the standard Euler-Euler model and the Euler-Euler model based on PCAM. Besides, the test results for a simplified two-dimensional case are presented. Chapter 3 compares and analyzes the simulation results of both Euler-Euler models with the data obtained in the bubbly flow experiments in different vertical pipes. Comparisons of simulation results and the experimental data for the bubbly flows in a cylindrical bubble column are shown in Chapter 4. Chapter 5 investigates the bubble shape effects on the simulation results of bubbly pipe flows. The conclusions for this work and the potential directions for future study are given in Chapter 6.
2 Theoretical and numerical methods

This chapter introduces the theoretical and the numerical methods for the Euler-Euler model based on PCAM. For comparison, the averaging method, the field equations, and the bubble force treatment for the standard Euler-Euler model are also presented. Finally, a simplified two-dimensional test case is used to demonstrate the problems in the standard Euler-Euler model and illustrate the ability of the PCAM to remedy these problems.

Before introducing the field equations of the Euler-Euler models, it is necessary to clarify what kind of problem this thesis tries to solve. This thesis focuses on recovering the consistency of the bubble force models for bubbly flow simulations with the PCAM and validating as well as applying this method. In this study, both phases are taken as incompressible Newtonian fluids. To avoid introducing other uncertain and complicated factors, heat transfer, bubble swarm effects, as well as bubble coalescence and breakup are not involved. Furthermore, it is not necessary to consider the gas density change along with the axial height of a pipe or a bubble column caused by the change of the local pressure. The reason is that the bubble size distribution obtained in the experiment is applied in the simulation setup.

2.1 Local instantaneous conservation equations

The local conservation equations, which are used to derive the field equations for the Euler-Euler model, are introduced in this section. According to Drew and Passman (1998), the local instantaneous mass conservation equation for the gas or the liquid phase in Eulerian form states

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,
\]  
(2.1)
\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = \nabla \cdot \sigma + \rho g, \]  

(2.2)

where \( \sigma \) and \( g \) are the stress tensor and the acceleration of gravity, respectively.

For the incompressible Newtonian fluids considered in this study, the stress tensor can be divided into a pressure term and a viscous stress term by

\[ \sigma = -pI + S, \]  

(2.3)

where \( p \) is the pressure, \( I \) is a unit tensor, and \( S \) is the viscous stress tensor.

Substituting Eq. (2.3) into Eq. (2.2), we obtain

\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot S + \rho g. \]  

(2.4)

\[ \text{2.2 Averaging method} \]

In gas-liquid bubbly flows, a spatial point in the fluid domain can be occupied by the gas and the liquid consecutively. Modeling the local instantaneous characteristic of bubbly flows is challenging because of the discontinuity of the properties across the gas-liquid interface, the quantity fluctuations induced by the turbulence, and the interface motion (Ishii and Hibiki, 2011). Fortunately, for the design of some industrial facilities and processes, the detailed flow information which does not influence the mean flow is not necessary (Drew, 1983). The fundamental information for the mean fluid motion and properties can be obtained by applying a proper averaging method to the local instantaneous conservation equations to filter the interface information and some unimportant fluctuations. This is the purpose of using an averaging method in the Euler-Euler model.

As mentioned in the introduction, generally, the basic averaging method used to derive the averaged field equations for the Euler-Euler model is time-averaging, volume-averaging, or ensemble-averaging. There are some restrictions or assumptions for the separation scale when the time-averaging or the volume-averaging is applied. The time interval used in the time-averaging should be large enough to smooth out the unwanted fluctuations but small enough compared with the macroscopic time constant of the unsteadiness of bulk flow (Ishii and Hibiki, 2011). Similarly, according to Nigmatulin (1979), the characteristic linear dimensions of the volume used in the volume-averaging should be several times larger than the nonuniformities (e.g. bubble diameter), but it should be smaller than the characteristic macrodimension (e.g. pipe diameter). Whereas, for the ensemble-averaging, such restrictions or assumptions are not required. Therefore, in this thesis, the ensemble-averaging is used as the basic averaging method.
2.2 Averaging method

2.2.1 Ensemble phase-averaging

According to Prosperetti (1998), the ensemble phase-average of a quantity $\Phi$ for phase $k$ is defined by

$$\overline{\Phi}_k(x, t) = \frac{1}{\alpha_k(x, t)} \int_{C^N} \Phi_k(x, t; N) X_k(x; N) P(N; t) \, dC^N, \quad (2.5)$$

where $C^N$ describes the set of all possible dynamic states for a system containing $N$ indistinguishable bubbles and $P(N; t)$ is the probability density function of a dynamic state at time $t$. Note, the indistinguishable bubble probability is used here, so

$$\int_{C^N} P(N; t) \, dC^N = 1. \quad (2.6)$$

Hence, $N!$ does not appear in Eq. (2.5). In this thesis, “particle” and “bubble” are used interchangeably since the formalism is the same, but only applications for bubbly flows are considered.

2.2.2 Ensemble particle-center-averaging

The PCAM is suitable for averaging the quantities that concern each bubble as a whole, like a bubble’s center-of-mass velocity. Therefore, a Dirac delta function $\delta$ indicating the location of the bubble center is involved in the averaging. The ensemble particle-center-average of a quantity $\Phi$ is defined by (Prosperetti, 1998)

$$\langle \Phi_{(x, t)} \rangle = \frac{1}{n(x, t)} \int_{C^N} \left[ \sum_{b=1}^{N} \delta(x - y^b) \Phi_{b}(N, t) \right] P(N; t) \, dC^N, \quad (2.7)$$

where $n$ is the number density of the bubble centers, $x$ is a spatial coordinate vector, $\Phi_{b}$ is the value of the quantity $\Phi$ for bubble $b$ ($b = \{1, \ldots, N\}$), and $y^b$ is the coordinate vector of the center location for bubble $b$. Here and in the following, the notation $\langle \cdot \rangle$ indicates the particle-center-averaged quantity. The involved Dirac delta function has the following property:

$$\delta(x - y^b) = \begin{cases} \infty, & x = y^b; \\ 0, & \text{otherwise}. \end{cases} \quad (2.8)$$

The bubble number density is defined by

$$n(x, t) = \int P(x, u^b, t) \, du^b. \quad (2.9)$$

Here $u^b$ is the velocity vector for bubble $b$, which is bubble’s center-of-mass velocity vector, while $P(x, u^b, t)$ is the one-bubble probability density function, which is related to $P(N; t)$ as

$$P(x, u^b, t) = \int P(N; t) \, dC^{N-1}. \quad (2.10)$$
In addition, the relation
\[ \int_{\Omega} n d\Omega = N \] (2.11)
justifies that \( n \) is the bubble number density. Herein, \( \Omega \) is the fluid domain.

### 2.3 Field equations for the standard Euler-Euler model

According to Drew and Passman (1998), the averaged field equations for the standard Euler-Euler model are derived by applying the phase-averaging method to average the local instantaneous conservation equations. After averaging Eq. (2.1), we obtain the following averaged mass conservation equation

\[
\frac{\partial (a_k \rho_k)}{\partial t} + \nabla \cdot (a_k \rho_k u_k) = 0, \tag{2.12}
\]

where the subscript \( k \) indicates the phase that this quantity belongs to. In this thesis, \( \rho \) is a constant, so the averaging method for it is not necessary to be shown. After averaging Eq. (2.4), we obtain the averaged momentum equation

\[
\frac{\partial (a_k \rho_k u_k)}{\partial t} + \nabla \cdot (a_k \rho_k u_k u_k) = -a_c \nabla p_k + \nabla \cdot (a_k \mathbf{S}_k) + \nabla \cdot (a_k \mathbf{T}_k) + \mathbf{f}_k + a_k \rho_k \mathbf{g}, \tag{2.13}
\]

where \( \mathbf{T} \) is the Reynolds stress tensor.

### 2.4 Theory of the particle-center-averaged Euler-Euler model

#### 2.4.1 Field equations for monodisperse simulations

In bubbly flows, if the gas volume fraction is relatively small, the spatial distribution of the equivalent diameter for the bubbles in the system is quite uniform. Such flows are called monodisperse bubbly flows. For the simulations of these bubbly flows, the bubble size is represented by an averaged bubble diameter, which is called monodisperse assumption. The simulations based on this assumption are called monodisperse simulations. In the simulations, the averaged continuity equation of the continuous phase is the same as the standard Euler-Euler model

\[
\frac{\partial (a_c \rho_c)}{\partial t} + \nabla \cdot (a_c \rho_c u_c) = 0. \tag{2.14}
\]
2.4 Theory of the particle-center-averaged Euler-Euler model

Here and in the following, a subscript \(c\) denotes a quantity for the continuous phase. For the disperse phase, the averaged continuity equation becomes

\[
\frac{\partial (\beta_d \rho_d)}{\partial t} + \nabla \cdot (\beta_d \rho_d \langle u_d \rangle) = 0, \tag{2.15}
\]

where \(\beta_d\) is gas volume fraction projecting all the bubble volume to the bubbles’ centers of mass. It is calculated by

\[
\beta_d = n V_B. \tag{2.16}
\]

According to Prosperetti (1998), the averaged momentum equation of the continuous phase is derived by averaging the local instantaneous conservation equation of the continuous phase with the ensemble phase-averaging method. The resulting equation is

\[
\frac{\partial (\alpha_c \rho_c \langle u_c \rangle)}{\partial t} + \nabla \cdot (\alpha_c \rho_c \langle u_c \rangle \langle u_c \rangle) = \alpha_c \nabla \cdot \mathbf{S}_c + \nabla \cdot (\alpha_c \langle T_c \rangle) + \langle f_c \rangle + \alpha_c \rho_c \mathbf{g}, \tag{2.17}
\]

where \(\mathbf{S}_c\) is the surface stress tensor that originates from the non-uniform distribution of the pressure force on the surface of a bubble (Zhang and Prosperetti, 1994a). In this study, the surface stress tensor is neglected since no closure model for it is known in a bubbly flow. After substituting Eq. (2.3) into Eq. (2.17) and neglecting the surface stress tensor, we obtain

\[
\frac{\partial (\alpha_c \rho_c \langle u_c \rangle)}{\partial t} + \nabla \cdot (\alpha_c \rho_c \langle u_c \rangle \langle u_c \rangle) = -\alpha_c \nabla \cdot \mathbf{p}_c + \alpha_c \nabla \cdot \mathbf{S}_c + \nabla \cdot (\alpha_c \langle T_c \rangle) + \langle f_c \rangle + \alpha_c \rho_c \mathbf{g}. \tag{2.18}
\]

The momentum equation of the disperse phase is derived by averaging the following equation of motion for a bubble (Prosperetti, 1998; Zhang and Prosperetti, 1994a)

\[
m_B \frac{Du_d}{Dt} = \int_{S_B} \sigma_s n_s dS_B + m_B \mathbf{g}, \tag{2.19}
\]

where \(m_B\) is the bubble mass, \(S_B\) is the surface area of the bubble, and \(n_s\) is the unit normal vector directed outward from the bubble surface. Applying the ensemble particle-center-averaging to average Eq. (2.19), we have the resulting equation as

\[
\frac{\partial (\beta_d \rho_d \langle u_d \rangle)}{\partial t} + \nabla \cdot (\beta_d \rho_d \langle u_d \rangle \langle u_d \rangle) = \beta_d \nabla \cdot \mathbf{p}_c + \beta_d \nabla \cdot (\beta_d \langle T_d \rangle) + \nabla \cdot \mathbf{S}_c + \nabla \cdot (\beta_d \langle T_d \rangle) + \langle f_d \rangle + \beta_d \rho_d \mathbf{g}, \tag{2.20}
\]

where \(\mathbf{S}_c\) is the collision stress due to direct bubble-bubble interactions. In this study, the collision stress is neglected. Substituting Eq. (2.3) into Eq. (2.20) and neglecting the collision stress, the resulting equation is

\[
\frac{\partial (\beta_d \rho_d \langle u_d \rangle)}{\partial t} + \nabla \cdot (\beta_d \rho_d \langle u_d \rangle \langle u_d \rangle) = -\beta_d \nabla \cdot \mathbf{p}_c + \beta_d \nabla \cdot \mathbf{S}_c + \nabla \cdot (\beta_d \langle T_d \rangle) + \langle f_d \rangle + \beta_d \rho_d \mathbf{g}. \tag{2.21}
\]
2.4.2 Field equations for fixed polydisperse simulations

In bubbly flows, as the gas volume fraction increases, the probability of the bubble coalescence and breakup becomes high in the system. As a result, the bubble size spectrum in the flows covers a large range. Such flows are called polydisperse bubbly flows. In the simulations of such bubbly flows, the bubble size cannot be represented by a single averaged bubble diameter. The reason is that the magnitude and the direction of some bubble forces depend on the bubble size and shape. For example, the magnitude of drag, shear-lift, wall-lift, and turbulent dispersion force depends on the bubble diameter. The direction of the shear-lift force depends on the bubble deformation. For bubbly flows in a clean air-water system, the shear-lift force of the bubble with an equivalent diameter smaller than 5 mm is directed to the wall, while the force is directed to the pipe center for the bubble with an equivalent diameter larger than 6 mm.

To simulate the polydisperse bubbly flows with the Euler-Euler model, Lo (1996) suggested dividing the bubbles in the system into several size groups and applying a population balance model to calculate the bubble size change induced by the bubble coalescence and breakup. In this model, each bubble size group has its continuity equation, but all the bubble size groups share the same momentum equation, which means at the same location, bubbles with different sizes move with the same velocity. This model is called homogeneous multiple size group (MUSIG) model. However, since some bubble forces depend on the bubble diameter and deformation, more than one bubble velocity group should be used for the gas phase for the simulations of the polydisperse bubbly flows. Therefore, based on the idea of using multiple size groups, Krepper et al. (2008) proposed an inhomogeneous MUSIG model. In this model, multiple bubble velocity groups are used for the gas phase and each velocity group has its continuity and momentum equation. Each velocity group can be further divided into several bubble size groups to calculate the mass transfer induced by the bubble coalescence and breakup, the phase change, and the density change.

In this thesis, the simulations using the setup of a fixed bubble size distribution is called fixed polydisperse simulations. Mass transfer, bubble coalescence and breakup are not involved. Hence, it is not necessary to use more than one bubble size group for each bubble velocity group in the simulations. Under this condition, each bubble velocity group works like an independent gas phase. The field equations of the continuous phase are the same as those for monodisperse simulations. The continuity equation of each bubble velocity group is

\[
\frac{\partial (\beta_{di} \rho_{di})}{\partial t} + \nabla \cdot (\beta_{di} \rho_{di} \langle u_{di} \rangle) = 0, \quad (2.22)
\]

where \( i = \{1, \cdots, N_g\} \), and \( N_g \) is the number of the bubble velocity groups. Here and in the following, a subscript \( di \) denotes the quantity for the bubble velocity group \( i \). In Eq. (2.22), the gas volume fraction projecting all the bubble volume to the bubble centers for each bubble velocity group is

\[
\beta_{di} = n_{di} V_{Bi}, \quad (2.23)
\]
where $V_{Bi}$ is the representative volume of the bubble velocity group $i$. The total gas volume fraction is calculated by

\[ \alpha_d = \sum_{i=1}^{N_g} \alpha_{di}. \]  

(2.24)

The momentum equation of each bubble velocity group is

\[ \frac{\partial (\beta_{di} \rho_{di} \langle u_{di} \rangle)}{\partial t} + \nabla \cdot (\beta_{di} \rho_{di} \langle u_{di} \rangle \langle u_{di} \rangle) = -\beta_{di} \nabla p_c + \beta_{di} \nabla \cdot \mathbf{S}_c + \nabla \cdot (\beta_{di} \langle T_{di} \rangle) + \langle f_{di} \rangle + \beta_{di} \rho_{di} \mathbf{g}. \]  

(2.25)

### 2.4.3 Quantity conversion method

As discussed above, phase-averaging and particle-center-averaging are used to average the solution variables for the continuous and the disperse phase, respectively. When the bubble diameter is smaller than the cell size, the difference between phase-averaged and particle-center-averaged quantities is not significant (Prosperetti, 1998). In this condition, it is reasonable to assume that a phase-averaged quantity approximately equals the corresponding particle-center-averaged quantity (e.g. $\alpha_d \approx \beta_d$). However, when the bubble diameter is larger than the cell size, the difference between the quantities averaged by different methods becomes significant, and the assumption is not appropriate. Therefore, in the conversion of phase-averaged and particle-center-averaged quantities, a comprehensive way that can be used no matter the bubble diameter is larger than the cell size or not is needed.

In principle, this way could be established by convolution using a kernel function that represents the spatial extent of a single bubble (Lyu et al., 2020). Whereas, if the convolution is employed in three-dimensional simulations directly, it leads to a high computational cost. In contrast, a diffusion-based method, which is equivalent to the convolution method with a Gaussian kernel function, requires fewer computational resources. Therefore, the diffusion-based method is used here to realize the Gaussian convolution to relate phase-averaged and particle-center-averaged quantities. The bubble influence region, over which the diffusion takes place, may be larger than the actual bubble volume to comprise also the effects of bubble shape and path oscillations. In this subsection, the quantity conversion method for monodisperse simulations is introduced. This method is also applied to convert the quantities for each bubble velocity group for fixed polydisperse simulations.

To calculate a phase-averaged quantity from the corresponding particle-center-averaged quantity, the quantity in the bubbles’ centers of mass should be distributed. For example, to calculate the gas volume fraction from the bubble number density, the bubble volume is distributed around the bubbles’ centers of mass by solving the following diffusion equation

\[ \frac{\partial a_d}{\partial t} - \nabla \cdot (C_{diff} \nabla a_d) = 0, \]  

(2.26)
with an initial condition of \( a_d(x_0, 0) = \beta_d(x_0) \). Herein, \( x_0 \) is a spatial coordinate vector. During the diffusion process, the bubble volume is conserved. In Eq. (2.26), \( \tau \) is the diffusion pseudo-time and \( C_{\text{diff}} \) is the diffusion coefficient, both determining the size of the bubble influence region. Note, the diffusion process takes place at every time step of the simulation such that \( \tau \) is unrelated to the physical time, and, hence, referred to as a pseudo-time. In the present study, \( C_{\text{diff}} \) is set to be \( 1 \, \text{m}^2 \, \text{s}^{-1} \) for all diffusion processes for the spherical bubbles. An optimized value is determined for \( \tau \) in Subsection 2.4.4. With the determined \( C_{\text{diff}} \) and the optimized \( \tau \), the diffusion process is optimized. Under the condition that the bubble deformation exists, \( C_{\text{diff}} \) becomes a tensor. The detailed information of the diffusion tensor for deformed bubbles is given in Subsection 2.4.5. To solve Eq. (2.26), a Neumann boundary condition with the derivative equal to zero is used for all boundaries. According to Haberman (2012), the solution of Eq. (2.26) in three-dimensional space is

\[
a_d(x, \tau) = \int_{\Omega} \beta_d(x_0) \frac{1}{(4\pi C_{\text{diff}} \tau)^{3/2}} \exp\left(-\frac{(x-x_0)^2}{4 C_{\text{diff}} \tau}\right) \, dx_0. \quad (2.27)
\]

Equation (2.27) shows that the diffusion-based method is equivalent to the convolution method with a Gaussian kernel function.

Similarly, to calculate a phase-averaged gas velocity \( \bar{u}_d \), the bubble momentum is distributed about the bubbles’ centers of mass by the following diffusion equation

\[
\frac{\partial(a_d \bar{u}_d)}{\partial \tau} - \nabla \cdot [C_{\text{diff}} \nabla (a_d \bar{u}_d)] = 0, \quad (2.28)
\]

with an initial condition of \( a_d(x_0, 0) \, \bar{u}_d(x_0, 0) = \beta_d(x_0) \langle \bar{u}_d \rangle (x_0) \). Other settings are as described above.

The forces acting on the bubble’s centers of mass are distributed to the bubble influence region by the following diffusion equation

\[
\frac{\partial \bar{f}_d}{\partial \tau} - \nabla \cdot (C_{\text{diff}} \nabla \bar{f}_d) = 0, \quad (2.29)
\]

with an initial condition of \( \bar{f}_d(x_0, 0) = \langle \bar{f}_d \rangle (x_0) \). At last, the forces acting on the continuous phase can be calculated by

\[
\bar{f}_c = -\bar{f}_d. \quad (2.30)
\]

For fixed polydisperse simulations, Eq. (2.30) is changed to be

\[
\bar{f}_c = -\sum_{i=1}^{N_g} \bar{f}_{di}. \quad (2.31)
\]

On the contrary, the continuous phase velocity at the bubbles’ centers of mass \( \langle \bar{u}_c \rangle \) can be calculated from the corresponding phase-averaged velocity of the continuous phase \( \bar{u}_c \).
2.4 Theory of the particle-center-averaged Euler-Euler model

with the following Gaussian convolution

$$\langle u_c \rangle (x_0, t) = \int_{\Omega} \overline{u_c}(x) \frac{1}{(4\pi C_{\text{diff}} t)^{\frac{3}{2}}} \exp \left\{ -\frac{(x_0 - x)^2}{4C_{\text{diff}} t} \right\} \, dx.$$  (2.32)

Equation (2.32) is the solution of the following equation in three-dimensional space

$$\frac{\partial \langle u_c \rangle}{\partial t} - \nabla \cdot (C_{\text{diff}} \nabla \langle u_c \rangle) = 0,$$  (2.33)

with an initial condition of $$\langle u_c \rangle (x, 0) = \overline{u_c}(x).$$

2.4.4 Diffusion pseudo-time optimization

A key parameter in the quantity conversion method with the diffusion-based method is the diffusion pseudo-time $$\tau.$$ The diffusion pseudo-time is independent of the physical time. It affects the size of the bubble influence region. The size of the bubble or particle influence region in the convolution or the diffusion-based method is still an open question. Deen et al. (2004) and Darmana et al. (2006) set the size to be 3 times the averaged bubble diameter, while Bokkers et al. (2006) and Lau et al. (2011) set it to be 6 and 2 times the averaged bubble diameter, respectively. Sun and Xiao (2015b) argued that the size should approximately equal the size of the particle wake. Since no agreement on the size of the influence region is found in the literature, this subsection aims to optimize the diffusion pseudo-time by minimizing the difference between expected and numerically computed gas volume fractions in a simplified one-dimensional case.

For a layer of equally sized and spherical bubbles slides on a wall, Lubchenko et al. (2018) derived a fixed profile for the gas volume fraction near the wall in the direction that is perpendicular to the wall. This profile can be used as the expected gas volume fraction for a one-dimensional case where a stream of spherical bubbles is injected at the location $$x = x_c.$$ Hence, the expected gas volume fraction reads

$$\alpha_d^{\text{exp}}(x) = \begin{cases} \alpha_d^{\text{max}} - 4\alpha_d^{\text{max}} (x - x_c)^2 / d_B^2, & |x - x_c| \leq d_B; \\ 0, & |x - x_c| > d_B. \end{cases}$$  (2.34)

Herein, $$x$$ is the spatial coordinate, $$\alpha_d^{\text{max}}$$ is the maximum gas volume fraction, and $$d_B$$ is the bubble diameter. The solved gas volume fraction is obtained by solving Eq. (2.26) in one dimension. According to Haberman (2012), the solution is

$$\alpha_d(x, t) = \int_D \beta_d(x_0) \frac{1}{\sqrt{4\pi C_{\text{diff}} t}} \exp \left\{ -\frac{(x - x_0)^2}{4C_{\text{diff}} t} \right\} \, dx_0.$$  (2.35)

In the one-dimensional case considered here, the initial bubble number density is concentrated only in the center computational cell. Consequently, the solved gas volume fraction
Figure 2.1 Sketch of gas volume fraction distribution for the one-dimensional case.

can be discretized as

\[
\alpha_{d}^{\text{sol}}(x, \tau) \approx \beta_{d}(x_{c}) \frac{1}{\sqrt{4\pi C_{\text{diff}} \tau}} \exp \left\{ -\frac{(x - x_{c})^{2}}{4C_{\text{diff}} \tau} \right\} \Delta_c, \tag{2.36}
\]

where \(\Delta_c\) is the spacing of the center computational cell.

Figure 2.1 shows the sketch of the expected and the solved gas volume fraction distribution for the one-dimensional case. In the comparison of the expected and the solved gas volume fractions, the gas volume is kept the same by setting

\[
\beta_{d}(x_{c}, 0) = \sum_{i=1}^{M} \alpha_{d}^{\text{exp}}(x_{i}) \frac{V_{i}}{V_{c}}, \tag{2.37}
\]

where \(x_{i}\) is the spatial coordinate of the computational cell \(i\) which is covered by the bubbles, \(M\) is the number of cells covered by the bubbles, while \(V_{i}\) and \(V_{c}\) are the volumes of the computational cells \(i\) and \(c\), respectively. The optimized diffusion pseudo-time is the time for the following error to reach its minimum value

\[
E(\tau) = \sum_{i=1}^{M} \left[ \alpha_{d}^{\text{exp}}(x_{i}) - \alpha_{d}^{\text{sol}}(x_{i}, \tau) \right]^{2}, \tag{2.38}
\]

where \(x_{i} \in (x_{c} \pm 0.5d_{B})\).

In Eq. (2.38), the discretized form of \(\alpha_{d}^{\text{exp}}\) and \(\alpha_{d}^{\text{sol}}\) are used. The influence of the parameter \(M\), which is used in the discretization, on the optimized diffusion pseudo-time should be analyzed. Since the optimized diffusion pseudo-time \(\tau_{\text{opt}}\) depends on \(C_{\text{diff}}\) as well as \(d_{B}\), a dimensionless optimized diffusion pseudo-time

\[
\tilde{\tau}_{\text{opt}} = \frac{\tau_{\text{opt}} C_{\text{diff}}}{d_{B}^{2}} \tag{2.39}
\]
is used in the analysis. The dependency of $\tilde{\tau}_{\text{opt}}$ on $M$ is shown in Fig. 2.2. As can be seen, $\tilde{\tau}_{\text{opt}}$ is almost a constant when $M$ is larger than 30. Hence, $\tilde{\tau}_{\text{opt}} = 0.03356$ is used in the following simulations. With the optimized diffusion pseudo-time, the distributions of the expected and the solved gas volume fractions for the one-dimensional case can be seen in Fig. 2.3. For this optimally solved gas volume fraction, 94.72% of the gas volume is contained within $x_c \pm 0.5d_B$.

**Figure 2.2** Dimensionless optimized diffusion pseudo-time dependency on $M$.

**Figure 2.3** Expected and optimally solved gas volume fraction for the one-dimensional case.
2.4.5 Treatment of bubble deformation

If the diffusion coefficient $C_{\text{diff}}$ is set to be $1 \text{ m}^2 \text{s}^{-1}$ in the quantity conversion with the diffusion-based method in three-dimensional space, the diffusion coefficient in the $x$, $y$ and $z$ axis direction will be $1 \text{ m}^2 \text{s}^{-1}$. In this condition, the diffusion is isotropic. As a result, the isosurface (or the isoline) of the diffused gas volume fraction of a single bubble forms a sphere (or a circle). This is suitable for spherical bubbles. Whereas, when the bubble diameter is relatively large, the bubble shape can deviate from a spherical shape (Grace et al., 1976), which is shown in Fig. 2.4.

In a clean air-water system, when the equivalent bubble diameter is larger than 1.3 mm, the bubble shape usually changes to be oblate ellipsoidal with its minor axis along the main flow direction (Jeong and Park, 2015). To determine the shape of such an oblate ellipsoid, the ratio between the major and the minor axis should be known. Based on the measurement projections for the liquid drops in experiments, Wellek et al. (1966) proposed an aspect ratio model for oblate ellipsoidal liquid drops, which is suitable for the contaminated systems (Hessenkemper et al., 2021; Lucas et al., 2020). Similarly, based on the measurements in a clean air-water system, Ziegenhein and Lucas (2019) and Hayashi et al. (2021) developed an aspect ratio model for oblate ellipsoidal bubbles, consecutively. For an air-water system, when the bubbles have a size of several millimeters, the system can be regarded as a clean system. This is the situation for the experimental cases used for the validations of the Euler-Euler model based on PCAM in the following chapters. Therefore, in this thesis, the model proposed by Ziegenhein and Lucas (2019) is used to describe the shape of deformed bubbles. This model has the following form:

$$\chi = 1 + 0.65 Eo^{0.35}, \quad (2.40)$$

where $\chi$ is the aspect ratio, and $\chi = d_H/d_V$. Herein, $d_H$ and $d_V$ are the horizontal (major) and the vertical (minor) axis of the oblate ellipsoidal bubbles, respectively. In the model, $Eo$ is the Eötvös number which is defined by

$$Eo = \frac{\Delta \rho |\mathbf{g}| d_H^2}{\sigma}, \quad (2.41)$$

where $\Delta \rho = \rho_c - \rho_d$, $\sigma$ is the surface tension coefficient and $|\mathbf{g}|$ is the norm of $\mathbf{g}$.

To consider bubble deformation, the diffusion of the bubble volume from the bubbles' cen-
ters of mass should be anisotropic. As a result, the diffusion coefficient becomes a tensor. In the following, the theory of a diffusion tensor imaging method is used to relate the diffusion tensor and the bubble shape. In three-dimensional space, all the gas molecules of a single bubble are put in the bubble’s center-of-mass location \( (x = 0) \) at the initial time of the diffusion process. After the gas molecules diffuse for a certain time \( \tau \), the displacement distribution of the gas molecules can be expressed as (Basser, 1995)

\[
P(x, \tau) = \frac{1}{\sqrt{|D|(4\pi \tau)^3}} \exp \left( -\frac{x^T D^{-1} x}{4\tau} \right).
\]  

(2.42)

Herein, \( P(x, \tau) \) is the probability of finding a gas molecule at the position \( x \) after diffusing for a certain time \( \tau \). In Eq. (2.42), \( D \) is the diffusion tensor and \( |D| \) is the determinant of \( D \). The tensor is symmetric, so it is determined by 6 components

\[
D = \begin{pmatrix}
D_{xx} & D_{xy} & D_{xz} \\
D_{xy} & D_{yy} & D_{yz} \\
D_{xz} & D_{yz} & D_{zz}
\end{pmatrix}
\]  

(2.43)

By setting the exponent part of Eq. (2.42) to a constant, Basser (1995) derived the expression for an isosurface of the probability \( P(x, \tau) \) as

\[
(D_{yy}D_{zz} - D_{xz}^2)x^2 + 2(D_{xz}D_{yz})xy + (D_{xx}D_{zz} - D_{xy}^2)y^2 + 2(D_{xy}D_{yz} - D_{xz}D_{yy})xz + 2(D_{xy}D_{xz} - D_{xx}D_{yy})yz + (D_{xx}D_{yy} - D_{xx}^2)z^2 = |D| \tau.
\]  

(2.44)

This surface can form an ellipsoid or a sphere, depending on the diffusion tensor components. For isotropic diffusion, it is a sphere, which is called “diffusion sphere”. Whereas, for anisotropic diffusion, it is an ellipsoid, which is called “diffusion ellipsoid”.

In the following, the relation between the diffusion ellipsoid and the oblate ellipsoidal bubble is established to determine the diffusion tensor for the bubble. The diffusion ellipsoid should have a similar shape as the deformed bubble and its center should be located at the bubble’s center-of-mass. Besides, it should have the same orientation as the bubble. Therefore, the diffusion ellipsoid should also be an oblate ellipsoid and its aspect ratio should equal the bubble’s aspect ratio. If the axes of the oblate ellipsoidal bubble are aligned with the axes of the laboratory frame of reference \( (x, y, z) \), only the diagonal components of \( D \) are non-zero. In this condition, \( |D| = D_{xx}D_{yy}D_{zz} \), and Eq. (2.44) can be simplified into

\[
\frac{x^2}{D_{xx} \tau} + \frac{y^2}{D_{yy} \tau} + \frac{z^2}{D_{zz} \tau} = 1.
\]  

(2.45)

If we assume the minor axis of the oblate ellipsoid along the main flow direction \( (z \text{ axis}) \), we obtain

\[
\sqrt{D_{xx} \tau} = \sqrt{D_{yy} \tau},
\]  

(2.46)
and

\[ \chi = \frac{\sqrt{D_{xx} \tau}}{\sqrt{D_{zz} \tau}} \]  

After simplifying Eqs. (2.46) and (2.47), we obtain

\[ D_{xx} = D_{yy}, \]  

and

\[ D_{xx} = \chi^2 D_{zz}. \]  

The volume of the diffusion ellipsoid is

\[ V_e = \frac{4}{3} \pi \sqrt{D_{xx} D_{yy} D_{zz} \tau_{opt,e}^3}, \]  

where \( \tau_{opt,e} \) is the optimized diffusion pseudo-time for the oblate ellipsoidal bubbles. The isotropic diffusion can be regarded as a special condition for anisotropic diffusion. The diffusion coefficient for the spherical bubbles (\( C_{diff} \)) is 1 \( m^2 s^{-1} \), which is equivalent to setting the diffusion tensor to be

\[ D_s = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \]  

Herein, \( D_s \) is the diffusion tensor for the spherical bubbles. The optimized diffusion pseudo-time for the spherical bubble (\( \tau_{opt,s} \)) is determined by Eq. (2.39). In this condition, the radius of the diffusion sphere is

\[ R_s = \sqrt{\tau_{opt,s}}. \]  

Hence, the volume of this diffusion sphere is

\[ V_s = \frac{4}{3} \pi R_s^3. \]  

During the bubble deformation, if the pressure change inside the bubble is not considered, the bubble volume will be constant. Therefore, the volume of the diffusion ellipsoid equals the volume of the diffusion sphere:

\[ V_e = V_s. \]  

Substituting Eqs. (2.50), (2.52), and (2.53) into Eq. (2.54) and simplifying the resulting equation, we have

\[ \sqrt{D_{xx} D_{yy} D_{zz} \tau_{opt,e}^3} = \tau_{opt,s}^{\frac{3}{2}}. \]  

If we keep \( \tau_{opt,e} = \tau_{opt,s} \), we obtain

\[ D_{xx} D_{yy} D_{zz} = 1. \]  

Based on Eqs. (2.48), (2.49), and (2.56), we derive the component of the diffusion tensor
2.4 Theory of the particle-center-averaged Euler-Euler model

for the oblate ellipsoidal bubbles as

\[ D_{xx} = D_{yy} = \chi^2, \]  

(2.57)

and

\[ D_{zz} = \chi^{-\frac{4}{3}}. \]  

(2.58)

For the simulations of bubbly pipe flows in the following chapters, a wedge computational domain is used because the flow in the location where the simulation results are compared with the experimental data is almost circumferentially symmetric. A quasi-two-dimensional mesh is used for the wedge computational domain. In this condition, the diffusion only appears in the radial and the axial direction, so it is two-dimensional. Therefore, Eq. (2.42) is changed to be (Painter and Hillen, 2013)

\[ P(x, \tau) = \frac{1}{4\pi \tau \sqrt{|D|}} \exp \left( -\frac{x^T D^{-1} x}{4\tau} \right). \]  

(2.59)

If we assume that the x-axis and the z-axis of the Cartesian coordinate system coincide with the radial and the axial direction of the computational domain, respectively, we obtain the diffusion tensor for the oblate ellipsoidal bubble as

\[ D = \begin{pmatrix} D_{xx} & 0 \\ 0 & D_{zz} \end{pmatrix}. \]  

(2.60)

In this condition, the isoline of the probability \( P(x, \tau) \) forms a circle with isotropic diffusion or forms an ellipse with anisotropic diffusion. Following a similar procedure as the three-dimensional case, we obtain the equation for a diffusion ellipse as

\[ \frac{x^2}{D_{xx}\tau} + \frac{z^2}{D_{zz}\tau} = 1. \]  

(2.61)

In this ellipse, the ratio between the major and the minor axis should equal \( \chi \). Therefore, the relation between \( D_{xx} \) and \( D_{zz} \) fits Eq. (2.49), which is the first constraint for the diffusion tensor.

In the two-dimensional diffusion, the area of the diffusion circle and the diffusion ellipse should be the same. The radius of the diffusion circle is \( R_c = \sqrt{\tau_{opt,s}} \). Therefore, the second constraint for the diffusion tensor is

\[ \sqrt{D_{xx}D_{zz}\tau_{opt,e}} = \tau_{opt,s}. \]  

(2.62)

Similar to three-dimensional condition, by keeping \( \tau_{opt,e} = \tau_{opt,s} \), we obtain

\[ D_{xx}D_{zz} = 1. \]  

(2.63)

Basing on Eqs. (2.49) and (2.63), we have \( D_{xx} = \chi \) and \( D_{zz} = \chi^{-1} \).
The calculated diffusion tensors for the three-dimensional and the two-dimensional condition are different because the second constraints used to calculate diffusion tensor in both conditions (Eq. (2.55) for a three-dimensional case and Eq. (2.62) for a two-dimensional case) are various. Therefore, when applying the theory, the diffusion tensor should be chosen based on the simulation condition.

2.5 Bubble force models

As mentioned before, closure models for bubble forces and turbulence are required in the Euler-Euler simulations because the gas-liquid interface is not resolved and an averaging method is applied to derive the field equations. The closure models for two-phase turbulence are introduced in Rzehak et al. (2017). This section introduces the bubble force models.

For the standard Euler-Euler model, the momentum interactions between the disperse and the continuous phase are usually assumed to be represented by a linear combination of some bubble forces (Ishii and Hibiki, 2011). The bubble forces typically include drag force, shear-lift force, virtual mass force, turbulent dispersion force, and wall-lift force (Rzehak et al., 2017). Moreover, for the Euler-Euler model based on PCAM, an additional wall-contact force has to be introduced to prevent the bubbles' centers of mass from coming nonphysically close to the wall.

**Drag force**

The drag force originates from the relative motion between a bubble and the surrounding liquid. It is the resistance to the bubble motion. According to Ishii and Zuber (1979), the drag force for a bubble is

\[
F_D^B = -\frac{\pi d_B^2}{8} C_D \rho_c \left| u_d - u_c \right| (u_d - u_c),
\]  

(2.64)

where \(C_D\) is the drag coefficient. Here and in the following, the averaging method for the quantities in the force of a single bubble is not specified because it depends on which Euler-Euler model the force is applied to.

**Shear-lift force and wall damping**

For a bubble moving in an unbounded shear flow, a shear-lift force appears. It is perpendicular to the direction of the bubble motion. The shear-lift force of a single bubble has the following form (Zun, 1980)

\[
F_L^B = -C_L V_B \rho_c (u_d - u_c) \times \nabla \times u_c.
\]  

(2.65)

Herein, \(C_L\) is the lift coefficient.
2.5 Bubble force models

In bubbly flow simulations with OpenFOAM (open source field operation and manipulation) by the standard Euler-Euler model, the shear-lift force is usually damped in the near-wall region. The reason comes from two aspects: On the one hand, in theory, the shear-lift force is influenced by the wall in the near-wall region. As a result, the force gradually decreases as the wall distance decreases and becomes zero on the wall (Takemura et al., 2009). The shear-lift force in the DNS results of Thomas et al. (2015) also supported this theory. Therefore, applying such a wall damping is a way to consider the wall effects on the shear-lift force in simulations (Shaver and Podowski, 2015). On the other hand, Li et al. (2019) pointed out that for bubbly flow simulations with OpenFOAM by the standard Euler-Euler model, even if a wall-lift force is employed to take into account the wall effects, the gas volume fraction can still be located on the wall if the shear-lift force is not damped near the wall. The reason is that near the wall, the gradient of the liquid velocity is relatively high.

In the present study, the following damping factor is applied to damp the shear-lift force in the region where the distance from the wall is smaller than the bubble diameter to obtain reasonable simulation results for the standard Euler-Euler model:

\[
\lambda = 0.5 - 0.5 \times \cos \left( \min \left( \frac{L}{d_B}, 1 \right) \pi \right),
\]

where \( \lambda \) is the damping factor. To compare the simulation results between the standard Euler-Euler model and the Euler-Euler model based on PCAM, such damping is also applied for the shear-lift force in the Euler-Euler model based on PCAM.

Virtual mass force

For a bubble moving in water, the change of the bubble velocity affects the motion of the surrounding water. For example, if the bubble accelerates, it will induce water motion behind it. This effect is expressed by the virtual mass force

\[
F_{VM}^B = -C_{VM} \rho_c \left( D_t u_d - D_t u_c \right),
\]

where \( C_{VM} \) is the virtual mass coefficient.

Turbulent dispersion force

Liquid turbulence influences the bubble motion, which is modeled by the turbulent dispersion force. Burns et al. (2004) proposed the following turbulent dispersion force model by applying Favre-averaging to the phase-averaged drag force

\[
\bar{f}_{TD} = -3 \alpha_d \rho_c \left( \nabla \frac{\nu^{\text{turb}}_c}{\sigma_{ac}} \left( \nabla \frac{\alpha_d}{\alpha_d} - \nabla \frac{\alpha_c}{\alpha_c} \right) \right),
\]

where \( \nu^{\text{turb}}_c \) is the turbulent eddy viscosity and \( \sigma_{ac} \) is the Schmidt number. The Schmidt number is typically set to be 0.9 and used in the following simulations (Rzehak et al., 2017).
Equation (2.68) is suitable for the standard Euler-Euler simulation because the first averaging method for the drag force is the phase-averaging. Based on the derivation procedure in Burns et al. (2004), a turbulent dispersion force model for the Euler-Euler model based on PCAM is developed (Appendix A.1). The resulting model is

$$\langle f_{d}^{TD} \rangle = \frac{3\beta_{d}}{4d_{B}} C_{D} \rho_{c} \langle (u_{d}) - \langle u_{c} \rangle \rangle \left( \frac{\nu_{turb}^{\beta_{d}}}{\sigma_{ac}} \right) \left( \nabla \beta_{d} - \nabla a_{c} \right). \quad (2.69)$$

Wall-lift force

A bubble moving in a static liquid near the wall experiences a force perpendicular to its motion direction. This force is referred to as wall-lift force and described by

$$F_{B}^{WL} = \frac{1}{3} \pi d_{B}^{2} C_{WL} \rho_{c} |u_{d} - u_{c}|^{2} n_{w}. \quad (2.70)$$

Herein, $C_{WL}$ is the wall-lift coefficient and $n_{w}$ is the unit wall-normal vector pointing into the fluid.

Wall-contact force

The wall-contact force model proposed by Lucas et al. (2007) is adapted for bubbles with an oblate ellipsoidal shape and used in the Euler-Euler simulations based on PCAM, which is shown in Appendix A.2. The resulting wall-contact force of a single bubble reads

$$F_{B}^{WC} = \pi d_{B} \sigma \left[ \frac{1}{L^{2}} - \frac{3\tilde{L}}{2G} \left( \left( \frac{4\sqrt{G}}{3} + \frac{\tilde{L}^{3}}{\sqrt{G}} \right) \arctanh \left( \sqrt{G} \right) - 1 \right) \right] n_{w}, \quad (2.71)$$

where $\tilde{L} = 2L/d_{B}$, $G = 1 - \tilde{L}^{3}$, and $L$ is the distance between the bubble’s center-of-mass and the wall.

2.6 Turbulence modeling

For bubbly flows, due to the small spatial scales of the disperse phase, it suffices to consider the turbulence of the continuous phase (Rzehak et al., 2017). The turbulence in bubbly flows is described by an SST model (Menter, 2009). The effects of bubble-induced turbulence are considered as source terms in the model. The SST model is a two-equation model. It blends the equations for the turbulent eddy frequency $\omega$ and the turbulent eddy dissipation rate $\varepsilon$. It combines the advantages of the $k - \varepsilon$ model away from the solid wall and the $k - \omega$ model inside the boundary layer.
The formulations for this model are
\[
\frac{\partial (\alpha_c \rho_c k_c)}{\partial t} + \nabla \cdot (\alpha_c \rho_c \mathbf{u}_c k_c) = \nabla \cdot \left( \alpha_c \left( \mu_c + \alpha_k \mu_{\text{turb}} \right) \nabla k_c \right) + \alpha_c \left( \rho_c - C \rho_c \omega_c k_c \right) + S_k, \tag{2.72}
\]
and
\[
\frac{\partial (\alpha_c \rho_c \omega_c)}{\partial t} + \nabla \cdot (\alpha_c \rho_c \mathbf{u}_c \omega_c) = \nabla \cdot \left( \alpha_c \left( \mu_c + \alpha_\omega \mu_{\text{turb}} \right) \nabla \omega_c \right) + \alpha_c \left( \frac{\rho_c P_k}{\mu_{\text{turb}}} - C \omega_0 \rho_c \omega_c^2 \right) + 2 \alpha_c \sigma_\omega \rho_c (1 - F_1) \frac{\nabla k_c \cdot \nabla \omega_c}{\omega_c} + S_\omega. \tag{2.73}
\]
Herein, \(S_k\) and \(S_\omega\) are the source terms, while \(F_1\) is the blending function. It assumes a value of one for the \(k-\omega\) model and zero for the \(k-\epsilon\) model. The model constant \(\sigma_k\) is calculated by interpolation between the value of the \(k-\omega\) model (with an index “1”) and the value of the \(k-\epsilon\) model (with an index “2”) using \(F_1\) as
\[
\sigma_k = F_1 \sigma_{k,1} + (1 - F_1) \sigma_{k,2}. \tag{2.74}
\]
This way is also used to calculate the other model constants \(C_\mu, \sigma_\omega, C_{\omega_P}\) and \(C_{\omega_D}\).

In Eqs. (2.72) and (2.73), \(P_k\) is the production term. It is calculated by
\[
P_k = \min \left( \tilde{P}_k, 10 C_\mu \rho_c \omega_c k_c \right),
\]
where \(\tilde{P}_k = 2 \mu_{\text{turb}} S_c : \nabla \mathbf{u}_c\) and \(S_c = \frac{1}{2} \left( \nabla \mathbf{u}_c + (\nabla \mathbf{u}_c)^T \right)\). The turbulent dynamic viscosity is calculated by
\[
\mu_{\text{turb}} = \frac{\rho_c k_c}{\max (\omega_c, C_\gamma F_2)} \tag{2.76}
\]
Herein, \(C_\gamma = 1/0.31\) is a model constant, \(F_2\) is another blending function, and \(\gamma = \sqrt{2S_c} : \mathbf{S}_c\).

For detailed information of the blending functions, the reader is referred to Menter (2009).

The bubble-induced turbulence is included in Eqs. (2.72) and (2.73) by the source terms. According to Ma et al. (2017), the total energy input from a bubble equals the work done by the buoyancy force acting on the bubble. For the steady state, the buoyancy force balances the drag force. Therefore, the total energy input from the bubble can be computed as
\[
F_d^D \mathbf{u}_d = F_d^D \mathbf{u}_c + F_d^D (\mathbf{u}_d - \mathbf{u}_c) \tag{2.77}
\]
The contribution \(F_d^D \mathbf{u}_d\) drives the mean flow, while the contribution \(F_d^D (\mathbf{u}_d - \mathbf{u}_c)\) indicates the energy converted into turbulence. Therefore, the source term for the \(k\) equation (Eq. (2.72)) is
\[
S_k^D = \min \left( 0.18 \frac{\text{Re}_B^{0.23}}{\text{Re}_B}, 1 \right) F_d^D (\mathbf{u}_d - \mathbf{u}_c), \tag{2.78}
\]
where \(\text{Re}_B = \rho_c |\mathbf{u}_d - \mathbf{u}_c| d_B / \mu_c\) is the bubble Reynolds number. The source term for \(\epsilon\) is modeled as
\[
S_\epsilon^D = 0.3 C_D \frac{S_k^D}{\tau_{\text{turb}}}. \tag{2.79}
\]
Herein, $\tau_{\text{turb}}$ is the life-time of a large-scale eddy. The source term for $\omega$ is calculated as

$$S_\omega^c = \frac{1}{\mu_k c} S_{\varepsilon}^c - \frac{\omega_c}{k_c} S_k^c.$$  \hfill (2.80)

### 2.7 Comparison of Euler-Euler models

#### 2.7.1 Averaging methods and field equations

Phase-averaging is used to derive the field equations of the continuous phase for the standard Euler-Euler model and the Euler-Euler model based on PCAM. To derive the field equations of the disperse phase, phase-averaging is used for the standard Euler-Euler model, while particle-center-averaging is used for the Euler-Euler model based on PCAM. In terms of field equations, the continuous phase continuity equation for both Euler-Euler models is the same. The disperse phase continuity equation for the standard Euler-Euler model is an equation of the gas volume fraction, while the equation for the Euler-Euler model based on PCAM is related to the bubble number density. The continuous phase momentum equation for the Euler-Euler model based on PCAM (Eq. (2.18)) is the same as the equation for the standard Euler-Euler model (Eq. (2.13) with $k = c$) except for the viscous stress term. In Eq. (2.18), the phase volume fraction in the viscous stress term is outside of the divergence since the part of the viscous stress term related to the gradient of the phase volume fraction is canceled by the interfacial contributions, which is similar to the pressure term (Prosperetti and Jones, 1984). For the disperse phase momentum equations, the differences are as follows:

1. Equation (2.21) is derived by averaging the equation of motion for bubbles, while the equation in the standard Euler-Euler model (Eq. (2.13) with $k = d$) is derived by averaging the local instantaneous momentum equation of the disperse phase.

2. The physical meaning of the disperse phase momentum equation for both Euler-Euler models is different. Equation (2.21) shows the momentum balance of the gas, which belongs to the bubbles having their centers located inside the control volume. This gas may only be partially contained within the control volume. However, for the standard Euler-Euler model, the equation refers to the momentum balance of all gas contained inside the control volume. This gas may belong partially or even completely to the bubbles with their centers outside of the control volume. Hence, Eq. (2.21) is related to the bubble number density, while Eq. (2.13) with $k = d$ is related to the gas volume fraction.

3. Equation (2.21) explicitly shows the response of bubbles to the pressure and the viscous stress tensor of the continuous phase. Hence, no additional closure model for the viscous stress tensor of the disperse phase is required. In contrast, in Eq. (2.13)
with $k = d$, the viscous stress tensor of the disperse phase appears in the equation and a closure model for it is required.

### 2.7.2 Bubble force treatments

As mentioned in Chapter 1, the bubble force model obtained from experimental data or DNS simulations is usually a resultant force for a single bubble that acts on the bubble’s center-of-mass. However, in the standard Euler-Euler model, each bubble force is a function of the gas volume fraction. The conversion from the developed bubble force to the force in the disperse phase momentum equation in the standard Euler-Euler model is given by Eq. (1.1). In the Euler-Euler model based on PCAM, each bubble force for the disperse phase is a function of the bubble number density and the conversion for the force is achieved by

$$\langle f_d \rangle = n F_B.$$  \hspace{1cm} (2.81)

### 2.8 Finite volume discretization

The field equations for the Euler-Euler models are partial differential equations. In numerical simulations, the equations need to be discretized. Before discretizing the equations, the solution domain and the solution time are also required to be discretized. The discretization for the solution domain is separating the domain into some computational cells, or control volumes. These cells do not overlap with one another and completely fill the domain. Temporal discretization is dividing the solution time into some finite time intervals, or time steps. The field equation discretization is deriving an algebraic equation from the partial differential equation so that the computer can solve the equation directly. In this study, for the numerical solution, the field equations are discretized by a cell-centered finite volume method.

The finite volume discretization for the following transport equation of a quantity $\Phi$

$$\frac{\partial (\rho \Phi)}{\partial t} - \nabla \cdot (\rho \mathbf{u} \Phi) = \nabla \cdot (\Gamma \nabla \Phi) + S(\Phi)$$ \hspace{1cm} (2.82)

is generated by integrating the equation over a cell and time $t$ to $t + \Delta t$

$$\int_t^{t+\Delta t} \left[ \int_{V_p} \frac{\partial (\rho \Phi)}{\partial t} dV - \int_{V_p} \nabla \cdot (\rho \mathbf{u} \Phi) dV \right] dt = \int_t^{t+\Delta t} \left[ \int_{V_p} \nabla \cdot (\Gamma \nabla \Phi) dV + \int_{V_p} S(\Phi) dV \right] dt.$$ \hspace{1cm} (2.83)

Herein, $\Gamma$ is the diffusivity and $S(\Phi)$ is the source term. Besides, $\Delta t$ is the time step, $V_p$ and $P$ are the volume and the center of the cell, respectively. In the discretization, the Gaussian divergence theorem is applied to transfer a volume integral to a surface integral. Furthermore, the surface integral is approximated by the product of the surface area vector
and the quantities in the face center of the cell. For example, the discretization for the convection term reads

$$
\int_{V_p} \nabla \cdot (\rho u \Phi) dV = \int_{S_p} dS_i(\rho u \Phi) \approx \sum_f S_i(\rho u) \Phi_f, \quad (2.84)
$$

where $S_p$ is the surface of the cell and $S_f$ is the surface area vector of the cell. This vector is a surface normal vector with its magnitude equal to the surface area. Here and in the following, the subscript $f$ denotes the quantities in the face centers of a cell. In this thesis, the quantities in the face center are calculated from the values in the centers of the cells by linear interpolations.

After such discretization, the flux on the cell face is also involved. For the discretization of the convection term, a flux-limiter is used to make the simulations stable. A first-order Euler implicit scheme is used for the temporal discretization. In addition, it is assumed that the cell does not change in time. As a result, Eq. (2.83) is simplified to be (Rusche, 2002)

$$
\frac{\rho^o \Phi^o s - \rho^o \Phi^o}{\Delta t} V_p + \sum_f S_i(\rho u) \Phi^o_i = \sum_f f^o_i (S_i \nabla (\Phi^o)) + S^o_i \Phi^o P V_p + S^o E V_p. \quad (2.85)
$$

Herein, the superscripts $n$ and $o$ denote the new and the old value, respectively, and the subscript $P$ indicates the quantity for the cell with its center at $P$. To derive Eq. (2.85), the relation $S(\Phi) = S_I \Phi_P + S_E$ is used. The relation divides the source term into an implicit part ($S_I \Phi_P$) and an explicit part ($S_E$). Similarly, for the discretization of the diffusion equations in the Subsection 2.4.3, a first-order Euler implicit scheme is used in the temporal discretization and a Gauss linear scheme is used for the discretization of the Laplacian term.

Simplifying Eq. (2.85), we obtain the following linear algebraic equation:

$$
a_P \Phi^o_P + \sum_N a_N \Phi^o_N = R_P. \quad (2.86)
$$

Herein, $a_P$ and $a_N$ are the coefficients, $R_P$ is the source term, $N$ is the center of a cell which is a neighboring cell of the cell with its center at $P$ and the subscript $N$ indicates the quantity for the cell with its center at $N$. For each cell, a linear algebraic equation similar to Eq. (2.86) exists. Therefore, after discretization, a system of linear algebraic equations is obtained as follows

$$
A \Phi^n = R, \quad (2.87)
$$

where $A$ is the matrix of coefficients, $\Phi$ is the column vector which consists of $\Phi$ for each cell, and $R$ is the source vector. In the solution, if the $\Phi$ in a term is treated explicitly in time, the value of $\Phi$ from the previous time or iteration step will be used and the term will contribute to $R$. In contrast, if the $\Phi$ in a term is treated implicitly in time, the $\Phi$ is remaining to be solved and the term will contribute to $A \Phi^n$. 


2.9 Implementation of the particle-center-averaged Euler-Euler model

The combination of the Euler-Euler framework based on PCAM and the Gaussian convolution method is implemented based on the solver *multiphaseEulerFoam* in the OpenFOAM Foundation release (The OpenFOAM Foundation Ltd., 2021). This section introduces some details for the implementation.

2.9.1 Correction terms for drag and virtual mass force

In the OpenFOAM multiphase flow solvers for the Euler-Euler model, the drag and the virtual mass force are treated semi-implicitly to make the solution stable. The drag and the virtual mass force for the disperse phase are

\[
\langle f_d^D \rangle = -\frac{3}{4d_B} C_D \rho_c \beta_d (\langle u_d \rangle - \langle u_c \rangle) (\langle u_d \rangle - \langle u_c \rangle) - \langle u_d \rangle) (\langle u_c \rangle - \langle u_c \rangle)
\]

(2.88)

and

\[
\langle f_d^{VM} \rangle = -C_{VM} \rho_c \beta_d \left( \frac{D_d \langle u_d \rangle}{Dt} - \frac{D_c \langle u_c \rangle}{Dt} \right),
\]

(2.89)

respectively. The quantities within the square brackets are treated implicitly in time. Note, \( \langle u_d \rangle \) in the other term of Eq. (2.88) is treated explicitly in time. These forces appear directly in the disperse phase momentum equation.

To keep the forces consistent between the disperse and the continuous phase, the forces \( \langle f_d^D \rangle \) and \( \langle f_d^{VM} \rangle \), which act on the bubbles’ centers of mass, are converted to the phase-averaged forces for the continuous phase using Eqs. (2.29) and (2.30). This conversion requires an explicit implementation, but the explicit implementation can cause numerical stability problems (Rusche, 2002). As a solution, a correction term

\[
f_{c,\text{correction}}^D = -\frac{3}{4d_B} C_D \rho_c \beta_d (\langle u_d \rangle - \langle u_c \rangle) (\langle u_c \rangle - \langle u_c \rangle)
\]

(2.90)

is added to the drag force of the continuous phase. Similarly, a correction term

\[
f_{c,\text{correction}}^{VM} = -C_{VM} \rho_c \beta_d \left( \left( \frac{D_c \langle u_c \rangle}{Dt} - \frac{D_c \langle u_c \rangle}{Dt} \right) \right)
\]

(2.91)

is added to the virtual mass force of the continuous phase. These correction terms do not exist in theory. Once the simulation has sufficiently converged to a steady state, these terms will be neglectable since the difference between the current value and the old value will be negligible.
2 Theoretical and numerical methods

2.9.2 Sink and source terms in the continuity equations

In the OpenFOAM multiphase flow solver for the Euler-Euler model, the continuity equations are not solved in the original forms. To make the simulations more stable, some additional terms are incorporated in the continuity equations to couple these equations with the pressure equation and the momentum equations (Haley, 2017). In this thesis, this treatment is also used in the solver for the Euler-Euler model based on PCAM. This subsection introduces how the additional terms are derived and added to the continuity equations.

In the Euler-Euler model based on PCAM, the continuity equation of the disperse phase including the mass source reads

\[
\frac{\partial (\beta_d \rho_d)}{\partial t} + \nabla \cdot (\beta_d \rho_d \langle u_d \rangle) = S^m_d. \tag{2.92}
\]

Herein, \(S^m_d\) is the mass source or sink. It is a source when it is larger than zero and it is a sink when it is smaller than zero. Equation (2.92) can be changed to

\[
\frac{\partial \beta_d}{\partial t} + \nabla \cdot (\beta_d \langle u_d \rangle) = \nabla \cdot u_d, \tag{2.93}
\]

where

\[
\nabla \cdot u_d = -\frac{\beta_d \rho_d}{\rho_d} \frac{D \rho_d}{Dt} + \frac{S^m_d}{\rho_d}. \tag{2.94}
\]

The continuity equation of the continuous phase including the mass source term is

\[
\frac{\partial (\alpha_c \rho_c)}{\partial t} + \nabla \cdot (\alpha_c \rho_c u_c) = S^m_c. \tag{2.95}
\]

Similarly, it can be changed to

\[
\frac{\partial \alpha_c}{\partial t} + \nabla \cdot (\alpha_c u_c) = \nabla \cdot u_c, \tag{2.96}
\]

where

\[
\nabla \cdot u_c = -\frac{\alpha_c \rho_c}{\rho_c} \frac{D \rho_c}{Dt} + \frac{S^m_c}{\rho_c}. \tag{2.97}
\]

Summing up the continuity equations for both phases (Eqs. (2.93) and (2.96)), we obtain

\[
\frac{\partial \beta_d}{\partial t} + \nabla \cdot (\beta_d \langle u_d \rangle) + \frac{\partial \alpha_c}{\partial t} + \nabla \cdot (\alpha_c u_c) = \nabla \cdot u_d + \nabla \cdot u_c. \tag{2.98}
\]

After defining a mixture velocity vector \(U_{PCAM}\) by

\[
U_{PCAM} = \beta_d u_d + \alpha_c u_c, \tag{2.99}
\]
and substituting Eq. (2.99) into Eq. (2.98), we have

\[ \nabla \cdot U_{\text{PCAM}} = -\frac{\partial \beta_d}{\partial t} - \frac{\partial a_c}{\partial t} + \nabla \cdot u_d + \nabla \cdot u_c. \]  
(2.100)

The right side of Eq. (2.93) can be changed to

\[ \nabla \cdot u_d = \nabla \cdot u_d + \beta_d \nabla \cdot U_{\text{PCAM}} - \beta_d \nabla \cdot U_{\text{PCAM}}. \]  
(2.101)

Substituting Eq. (2.100) into Eq. (2.101) to replace the second \( \nabla \cdot U_{\text{PCAM}} \) and simplifying the resulting equation, we obtain

\[ \nabla \cdot u_d = (1 - \beta_d) \nabla \cdot u_d + \beta_d \nabla \cdot U_{\text{PCAM}} + \beta_d \left( \frac{\partial \beta_d}{\partial t} + \frac{\partial a_c}{\partial t} - \nabla \cdot u_c \right). \]  
(2.102)

Similarly, the right side of Eq. (2.96) can be changed to

\[ \nabla \cdot u_c = \nabla \cdot u_c + a_c \nabla \cdot U_{\text{PCAM}} - a_c \nabla \cdot U_{\text{PCAM}}. \]  
(2.103)

Substituting Eq. (2.100) into Eq. (2.103) to replace the second \( \nabla \cdot U_{\text{PCAM}} \) and simplifying the resulting equation, we obtain

\[ \nabla \cdot u_c = (1 - a_c) \nabla \cdot u_c + a_c \nabla \cdot U_{\text{PCAM}} + a_c \left( \frac{\partial \beta_d}{\partial t} + \frac{\partial a_c}{\partial t} - \nabla \cdot u_d \right). \]  
(2.104)

The right side of Eqs. (2.102) and (2.104) is the right side of the continuity equations in the solver.

### 2.9.3 Degassing boundary condition

For simulation of bubbly flows in a bubble column, a degassing boundary is used on the top of the column. The boundary works like an outlet for the disperse phase, while it works like a free slip wall for the continuous phase. Therefore, the disperse phase can leave the computational domain, while the continuous phase remains inside the domain. To obtain such effects, a mass sink is added for the disperse phase in the layer of cells nearest to the degassing boundary. Meanwhile, in the same cells, a mass sink or source is added for the continuous phase to keep the water level as high as the computational domain. This subsection introduces the content of the sink and source terms.

In the Euler-Euler model based on PCAM, the sink for the disperse phase is related to \( \beta_d \) because \( \beta_d \) is the solution variable related to the mass (volume) of the disperse phase in the continuity equation. Therefore, after the temporal discretization, the mass sink for the disperse phase is

\[ S_{m_d}^n = -\frac{\beta_d \rho_d}{\Delta t}. \]  
(2.105)
Note, $\beta_d$ is the gas volume fraction that attaches all the bubble volume to the bubble’s center-of-mass. Hence, once a bubble’s center-of-mass appears in the layer of cells nearest to the degassing boundary, all the gas volume belonging to this bubble will be removed from the domain by the sink term (Eq. (2.105)). If the bubble diameter is larger than the cell size, this sink term may give nonphysical gas volume fractions near the degassing boundary. Whereas, if the location of interest in the computational domain is not close to the degassing boundary, the influence of the nonphysical gas volume fractions near can be neglected.

For the continuous phase, the sink or source comes from three aspects. The first part corresponds to the sink of the disperse phase set by Eq. (2.105). The second part corresponds to the other source of the disperse phase in the fluid domain. For example, gas sources are usually set near the inlet to simulate gas injections by the nozzles. The third part corresponds to the sink or source of the disperse phase from the boundaries of the fluid domain (e.g. inlet and outlet). As a result, the formulation of the mass sink or source for the continuous phase is

$$S_m^c = \rho_c \left[ \frac{\beta_d}{\Delta t} - \frac{S_{m,\text{other}}^m V_{\text{cell}}^m}{\rho_d V_{\text{total}}^\text{cell}} + \sum_j (\beta_d u_d S_i) \right], \quad (2.106)$$

where $S_{m,\text{other}}^m$ is the mass sink or source for the disperse phase within the fluid domain except the mass sink for the degassing boundary, and $V_{\text{cell}}^m$ is the volume of the cell where $S_{m,\text{other}}^m$ is applied. In addition, $V_{\text{total}}^\text{cell}$ is the total volume of the layer of cells nearest to the degassing boundary. Moreover, the index $j$ indicates the boundary cells.

### 2.9.4 Pressure equation

Similar to the standard Euler-Euler model, a projection method is used in the solution of the Euler-Euler model based on PCAM. The method splits the calculation of the pressure and the velocity into three steps: velocity and flux predictions, pressure equation solution, and velocity and flux corrections (Chorin, 1968). The pressure equation does not appear in the field equations of the Euler-Euler model based on PCAM. It is derived from the continuity equations by assuming that the particle-center-averaged and the phase-averaged pressure are the same. It has become customary to use the shared pressure assumption in the solution of the Euler-Euler model. After correcting the velocities by the updated pressure, the velocities satisfy both momentum and continuity equations. Therefore, the pressure equation is a bridge between the continuity and the momentum equations.

For incompressible flows, the continuity equations can be simplified to be

$$\frac{\partial \alpha_c}{\partial t} + \nabla \cdot (\alpha_c \mathbf{u}_c) = 0, \quad (2.107)$$

and

$$\frac{\partial \beta_d}{\partial t} + \nabla \cdot (\beta_d \langle \mathbf{u}_d \rangle) = 0. \quad (2.108)$$
Summing up Eqs. (2.107) and (2.108), we obtain

\[
\frac{\partial (\alpha_c + \beta_d)}{\partial t} + \nabla \cdot (\alpha_c \mathbf{u}_c + \beta_d (\mathbf{u}_d)) = 0.
\] (2.109)

After discretizing the momentum equations, we obtain the relation between the corrected velocity and the predicted velocity as

\[
\mathbf{u}_c = \mathbf{u}_c^* - \frac{\alpha_c}{(A_c)_D} \nabla p_{rgh},
\] (2.110)

and

\[
\langle \mathbf{u}_d \rangle = \langle \mathbf{u}_d \rangle^* - \frac{\beta_d}{(A_d)_D} \nabla p_{rgh}.
\] (2.111)

Herein, the superscript “*” denotes the predicted quantity, while \((A_c)_D\) and \((A_d)_D\) are the diagonal matrices decomposed from the coefficient matrices of the discretized momentum equations for the continuous and the disperse phase, respectively, and \(p_{rgh}\) is a pseudo pressure. To treat the machine precision issues, the OpenFOAM solver works with the \(p_{rgh}\) instead of \(p\). The relation between \(p_{rgh}\) and \(p\) is

\[
p_{rgh} = p - \rho_m gh,
\] (2.112)

where \(\rho_m\) is the mixture density and \(h\) is the position vector to the point of zero potential. The mixture density is calculated by

\[
\rho_m = \alpha_d \rho_d + \alpha_c \rho_c.
\] (2.113)

After substituting Eqs. (2.110) and (2.111) into Eq. (2.109) and simplifying the resulting equation, we obtain the following pressure equation:

\[
\frac{\partial (\alpha_c + \beta_d)}{\partial t} + \nabla \cdot \left( \alpha_c \mathbf{u}_c^* + \beta_d \langle \mathbf{u}_d \rangle^* \right) = \nabla \cdot \left( \frac{\alpha_c}{(A_c)_D} + \frac{\beta_d}{(A_d)_D} \right) \nabla p_{rgh}.
\] (2.114)

### 2.9.5 Solution procedure

The discretized field equations are solved by a segregated solution procedure, which is introduced in this subsection. In the solution procedure, the continuity equations for both phases including the mass sink and source terms are solved to facilitate the independent treatment of the sink and source terms for both phases. This is necessary for the degassing boundary because in this boundary, a sink term exists for the disperse phase and a sink or source term exists for the continuous phase. If the PISO (pressure implicit with splitting of operator) algorithm is used, the solution procedure is as follows:

1. Solution of the disperse phase continuity equation (Eq. (2.93)) to obtain \(\beta_d\).

2. Solution of \(\alpha_d\) from \(\beta_d\) by a Gaussian convolution (Eq. (2.26)).
3. Solution of the continuous phase continuity equation (Eq. (2.96)) by the multidimensional limiting of fluxes (MULES) to maintain the boundedness of the $\alpha_c$. In this process, the total volume fraction of both phases is guaranteed to equal 1.

4. PISO loop.
   a) Flux prediction. The coefficient matrix of the discretized momentum equations is constructed and the flux for both phases is predicted based on the discretized momentum equations excluding the pressure gradient term.
   b) Pressure solution. The discretized form of Eq. (2.114) is constructed and solved to obtain a pressure field that meets the continuity of the gas-liquid mixture volume.
   c) Flux correction. The flux for both phases is corrected with the discretized form of Eqs. (2.110) and (2.111) based on the updated pressure field.
   d) Velocity calculation. The velocity for both phases is calculated from the updated phase volumetric flux.

5. Optional solution of the equations for the selected turbulence model.

The scheme of the solution procedure is shown in Fig. 2.5. The conversion between $\beta_d$ and $\alpha_d$ is shown in the scheme, while the other quantity conversions mentioned in Subsection 2.4.3 are required in the solution of velocities. The conversion from $\langle u_d \rangle$ to $\bar{u}_d$ is required in the calculation of phase-averaged relative velocity. This relative velocity is needed in the modeling of bubble-induced turbulence. Conversion from $\bar{u}_c$ to $\langle u_c \rangle$ is necessary for the calculation of $\langle f_d \rangle$ for the disperse phase momentum equation. Transferring $\langle f_d \rangle$ to $\bar{f}_d$ is needed when calculating the phase-averaged force for the continuous phase momentum equation. Therefore, these conversions appear in the calculation of the phase flux which is a function of velocity, including phase flux prediction and correction.
2.10 Verification

In this section, the simplified two-dimensional test case used in Tomiyama et al. (2006, 2003) is employed to reveal the numerical problems and nonphysical results of the standard Euler-Euler model caused by the inconsistency in the bubble force models. Meanwhile, the improvement by changing the bubble forces to act on the bubbles’ centers of mass by the PCAM is shown.

2.10.1 Simulation setup

The computational domain and boundary settings of the test case are shown in Fig. 2.6 (a). It is a rectangle with a size of 0.03 m × 0.5 m. A stream of air bubbles with a diameter of 10 mm is injected at x = 0 m and y = 0.15 m into the domain that contains only water at the beginning. At the inlet, the value of the volume fraction and velocity for both phases are given. As shown in Fig. 2.6 (b), the profile for the inlet liquid velocity is parabolic to introduce a shear flow field. For the standard Euler-Euler simulations, the inlet gas velocity is uniform with a value of 0.1 m s\(^{-1}\). The inlet gas volume fraction distribution is presented in Fig. 2.6 (c). In the profile, the lateral length over which the gas volume fraction is non-zero equals the bubble diameter.

For the Euler-Euler simulations based on PCAM, the bubble number density at the inlet is non-zero only in the center cell of the mesh. The inlet gas velocity is 0.1 m s\(^{-1}\) in the center cell and it is zero in the other cells. To keep the inlet gas flow rate the same as the standard Euler-Euler simulations, the inlet bubble number density is calculated by

\[
n = \frac{1}{V_B} \sum_{j=1}^{M} a_{d,j},
\]  

(2.115)

where \(a_{d,j}\) is the gas volume fraction in the computational cell \(j\), and \(M\) is the number of computational cells in the first layer near the inlet containing non-zero gas volume fraction. The aspect ratio of the cells is kept at 1 (i.e. cell spacing \(\Delta = \Delta_x = \Delta_y\); Herein, \(\Delta_x\) and \(\Delta_y\) are the cell spacing in the \(x\) and \(y\) axis direction, respectively). The cell spacing is uniform in the \(x\) and \(y\) axis direction.

At the wall, a slip boundary is used for the gas phase velocity, while a no-slip boundary is used for the liquid phase velocity. For all simulations, the Courant number (\(Co = u\Delta t/\Delta y\)) is

<table>
<thead>
<tr>
<th>(\rho_c) [kg m(^{-3})]</th>
<th>(\rho_d) [kg m(^{-3})]</th>
<th>(\mu_c) [kg m(^{-1}) s(^{-1})]</th>
<th>(\mu_d) [kg m(^{-1}) s(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>995.6</td>
<td>1.165</td>
<td>7.97e-4</td>
<td>1.86e-05</td>
</tr>
</tbody>
</table>

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2 Theoretical and numerical methods

(a) Computational domain and boundaries
(b) Inlet liquid velocity
(c) Inlet gas volume fraction

Figure 2.6 Computational domain and boundary settings.

Table 2.2 HZDR baseline model for bubbly flow simulations.

<table>
<thead>
<tr>
<th>Force and turbulence</th>
<th>Selected model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drag force</td>
<td>Ishii and Zuber (1979)</td>
</tr>
<tr>
<td>Shear-lift force</td>
<td>Hessenkemper et al. (2021) with cosine wall damping</td>
</tr>
<tr>
<td>Turbulent dispersion force</td>
<td>Burns et al. (2004)</td>
</tr>
<tr>
<td>Wall-lift force</td>
<td>Hosokawa et al. (2002)</td>
</tr>
<tr>
<td>Virtual mass force</td>
<td>Constant coefficient, $C_{VM} = 0.5$ (Auton et al., 1988)</td>
</tr>
<tr>
<td>Turbulence</td>
<td>$k - \omega$ SST (Menter, 2009)</td>
</tr>
<tr>
<td>Bubble-induced turbulence</td>
<td>Ma et al. (2017)</td>
</tr>
</tbody>
</table>
0.002. The temperature of air and water is 298.15 K and the pressure is 101325 Pa. The physical properties of the fluids are listed in Table 2.1.

The selected closure models for the bubble forces and turbulence according to the current Helmholtz-Zentrum Dresden-Rossendorf (HZDR) baseline model, which is based on the standard Euler-Euler model, are listed in Table 2.2 (Hänsch et al., 2021). The bubble shape model proposed by Ziegenhein and Lucas (2019) is used. Using this bubble shape model, the shear-lift force of Hessenkemper et al. (2021) is expected to change its sign when the bubble diameter is around 5.2 mm. Furthermore, for the simulations, the pressure treatment of Rzehak et al. (2021) is used. For the Euler-Euler model based on PCAM, the wall-contact force model mentioned in Subsection 2.5 is employed.

### 2.10.2 Mesh sensitivity analysis

A mesh sensitivity is carried out for the standard Euler-Euler simulations and the Euler-Euler simulations based on PCAM. In the analysis, the ratio between the bubble diameter and the cell spacing ranges from 2.5 to 20. The results for the gas volume fraction were averaged between 5 s and 20 s of simulation time at an axial height of $y = 0.4$ m because the standard Euler-Euler simulations did not reach a steady state. Laminar and turbulent flow cases are considered separately.

For a laminar flow, the results of the mesh sensitivity analysis are shown in Fig. 2.7. For the standard Euler-Euler model, the peak of the gas volume fraction increases continuously with decreasing cell spacing. This results from the fact that the shear-lift force acts on the distributed gas and drives it to the computational cells in the channel center. The resulting gas concentration in the channel center becomes higher when the mesh is refined and mesh-independent results cannot be found.

In contrast, in the results of the Euler-Euler model based on PCAM, the gas volume fraction distributions are similar upon refining the mesh. The reason is that with the PCAM, the bubble forces are changed to act on the bubbles’ centers of mass and the centers are located at the centreline of the channel, where the shear gradient vanishes. Therefore, the PCAM remedies the numerical deficiency in the standard Euler-Euler approach and provides a mesh-independent solution for the laminar flow.

For a turbulent flow, the results of the mesh sensitivity analysis are shown in Fig. 2.8. The results show similar phenomena as that in the laminar flow. In the results of the standard Euler-Euler model, the gas volume fraction peak for a cell spacing of 0.5 mm is slightly lower than that in the laminar flow. The reason is that the turbulent dispersion force which is activated in the turbulent flow simulation flattens the gas volume fraction peak. For other cell spacings, the gas volume fraction peaks in the laminar and the turbulent flow cases are almost the same. As a result, the phenomenon that the gas volume fraction peak grows with decreasing cell spacing is still significant. After using the PCAM, the gas volume fractions remain similar upon refining the mesh.
In summary, using the PCAM in the Euler-Euler model yields a mesh-independent solution, whereas the standard Euler-Euler model does not. However, the test cases are simplified. It is conceivable that mesh-independent solutions may exist also for the standard Euler-Euler model when the turbulent dispersion force is strong enough.

### 2.10.3 Axial development of gas volume fraction

In this subsection, the axial development of the gas volume fractions is analyzed. The grid spacing for all simulations in this subsection is 0.5 mm. At the inlet, the lateral region between \( x = 0.01 \) m and \( x = 0.02 \) m has non-zero gas volume fractions. The width of this region equals the bubble diameter. For a laminar flow, the gas volume fractions at different downstream positions are shown in Fig. 2.9. In the results for the standard Euler-Euler model, the gas volume fraction profiles are narrow with a high center peak, which means
2.10 Verification

(a) Standard Euler-Euler model

(b) Euler-Euler model based on PCAM

Figure 2.9  Gas volume fraction for laminar flow at different downstream positions.

(a) Standard Euler-Euler model

(b) Euler-Euler model based on PCAM

Figure 2.10  Gas volume fraction for turbulent flow at different downstream positions.

that gas concentrates in the channel center following the flow downstream. The width of the lateral region covered by the gas becomes smaller than the bubble diameter, which is nonphysical. This phenomenon is caused again by the shear-lift force, which transports the distributed gas to the channel center even though it belongs to the same bubble. In contrast, by using the PCAM in the Euler-Euler model, the distribution of the gas volume fraction remains almost unchanged after the inlet and the width of the region covered by the gas is close to the bubble diameter. Therefore, the gas volume fractions predicted by the PCAM are considered to be more reasonable.

For a turbulent flow, the gas volume fractions at different downstream positions are shown in Fig. 2.10. In the results of the standard Euler-Euler model, the peak of the gas volume fraction profiles is lower than that in the laminar flow case because of the effects of the turbulent dispersion force. Similar to the results in the laminar flow, the gas over-concentration in the channel center downstream of the inlet is significant and the width of
the region covered by the gas, which is slightly larger than that in the laminar flow case, is still much smaller than the bubble diameter. After changing the bubble forces to act on the bubbles’ centers of mass by the PCAM, the gas over-concentration in the channel center disappears from the simulation results. Furthermore, the width of the region covered by the gas is close to the bubble diameter.

In conclusion, no matter it is a laminar or turbulent flow case, gas over-concentration can appear in the channel center in the standard Euler-Euler simulations. This gas over-concentration is avoided by changing the bubble forces to act on the bubbles’ centers of mass as done by the PCAM. Therefore, using the PCAM in the Euler-Euler simulation recovers the consistency of the bubble force models for the Euler-Euler simulations.
3 Simulation of bubbly flows in vertical pipes

This chapter considers bubbly flows in different vertical pipes to evaluate the Euler-Euler model based on PCAM. For the bubbly flow cases, the experimental conditions and simulation setup are presented. Afterward, the predictions of the standard Euler-Euler model and the Euler-Euler model based on PCAM are compared with experimental data and discussed.

3.1 Description of the experiment

Experimental data are from the measurement test loop (MTLoop) facility (Lucas et al., 2005; Prasser et al., 2003) as well as from the experiments reported by Hosokawa and Tomiyama (2009), Shawkat et al. (2008) and Hibiki et al. (2001). The experimental data were obtained by different techniques, including intrusive and non-invasive methods. The experimental conditions are summarized briefly in Table 3.1 and a schematic for the test facility is shown in Fig. 3.1. In the MTLoop experiment and the experiments of Hibiki et al. (2001), the measurements were performed in several axial heights. In this chapter, the data obtained at the location that is the furthest away from the gas injection are used for comparison with the simulations. This location is referred to as the measurement plane in Table 3.1.

In the MTLoop experiment, a co-current air-water flow in a vertical pipe with an inner diameter of 51.2 mm and a height of 3.5 m was investigated. The water with a temperature of 303.15 K is supplied to the test section by a circulation pump, while the pressurized air is injected into the test section by some distributed nozzles at the bottom of the test section. After the two-phase flow leaves the test section, the air is separated by a cyclone-separator and released to the environment, while the water is recycled. The bubble characteristics, including local gas volume fraction, bubble size, and axial bubble velocity, were obtained at
Table 3.1 Experimental conditions (z: the axial distance from the location of gas injection or the top of the mixing section; LDV: laser Doppler velocimetry system).

<table>
<thead>
<tr>
<th></th>
<th>MTL Loop</th>
<th>Hosokawa</th>
<th>Shawkat</th>
<th>Hibiki</th>
</tr>
</thead>
<tbody>
<tr>
<td>Disperse phase</td>
<td>air</td>
<td>air</td>
<td>air</td>
<td>air</td>
</tr>
<tr>
<td>Continuous phase</td>
<td>water</td>
<td>tap water</td>
<td>filtered water</td>
<td>purified water</td>
</tr>
<tr>
<td>Temperature [K]</td>
<td>303.15</td>
<td>298.15</td>
<td>297.65</td>
<td>293.15</td>
</tr>
<tr>
<td>Pressure [Pa]</td>
<td>101325</td>
<td>101325</td>
<td>101325</td>
<td>101325</td>
</tr>
<tr>
<td>Pipe diameter $D$ [mm]</td>
<td>51.2</td>
<td>25.0</td>
<td>200</td>
<td>50.8</td>
</tr>
<tr>
<td>Pipe length [m]</td>
<td>3.5</td>
<td>2.0</td>
<td>9.56</td>
<td>3.061</td>
</tr>
<tr>
<td>Measurement plane $z$ [m]</td>
<td>3.03</td>
<td>1.7</td>
<td>8.4</td>
<td>2.7178</td>
</tr>
<tr>
<td>Measurement plane $z/D$</td>
<td>59.2</td>
<td>68.0</td>
<td>42.0</td>
<td>53.5</td>
</tr>
<tr>
<td>Bubble characteristic</td>
<td>wire-mesh</td>
<td>image</td>
<td>dual optical</td>
<td>double sensor</td>
</tr>
<tr>
<td>measurement</td>
<td>sensor</td>
<td>processing</td>
<td>probe</td>
<td>probe</td>
</tr>
<tr>
<td>Liquid characteristic</td>
<td>-</td>
<td>LDV</td>
<td>anemometry</td>
<td>anemometry</td>
</tr>
</tbody>
</table>

Figure 3.1 Schematic of test facility.

According to Beyer et al. (2008), the sensors distinguish air from water based on the different electrical conductivity of the two phases. Air can be regarded as an ideal insulator, while water is slightly conducting. Having two nearby measurement planes along with the axial height allows measuring the axial bubble velocity. The data obtained at an axial height of 3.03 m are compared with the simulation results. The experiment covered a wide range of air superficial velocities (from 0.0025 m s$^{-1}$ to 0.534 m s$^{-1}$) and water superficial velocities (from 0.0405 m s$^{-1}$ to 4.047 m s$^{-1}$). The superficial velocity for a phase is a hypothetical phase velocity calculated as if this phase was the only one flowing through the cross-sectional area. When the water superficial velocity is as high as 4.047 m s$^{-1}$, a finely dispersed flow
3.1 Description of the experiment

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Quantity</th>
<th>Uncertainty</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>MTLoop</td>
<td>(a_d)</td>
<td>1% (small bubbles) 4% (Taylor bubbles)</td>
<td>Prasser et al. (2005)</td>
</tr>
<tr>
<td></td>
<td>(u_d)</td>
<td>10%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(d_B)</td>
<td>4%</td>
<td>Hosokawa and Tomiyama (2009)</td>
</tr>
<tr>
<td></td>
<td>(u_c)</td>
<td>1%</td>
<td></td>
</tr>
<tr>
<td>Hosokawa</td>
<td>(a_d)</td>
<td>14%</td>
<td>Shawkat (2007)</td>
</tr>
<tr>
<td></td>
<td>(u_d)</td>
<td>2%-7.5%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(u_c)</td>
<td>3.7%</td>
<td></td>
</tr>
<tr>
<td>Shawkat</td>
<td>(a_d)</td>
<td>5.74%</td>
<td>Hibiki et al. (2001)</td>
</tr>
<tr>
<td></td>
<td>(u_d)</td>
<td>(\leq) 12%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(u_c)</td>
<td>(\leq) 3%</td>
<td>Hibiki et al. (1998)</td>
</tr>
<tr>
<td>Hibiki</td>
<td>(a_d)</td>
<td>5.74%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(u_d)</td>
<td>(\leq) 12%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(u_c)</td>
<td>(\leq) 3%</td>
<td></td>
</tr>
</tbody>
</table>

Table 3.2 Measurement uncertainty.

Regime appears. Prasser et al. (2005) analyzed the measurement uncertainty of the gas volume fraction by comparing the data obtained by the wire-mesh sensor and by ultrafast X-ray computed tomography. The results are summarized in Table 3.2.

In the experiment of Hosokawa and Tomiyama (2009), turbulent bubbly flows in a vertical pipe with an inner diameter of 25.0 mm and a height of 2.0 m were studied. The tap water at room temperature and atmospheric pressure is supplied to the mixing section by a circulation pump from a water tank. Air is compressed by a compressor and injected into the mixing section through holes with a diameter of 1 mm on the pipe wall. The mixing section is located upstream of the test section. It is designed to mix air and water so that an approximately uniform bubble size can be obtained. After the air-water mixture leaves the test section, the water comes back to the tank. Meanwhile, the air is released into the environment. The pipe of the test section was made of FEP (fluorinated ethylene-propylene resin). It is transparent and its refractive index is close to that of water.

The data were obtained at 1.7 m above the mixing section. The bubble images were recorded by two high-speed cameras. The bubble characteristics, including gas volume fraction, bubble size, and axial bubble velocity, were obtained by post-processing the recorded images. The liquid velocities were obtained by a laser Doppler velocimetry system (LDV). The LDV measures the local, instantaneous fluid velocities by detecting the frequency of light scattered by the small particles suspended in the fluid as they pass through a fringe or interference pattern. According to the Doppler principle, the frequency of the scattered light is shifted by an amount that is directly proportional to the flow velocity. The mean and fluctuating velocity components are determined from the frequency and the Doppler shifts. The measurement uncertainties estimated at 95% confidence are summarized in Table 3.2.

In the experiment of Shawkat et al. (2008), bubbly flows in a large vertical pipe with an inner diameter of 200 mm and a height of 9.56 m were investigated. In the experiment, the filtered water is introduced to the test section by a pump. The air is injected into the
test section through a shower-head injector at its bottom. On the top of the test section, a separation tank is connected to collect the water and separate the air from the mixture. The water temperature was held at around 297.65 K by a cooling system and a chiller.

The data were obtained at 8.4 m above the gas injection. The bubble characteristics, including gas volume fraction, bubble frequency, bubble diameter, and axial bubble velocity, were recorded with a dual optical probe. The optical probe distinguishes air from water based on the difference of refractive indices between air and water. The dual optical probe has two optical sensors which are installed in different axial locations. Each sensor has a photoelectric conversion circuit and an independent phase identifier. Using the two sensors allows measuring the axial bubble velocity and the instantaneous gradient of the phase interface. In the experiment, the liquid velocities and turbulence were obtained by a hot-film anemometry based on the heat transfer from the electrically-heated element (film) exposed to the liquid. Heat is convected away from the film to the fluid, which decreases the temperature of the film and changes the resistance of the wire. The change of the resistance is converted to a voltage signal which is calibrated to the fluid velocity. The uncertainties of the data are listed in Table 3.2.

In the experiment of Hibiki et al. (2001), bubbly flows in a vertical pipe with an inner diameter of 50.8 mm and a height of 3.061 m were investigated. The inner diameter of the test section is close to the MTLoop experiment. The purified water from a reservoir is supplied to a mixing chamber which is located at the bottom of the test section. The water temperature was held at around 293.15 K using a heat exchanger in the reservoir. The pressurized air is injected into the mixing chamber. The air and water are mixed in the mixing chamber and supplied to the test section. After the air-water mixture leaves the test section, the air is separated from the mixture by a separator and released to the environment. Meanwhile, the water is reused and fed back to the reservoir.

The local parameters, including gas volume fraction, interfacial area concentration, interfacial velocity, and bubble diameter, were obtained with a double sensor probe. Similar to the wire-mesh sensor, the measurement of the sensor probe is also based on the difference in the electrical conductivity between water and air. For the double sensor probe, two sensors are installed with a typical distance of approximately 2 mm to 3 mm in the axial direction. This setting allows the measurement of the axial bubble velocity. The local liquid velocities and their fluctuations were obtained by a hot-film anemometer system. The measurement data at the axial height of 2.7178 m are compared with the simulation results in the following. The measurement uncertainties of the data are listed in Table 3.2. In the table, the uncertainty of the gas volume fraction was determined by comparing the data obtained by the double sensor probe and by the γ-densitometer. According to Hibiki et al. (2001), the intrusive measurement using the double sensor probe does not work in the vicinity of a wall with \( r/R < 1 - d_B/(2R) \) because the presence of the wall and the probe do not allow a bubble to pass the near-wall region randomly. This causes a measurement error for the axial bubble velocity and the bubble diameter.
3.2 Simulation setup

In the experiments of MTLoop and Shawkat et al. (2008), the cross-sectional distribution of the nozzles used for gas injection is relatively uniform (Fig. 3 in Lucas et al. (2005)). The gas volume fractions obtained in the experiment made by Prasser et al. (2003, Fig. 4.37) can also be regarded as circumferentially symmetric. In the experiments of Hosokawa and Tomiyama (2009) as well as Hibiki et al. (2001), a mixing section and a mixing chamber were used, respectively. Moreover, in this thesis, the locations where the simulation results are compared with the measurement data are far away from the gas injection ($z/D \geq 42.0$). Hence, the flows in the locations where a comparison is made for simulation results and experimental data can be regarded as fully developed and circumferentially symmetric. Therefore, to save computational cost, the computational domain for the simulations is a narrow sector of the test-section pipe with wedge boundary conditions imposed on the side faces. The same was done in Lehnigk (2020), Liao et al. (2020), and Rzehak et al. (2017).

The simulations were run in a stationary mode. The computational domain and the boundary settings for the simulations are shown in Fig. 3.2. The central angle of the computational domain for MTLoop cases is $1.0^\circ$. For the simulations of the other experimental cases, the angle is $2.5^\circ$. The different choices for the central angle are not on purpose and they should not make any difference in the simulation results. According to the test results (not shown here), the simulation results of some MTLoop cases with the central angle equal to $1.0^\circ$ are about the same as that with the central angle equal to $2.5^\circ$.

The parameters for the selected cases are listed in Table 3.3. The case name indicates the experiment the case belongs to. The name of the MTLoop cases starts with “MT”, while the name of the experimental cases of Hosokawa et al., Shawkat et al., and Hibiki et al.
Table 3.3 Parameters for the selected cases (\(J\): superficial velocity; “\(\bar{\alpha}^{cs}\)”: cross-section averaged value; \(\Delta r\): radial cell spacing).

<table>
<thead>
<tr>
<th>Name</th>
<th>(J_c) [m s(^{-1})]</th>
<th>(J_d) [m s(^{-1})]</th>
<th>(\bar{\alpha}^{cs})% [-]</th>
<th>(d_B^{cs}) [mm]</th>
<th>(d_B^{cs}/\Delta r) [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Wall-peaking cases</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>MT17</td>
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<td>0.004</td>
<td>0.36</td>
<td>4.44</td>
<td>8.7</td>
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<tr>
<td>MT42</td>
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<td>0.53</td>
<td>3.89</td>
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<td>3.21</td>
<td>10.3</td>
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<tr>
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<td>3.99</td>
<td>4.25</td>
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<tr>
<td>HO21</td>
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<td>0.02</td>
<td>1.46</td>
<td>3.52</td>
<td>11.3</td>
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<td>HO22</td>
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<td>SH21</td>
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<td>6.56</td>
</tr>
<tr>
<td>SH31</td>
<td>0.68</td>
<td>0.015</td>
<td>1.70</td>
<td>3.20</td>
<td>5.12</td>
</tr>
<tr>
<td>HI11</td>
<td>0.491</td>
<td>0.0275</td>
<td>4.90</td>
<td>2.60</td>
<td>4.10</td>
</tr>
<tr>
<td>HI12</td>
<td>0.491</td>
<td>0.0556</td>
<td>9.20</td>
<td>2.80</td>
<td>4.40</td>
</tr>
<tr>
<td><strong>Center-peaking cases</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MT35</td>
<td>0.0641</td>
<td>0.0096</td>
<td>3.37</td>
<td>6.36</td>
<td>12.4</td>
</tr>
<tr>
<td>MT48</td>
<td>0.161</td>
<td>0.0151</td>
<td>3.75</td>
<td>6.23</td>
<td>12.2</td>
</tr>
<tr>
<td>MT107</td>
<td>1.017</td>
<td>0.14</td>
<td>9.30</td>
<td>6.55</td>
<td>12.8</td>
</tr>
<tr>
<td>MT142</td>
<td>2.554</td>
<td>0.534</td>
<td>12.51</td>
<td>5.87</td>
<td>11.5</td>
</tr>
<tr>
<td><strong>Finely dispersed flow cases</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MT22</td>
<td>4.047</td>
<td>0.004</td>
<td>0.07</td>
<td>4.08</td>
<td>8.0</td>
</tr>
<tr>
<td><strong>Fixed polydisperse simulations</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MT38</td>
<td>0.255</td>
<td>0.0096</td>
<td>1.94</td>
<td>4.77</td>
<td>9.3</td>
</tr>
<tr>
<td>MT39</td>
<td>0.405</td>
<td>0.0096</td>
<td>1.53</td>
<td>4.92</td>
<td>9.6</td>
</tr>
<tr>
<td>MT40</td>
<td>0.641</td>
<td>0.0096</td>
<td>1.09</td>
<td>5.06</td>
<td>9.9</td>
</tr>
<tr>
<td>MT41</td>
<td>1.017</td>
<td>0.0096</td>
<td>0.78</td>
<td>4.86</td>
<td>9.5</td>
</tr>
<tr>
<td>MT42</td>
<td>1.611</td>
<td>0.0096</td>
<td>0.53</td>
<td>3.89</td>
<td>7.6</td>
</tr>
<tr>
<td>MT50</td>
<td>0.405</td>
<td>0.0151</td>
<td>2.35</td>
<td>4.94</td>
<td>9.6</td>
</tr>
<tr>
<td>MT52</td>
<td>1.017</td>
<td>0.0151</td>
<td>1.19</td>
<td>4.95</td>
<td>9.7</td>
</tr>
<tr>
<td>MT86</td>
<td>1.611</td>
<td>0.0574</td>
<td>2.86</td>
<td>4.99</td>
<td>9.7</td>
</tr>
</tbody>
</table>

begins with “HO”, “SH”, and “HI”, respectively. In the simulation setup, the bubble diameter, the inlet velocities and volume fractions for the continuous and the disperse phase or for each bubble velocity group are required. For monodisperse simulations, the bubble diameters listed in Table 3.3 are used in the simulation setup directly. The cross-sectional distributions of inlet velocities and volume fractions are assumed to be uniform. At the inlet, by assuming a vanishing relative velocity between the gas and the liquid, the axial
velocities are calculated by

\[ u_{d,\text{in}} = u_{c,\text{in}} = J_d + J_c. \] (3.1)

Herein, \( u_{d,\text{in}} \) and \( u_{c,\text{in}} \) are the axial velocity components at the inlet for the disperse and the continuous phase, respectively. The lateral velocity components at the inlet are zero. The inlet volume fraction for the disperse phase, which is denoted as \( \alpha_{d,\text{in}} \), is computed by

\[ \alpha_{d,\text{in}} = \frac{J_d}{J_d + J_c}. \] (3.2)

Based on Eq. (3.2), the inlet volume fraction for the continuous phase, which is denoted as \( \alpha_{c,\text{in}} \), is calculated by

\[ \alpha_{c,\text{in}} = 1 - \alpha_{d,\text{in}}. \] (3.3)

For the Euler-Euler simulations based on PCAM, at the inlet, the particle-center-averaged axial velocity component is assumed to be the same as the corresponding phase-averaged axial velocity component which is calculated with Eq. (3.1). The particle-center-averaged lateral velocity components are also zero. In addition, the following relation is assumed:

\[ \beta_{d,\text{in}} = \alpha_{d,\text{in}}. \] (3.4)

For fixed polydisperse simulations, more than one bubble velocity group is used. To divide the bubbles into different velocity groups, the boundaries used to determine the bubble size range for the groups are required. It is a natural choice to use the critical diameter for the shear-lift coefficient to change its sign (about 5.2 mm) as one boundary. The reason is that the aim of using more than one bubble velocity group for simulations is to allow bubbles of different sizes to move with various velocities. In this thesis, with respect to the computational cost, the bubbles are divided into three or four velocity groups. For the simulations using four bubble velocity groups, the bubble size ranges for the groups are \( 0 \text{ mm} < d_B \leq 3.0 \text{ mm}, 3.0 \text{ mm} < d_B \leq 5.2 \text{ mm}, 5.2 \text{ mm} < d_B \leq 7.0 \text{ mm} \) and \( d_B > 7.0 \text{ mm} \). For the simulations using three bubble velocity groups, the last two bubble size ranges are merged to be the range for one bubble velocity group.

The bubble size distributions obtained in the experiments is used to calculate the parameters required in the simulation setup for each bubble velocity group. The measurement distributions provides the volume fraction and the bubble size range for each bubble size group. Usually, the number of bubble size groups in the measurement is much larger than the number of bubble velocity groups used in the simulations. Based on the bubble size distribution data, the volumetric flow rate fraction for the bubble velocity group \( i \), which is denoted as \( f_{vi} \), is calculated by

\[ f_{vi} = \sum_j f_j. \] (3.5)

Herein, the index \( j \) denotes the bubble size group that belongs to the bubble velocity group \( i \), and \( f_j \) is the volume fraction of the bubble size group \( j \), which is the ratio between the gas volume of the bubble size group \( j \) and the total gas volume of the bubble velocity
Table 3.4 Parameters for fixed polydisperse simulations of MTLoop cases.

<table>
<thead>
<tr>
<th>Name</th>
<th>(d_{B1}) [mm]</th>
<th>(d_{B2}) [mm]</th>
<th>(d_{B3}) [mm]</th>
<th>(d_{B4}) [mm]</th>
<th>(f_{v1})%</th>
<th>(f_{v2})%</th>
<th>(f_{v3})%</th>
<th>(f_{v4})%</th>
</tr>
</thead>
<tbody>
<tr>
<td>MT38</td>
<td>2.46</td>
<td>4.40</td>
<td>5.77</td>
<td>7.30</td>
<td>0.2</td>
<td>67.8</td>
<td>31.0</td>
<td>1.0</td>
</tr>
<tr>
<td>MT39</td>
<td>2.58</td>
<td>4.66</td>
<td>5.68</td>
<td>7.25</td>
<td>0.2</td>
<td>69.3</td>
<td>30.4</td>
<td>0.1</td>
</tr>
<tr>
<td>MT40</td>
<td>2.63</td>
<td>4.78</td>
<td>5.60</td>
<td>7.13</td>
<td>0.2</td>
<td>61.5</td>
<td>38.2</td>
<td>0.1</td>
</tr>
<tr>
<td>MT41</td>
<td>2.63</td>
<td>4.61</td>
<td>5.62</td>
<td>7.13</td>
<td>0.5</td>
<td>68.6</td>
<td>30.8</td>
<td>0.1</td>
</tr>
<tr>
<td>MT42</td>
<td>2.55</td>
<td>4.00</td>
<td>5.52</td>
<td>-</td>
<td>6.9</td>
<td>89.2</td>
<td>3.9</td>
<td>-</td>
</tr>
<tr>
<td>MT50</td>
<td>2.48</td>
<td>4.51</td>
<td>5.75</td>
<td>7.37</td>
<td>0.1</td>
<td>60.6</td>
<td>38.3</td>
<td>1.0</td>
</tr>
<tr>
<td>MT52</td>
<td>2.64</td>
<td>4.60</td>
<td>5.66</td>
<td>7.22</td>
<td>0.4</td>
<td>59.9</td>
<td>39.6</td>
<td>0.1</td>
</tr>
<tr>
<td>MT86</td>
<td>2.64</td>
<td>4.47</td>
<td>5.82</td>
<td>7.33</td>
<td>0.6</td>
<td>53.4</td>
<td>44.2</td>
<td>1.8</td>
</tr>
</tbody>
</table>

The representative bubble diameter of the bubble velocity group \(i\), which is denoted as \(d_{Bi}\), is computed by

\[
d_{Bi} = \frac{1}{\sum_j (f_j / d_{Bj})}
\]  

(3.6)

Herein, \(d_{Bj}\) is the representative bubble diameter of the bubble size group \(j\). In this thesis, the mid-point value of the bubble size range for a bubble size group is used as the representative diameter for this group. The calculation results of volumetric flow rate fraction and representative bubble diameter for each bubble velocity group are listed in Table 3.4. The fixed polydisperse simulations are performed only for some MTLoop cases because the measurement data for each bubble velocity group are available only for the MTLoop cases.

At the inlet, the cross-sectional distributions of velocities and volume fractions are also assumed to be uniform. The inlet axial velocity for each bubble velocity group is assumed to be the same as the inlet axial velocity for the disperse phase used for monodisperse simulations. Based on these assumptions, the inlet gas volume fraction of the bubble velocity group \(i\), which is denoted as \(a_{dl, in}\), is calculated by

\[
a_{dl, in} = f_i a_{d, in}
\]  

(3.7)

In terms of closure models, the selected models are the same as those in the verification case in Section 2.10. The maximum Courant number in simulations is smaller than 1 for the experimental cases of MTLoop, Hosokawa et al., and Hibiki et al. For the simulations of the experimental cases of Shawkat et al., the maximum Courant number is around 2 but the mean Courant number is around 0.1.
3.3 Mesh sensitivity analysis

This section illustrates the necessity of damping the shear-lift force near the wall for the standard Euler-Euler model to obtain mesh-independent solutions. Moreover, it aims to find a proper mesh resolution for the subsequent simulations of the experimental cases in the following sections or chapters. The simulation results with the proper mesh resolution are expected to be mesh-independent.

A quasi-two-dimensional mesh is applied to the computational domain for the simulations. Only one layer of computational cells is used in the circumferential direction. Besides, the cell spacing is uniform in the axial and the radial direction. To find a proper mesh resolution for the simulations, three or four different mesh resolutions are used to test the influence of cell size on the simulation results of the same experimental case. To show the influence clearly, the radial cell spacing decreases with a constant factor of 0.5. Moreover, to study the damping effects of the shear-lift force carefully, the aspect ratio of computational cells in different mesh for the MTLoop case is kept the same. In the mesh for the other experimental cases, the axial cell spacing does not change. The reason is that the axial cell spacing has little influence on the simulation results and keeping it constant can save computational cost. For each mesh, the radial and axial cell spacing are listed in Table 3.5.

To study the effects of damping the shear-lift force near the wall, the mean Courant number is kept the same for the simulations. This is achieved by decreasing the time step to half

<table>
<thead>
<tr>
<th>Name</th>
<th>$\Delta_r$ [mm]</th>
<th>$\Delta_z$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>MTLoop cases</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MT64-M1</td>
<td>1.02</td>
<td>8.75</td>
</tr>
<tr>
<td>MT64-M2</td>
<td>0.51</td>
<td>4.38</td>
</tr>
<tr>
<td>MT64-M3</td>
<td>0.26</td>
<td>2.19</td>
</tr>
<tr>
<td>MT64-M4</td>
<td>0.13</td>
<td>1.09</td>
</tr>
<tr>
<td><strong>Experimental cases of Hosokawa et al.</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HO22-M1</td>
<td>0.63</td>
<td>2.50</td>
</tr>
<tr>
<td>HO22-M2</td>
<td>0.31</td>
<td>2.50</td>
</tr>
<tr>
<td>HO22-M3</td>
<td>0.16</td>
<td>2.50</td>
</tr>
<tr>
<td><strong>Experimental cases of Shawkat et al.</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SH21-M1</td>
<td>1.25</td>
<td>11.95</td>
</tr>
<tr>
<td>SH21-M2</td>
<td>0.63</td>
<td>11.95</td>
</tr>
<tr>
<td>SH21-M3</td>
<td>0.31</td>
<td>11.95</td>
</tr>
<tr>
<td><strong>Experimental cases of Hibiki et al.</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HI12-M1</td>
<td>1.27</td>
<td>3.83</td>
</tr>
<tr>
<td>HI12-M2</td>
<td>0.64</td>
<td>3.83</td>
</tr>
<tr>
<td>HI12-M3</td>
<td>0.32</td>
<td>3.83</td>
</tr>
</tbody>
</table>

3.3 Mesh sensitivity analysis

This section illustrates the necessity of damping the shear-lift force near the wall for the standard Euler-Euler model to obtain mesh-independent solutions. Moreover, it aims to find a proper mesh resolution for the subsequent simulations of the experimental cases in the following sections or chapters. The simulation results with the proper mesh resolution are expected to be mesh-independent.

A quasi-two-dimensional mesh is applied to the computational domain for the simulations. Only one layer of computational cells is used in the circumferential direction. Besides, the cell spacing is uniform in the axial and the radial direction. To find a proper mesh resolution for the simulations, three or four different mesh resolutions are used to test the influence of cell size on the simulation results of the same experimental case. To show the influence clearly, the radial cell spacing decreases with a constant factor of 0.5. Moreover, to study the damping effects of the shear-lift force carefully, the aspect ratio of computational cells in different mesh for the MTLoop case is kept the same. In the mesh for the other experimental cases, the axial cell spacing does not change. The reason is that the axial cell spacing has little influence on the simulation results and keeping it constant can save computational cost. For each mesh, the radial and axial cell spacing are listed in Table 3.5.

To study the effects of damping the shear-lift force near the wall, the mean Courant number is kept the same for the simulations. This is achieved by decreasing the time step to half
when the number of axial cells is doubled. In the following, the simulation results of case MT64 with different mesh resolutions are shown. The simulated gas volume fractions were averaged between 5 s and 10 s of simulation time because some simulations did not reach a steady state.

Figure 3.3 presents the gas volume fractions simulated by both Euler-Euler models without damping the shear-lift force near the wall. Here and in the following, \( r \) is the radial coordinate and \( R \) is the pipe radius for the bubbly pipe flow cases. In the standard Euler-Euler simulation results, the peak of the gas volume fraction profiles for mesh MT64-M1 and mesh MT64-M2 is located on the wall, and the peak increases as the cell size decreases from mesh MT64-M1 to mesh MT64-M2. As the cell size continues to decrease with mesh MT64-M3, the peak is left from the wall. As the cell size further decreases with mesh MT64-M4, the peak becomes higher than the peak for mesh MT64-M3. The peak is located slightly closer to the wall than the one for mesh MT64-M3. These phenomena are similar to those
3.3 Mesh sensitivity analysis

that appear in the channel center of the two-dimensional test case in Section 2.10. The reason for these phenomena is that the shear-lift force and wall-lift force drive more gas to the peak when the cell size decreases. As a result, a mesh-independent solution is not found. In contrast, the gas volume fraction simulated with the Euler-Euler model based on PCAM using mesh MT64-M2 is close to that using mesh MT64-M3 and can be regarded as a mesh-independent solution.

With the wall damping, the gas volume fractions simulated by damping the shear-lift force near the wall are shown in Fig. 3.4. All the simulations reach a steady state and mesh convergence is obtained. The peak of the gas volume fraction simulated with the standard Euler-Euler model is not located on the wall, and the peak becomes much lower than the one simulated without wall damping. More importantly, the gas volume fraction simulated with mesh MT64-M2 is almost the same as that with mesh MT64-M3 and can be regarded as a mesh-independent solution. The peak of the gas volume fraction simulated by the Euler-Euler model based on PCAM is also lower than the one simulated without wall damping. The gas volume fraction simulated with mesh MT64-M2 is also regarded as a mesh-independent solution because it is almost the same as the result simulated with mesh MT64-M3.

In summary, it is necessary to damp the shear-lift force near the wall to obtain a mesh-independent solution for the standard Euler-Euler simulations. Therefore, the wall damping is applied in the subsequent standard Euler-Euler simulations. To keep the setting the same, the wall damping is also applied in the subsequent particle-center-averaged Euler-Euler simulations. Mesh MT64-M2 is regarded as a proper mesh resolution for the subsequent simulations of the MTLoop cases.

Figure 3.5 gives the gas volume fractions simulated by both Euler-Euler models with different mesh resolutions for the experimental cases of Hosokawa et al., Shawkat et al., and Hibiki et al. The selected cases for the simulations are listed in the label of the figure. The time-averaged gas volume fractions are used in comparisons because a few simulations did not reach a steady state. For cases HO22 and HI12, the gas volume fractions were averaged between 6 s and 10 s of simulation time. For case SH21, the gas volume fractions were averaged between 20 s and 25 s of simulation time.

For case HO22, the gas volume fraction simulated by the standard Euler-Euler model using mesh HO22-M1 has a lower peak than that using mesh HO22-M2. Nevertheless, the gas volume fraction for mesh HO22-M2 is close to that for mesh HO22-M3. Similar phenomena appear in the gas volume fractions simulated with the Euler-Euler model based on PCAM using these mesh resolutions. Therefore, the gas volume fractions simulated by both Euler-Euler models using mesh HO22-M2 can be regarded as mesh-independent solutions. Furthermore, mesh HO22-M2 is regarded as a proper mesh resolution for the subsequent simulations of the experimental cases of Hosokawa et al.

For case SH21, the gas volume fraction simulated by the standard Euler-Euler model with mesh SH21-M1 has a slightly lower peak than the one with mesh SH21-M2. Whereas, the
Figure 3.5 Mesh sensitivity analysis for other experimental cases.
3.4 Monodisperse simulation

gas volume fraction for mesh SH21-M2 is almost the same as that for mesh SH21-M3. For the Euler-Euler model based on PCAM, the gas volume fraction simulated with mesh SH21-M2 is also close to that simulated with mesh SH21-M3. Therefore, the gas volume fractions simulated by both Euler-Euler models with mesh SH21-M2 are regarded as mesh-independent solutions, and mesh SH21-M2 is used in the subsequent simulations of the experimental cases of Shawkat et al.

For case HI12, in the simulation results with the standard Euler-Euler model, the shape of the gas volume fraction profile for mesh HI12-M1 is different from the one for mesh HI12-M2. Whereas, the gas volume fraction simulated with mesh HI12-M2 is almost the same as that simulated with mesh HI12-M3 and can be regarded as a mesh-independent solution. In the gas volume fractions simulated with the Euler-Euler model based on PCAM, the difference between the results for mesh HI12-M2 and mesh HI12-M3 is smaller than the difference between the results for mesh HI12-M1 and mesh HI12-M2. This indicates that the gas volume fraction simulated with mesh HI12-M2 is close to a mesh-independent solution. Hence, to save the computational cost, mesh HI12-M2 is used in the subsequent simulations of the experimental cases of Hibiki et al.

The correction terms proposed in Subsection 2.9.1 do not exist in theory, but they are negligible when the simulation has sufficiently converged to a steady state. With the above-chosen mesh resolutions, the Euler-Euler simulations based on PCAM reach a steady state, which meets the prerequisite of using the correction terms in the simulations. The ratio between the averaged bubble diameter and the radial cell spacing for the chosen mesh resolutions is listed in Table 3.3. For all simulations, the ratio is larger than 4. For the simulations of the experimental cases of Hosokawa et al. and the center-peaking cases of the MTLoop experiment, the ratio is larger than 10. Therefore, the chosen mesh resolutions are suitable for the simulations to reveal the nonphysical phenomena caused by the inconsistency of the bubble force models used in the standard Euler-Euler simulations. They are also proper for the simulations to illustrate the ability of the PCAM in recovering the consistency.

3.4 Monodisperse simulation

This section compares the simulation results of the Euler-Euler model based on PCAM and the standard Euler-Euler model with the experimental data. In the simulations, a fixed bubble size (monodisperse) is assumed. The selected cases comprise different flow regimes, namely flows with wall-peaking and center-peaking gas volume fraction profiles as well as finely dispersed bubbly flows. The gas volume fraction profile is wall-peaking when the shear-lift force of the bubbles points to the wall of a pipe, while the profile is center-peaking when the shear-lift force points to the pipe center.
### 3.4.1 Comparison of wall-peaking cases

**Gas volume fraction**

Figure 3.6 shows the profiles for the gas volume fractions simulated by both Euler-Euler models in comparison with the profiles obtained in the MTLoop experiment. In the pipe-center region with $0 < r/R < 0.6$, the gas volume fractions simulated with both Euler-Euler models are similar. In this region, the simulated gas volume fractions of the cases, except case MT17, agree well with the experimental data. For all cases, the deviation between the simulation results and the experimental data appears in the region near the gas volume fraction peaks. The peak of the gas volume fraction profiles simulated with the standard Euler-Euler model is higher than the peak in the experimental data. The simulated peak is about 1.17, 1.37, 5.84, 4.72, 2.30, and 2.13 times the peak of the experimental data for cases MT17, MT19, MT20, MT42, MT64, and MT120, respectively. Herein, the maximum of the simulation results and the measurement data are used in the comparisons and these maxima can appear in different radial locations. In addition, for cases MT20 and MT42, the simulated peak is narrower than the peak in the experimental data. The reason for the over-predicted and narrow peaks is that the shear-lift force and the wall-lift force drive the gas to the peak without considering the bubble dimension because these forces are the functions of the local gas volume fraction.

After using the PCAM in the Euler-Euler simulations, the over-prediction of the gas volume fraction peaks is alleviated. The simulated peak turns to be around 1.07, 1.05, 2.12, 1.99, 1.55, and 1.65 times the peak in the experimental data for the cases. Moreover, for cases MT20 and MT42, the width of the simulated peak agrees well with the experimental data. The reason is that using the PCAM in the Euler-Euler simulations changes the bubble forces to act on the bubbles’ centers of mass by introducing the bubble number density.

Another phenomenon in Fig. 3.6 is that the gas volume fraction peaks simulated with the Euler-Euler model based on PCAM are located further away from the wall than those simulated with the standard Euler-Euler model. This results from the wall-contact force model used in the Euler-Euler simulations based on PCAM. The wall-contact force is relatively strong. It will drive too much gas from the wall in the near-wall region if the model would be used in the standard Euler-Euler simulations. Therefore, in the present study, this model was not used in the standard Euler-Euler simulations.

Except for case MT120, the simulated gas volume fractions are under-predicted in the near-wall region with $0.95 < r/R < 1$. The gas volume fraction peak in the simulation results is located further away from the wall than the peak location in the experimental data. The peak in the experimental data is almost located on the wall. There are two possible reasons for the deviation between the simulation results and the experimental data: The first reason is the assumption of a monodisperse bubble size in the simulations. Without such an assumption, it will be possible that bubbles smaller than the averaged bubble diameter slide on the wall or flow near the wall, and the gas volume fraction peak can be located closer to the wall. The second reason is that the spatial resolution of the wire-mesh sensor
3.4 Monodisperse simulation

Figure 3.6 Gas volume fraction for wall-peaking cases in MTLoop experiment (“E-E”: Euler-Euler model).
used in the experiments is limited. As a result, the gas volume fraction obtained in the
measurement cell nearest to the wall can be the highest if there are a lot of small bubbles
moving along the wall. For case MT17, the shape of the simulated gas volume fraction
profiles is different from the shape of the measurement one. This comes from insufficiencies
in the models for the radial bubble forces. However, comparing the existing bubble force
models to find a better selection or developing a new bubble force model is beyond the
scope of this thesis.

The gas volume fractions simulated by both Euler-Euler models together with the data
obtained in the experiment of Hosokawa et al. (“E-E”: Euler-Euler model; measurement uncertainty: 10%).
3.4 Monodisperse simulation

Figure 3.8  Gas volume fraction for wall-peaking cases in experiment of Shawkat et al. ("E-E": Euler-Euler model; measurement uncertainty: 14%).

The gas velocity is over-estimated, which leads to the under-prediction of gas volume fraction when the gas volumetric flow rate is fixed.

For the remaining cases, the gas volume fraction peak simulated with the standard Euler-Euler model is higher and narrower than the peak in the experimental data. It is about 2.29, 1.56, and 1.54 times the peak in the experimental data for cases HO11, HO21, and HO22, respectively. Similar to the condition in the MTLoop cases, the reason for the over-predictions is that the bubble forces are functions of the local gas volume fraction, and the shear-lift and the wall-lift force induce gas over-concentration in the wall peak. After changing the bubble forces to act on the bubbles’ centers of mass by the PCAM, the over-prediction of the gas volume fraction peak for case HO11 is alleviated. The simulated peak is 1.89 times the peak in the experimental data. However, for case HO11, the gas volume fractions simulated with both Euler-Euler models are over-estimated near the wall and under-estimated in the pipe center region with \(0 < r/R < 0.6\). This results from the fact that in the simulations, the shear-lift force is too strong or the wall-lift force is not strong enough. For cases HO21 and HO22, the gas volume fraction peaks simulated with the PCAM are close to the peaks in the experimental data. Furthermore, compared with the standard Euler-Euler simulation results, the shape of the gas volume fraction profile for cases HO21 and HO22 simulated with the PCAM is closer to the shape of the measurement profiles.

The comparisons of the simulated and the experimental gas volume fraction distributions for the experimental cases of Shawkat et al. are presented in Fig. 3.8. For case SH21, the gas volume fractions simulated with both Euler-Euler models are about the same. The simulation results are under-estimated in the pipe-center region with \(0 < r/R < 0.8\), but near the wall, they have a peak that is more significant than the peak in the measurement data. The deviation also originates from the fact that in the simulations, the strong shear-lift force pushes too much gas to the near-wall region or the wall-lift force is not strong enough to push the gas to the pipe-center region. For case SH31, the gas volume fractions
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 simulated with both Euler-Euler models coincide with each other except for the peaks. They agree well with the experimental data in the region with \( 0 < r/R < 0.95 \). Near the wall, the peaks of the simulated gas volume fractions are much higher than the peak in the experimental data. The peak simulated with the standard Euler-Euler model is 3.09 times the peak in the experimental data. This over-prediction is alleviated when the PCAM is applied in the simulations. The peak in the results simulated with PCAM is 2.36 times the peak in the experimental data. The reason for the deviation between the simulation results of both Euler-Euler models and the measurement data is that the measurement with the optical probe is an intrusive technique, and the presence of the probe and a pipe wall stops bubbles passing through the near-wall region.

Figure 3.9 shows the gas volume fraction profiles simulated by both Euler-Euler models in comparison with the data obtained in the experiment of Hibiki et al. For case HI11, the gas volume fractions simulated by both Euler-Euler models agree well with the experimental data in the pipe-center region with \( 0 < r/R < 0.7 \). Near the wall, the gas volume fraction simulated with the standard Euler-Euler model fits the measurement data well, but its peak is 2.02 times the peak in the experimental data. The reason for the over-prediction originates from the shear-lift force and the wall-lift force, which are the functions of the local gas volume fraction, drive the gas to the peak without considering the bubble dimension. After changing the forces to act on the bubbles' centers of mass by the PCAM, the over-prediction is alleviated. The peak simulated by the Euler-Euler model based on PCAM is 1.14 times the peak in the experimental data. However, the simulated peak is located further away from the wall than the peak in the experimental data, which is due to the strong wall-contact force used in the simulation.

For case HI12, the shape of the gas volume fraction profiles simulated with both Euler-Euler models are about the same as the experimental profile, but the simulation results are under-estimated in the majority of the radial locations. This is caused by the measure-
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ment uncertainty in the experimental data. The gas volumetric flow rate calculated from the measurement gas volume fraction and axial gas velocity is about 33% higher than the flow rate calculated from the superficial gas velocity (Table 3.3), which indicates that the measurement gas volume fraction is too high. The difference between the gas volume fraction profiles simulated with both Euler-Euler models is the peak location, which also results from the wall-contact force used in the Euler-Euler simulations based on PCAM.

Axial gas velocity

In the following, the axial gas velocities simulated by both Euler-Euler models are compared with the experimental data. As a prerequisite, the simulated gas velocities selected for comparisons have to be determined because there are two gas velocities available in the simulation results of the Euler-Euler model based on PCAM. In the simulation results of the standard Euler-Euler model, only one gas velocity is available, so it is used in the comparisons. Whereas, in the simulation results of the Euler-Euler model based on PCAM, the phase-averaged and the particle-center-averaged gas velocity are available. The particle-center-averaged gas velocity is the bubbles’ centers of mass velocity which is the gas velocity obtained in the experiment. Consequently, it is used in the comparisons. In the region very close to the wall, the bubbles’ centers of mass do not exist, so the particle-center-averaged gas velocity does not have any physical meaning. Therefore, in this region, it makes no sense to compare the particle-center-averaged gas velocity with the other gas velocities. In this study, if the calculated bubble number density is smaller than $10^{-6} \text{m}^{-3}$, it is regarded as no bubble’s center-of-mass exists in this region. Using $10^{-6} \text{m}^{-3}$ is reasonable because the simulated bubble number density is usually a high value. For example, for case MT19, it can be as high as $10^5 \text{m}^{-3}$.

Figure 3.10 shows the axial gas velocity profiles simulated by both Euler-Euler models in comparison with the data obtained in the MTLoop experiment. Here and in the following, the black dotted line in the subfigure marks the location where the simulated bubble number density is smaller than the threshold value $10^{-6} \text{m}^{-3}$. This line is called zero bubble number density line in the following. Between the line and the wall, it is regarded as no bubble’s center-of-mass exists. For all cases, in the region between $r/R = 0.9$ and the zero bubble number density line, the gas velocities simulated with the standard Euler-Euler model have a larger gradient than that simulated with the Euler-Euler model based on PCAM. In addition, the velocity simulated with the standard Euler-Euler model is also slightly higher. The reason is that in this region, the gas volume fraction simulated with the standard Euler-Euler model is higher, which induces a higher buoyancy force for the gas phase. Overall, the gas velocities simulated with both Euler-Euler models are almost the same. The simulated gas velocities of the cases except for case MT120 agree well with the experimental data. For case MT120, the simulated gas velocities are lower than the experimental data, which results from the fact that the drag force in the simulations is too strong.

For the experimental cases of Hosokawa et al., the comparisons of the simulated and the measurement axial gas velocities are shown in Fig. 3.11. In the pipe-center region with
Figure 3.10  Axial gas velocity for wall-peaking cases in MTLoop experiment (“E-E”: Euler-Euler model; right side of the black dotted line: \( n < 10^{-6} \text{ m}^{-3} \)).
0 < r/R < 0.8, the gas velocities simulated with both Euler-Euler models are approximately the same. Near the wall, a difference between the simulated gas velocities appears. Similar to the results of the MTLoop cases, in the region between r/R = 0.8 and the zero bubble number density line, the gas velocities simulated with the standard Euler-Euler model are higher than that simulated with the Euler-Euler model based on PCAM. This is also because the gas volume fractions simulated with the standard Euler-Euler model are higher and they introduce a higher buoyancy force for the gas phase. In this region, the gas velocities simulated with the Euler-Euler model based on PCAM fit the experimental data better than the results of the standard Euler-Euler simulations. For all cases, the results simulated with both Euler-Euler models are over-predicted. The deviation is higher than the reported measurement uncertainty (3%), but further analysis is stopped by the fact that the measurement data do not cover the whole cross-section of the pipe.

The axial gas velocity profiles simulated with both Euler-Euler models in comparison with the data obtained in the experiment of Shawkat et al. are presented in Fig. 3.12. For
both cases, the simulated gas velocities are much lower than the measurement data in the whole cross-section of the pipe. Besides, the shape of the simulated gas velocity profiles is also different from the measurement profile. The deviation is because the drag force model used in the simulations is not suitable for the simulation of the two cases. The measurement relative velocity between the gas and the liquid can be as high as 0.45 m s\(^{-1}\), but the relative velocity determined by the drag force model used in the simulations is around 0.23 m s\(^{-1}\). For case SH21, the gas velocities simulated with both Euler-Euler models fit each other. For case SH31, the simulated gas velocities are also close to each other except for some difference in the pipe-center region with 0 < \(r/R\) < 0.5. In this region, compared with the standard Euler-Euler simulation results, the axial gas velocity simulated with the Euler-Euler model based on PCAM is closer to the experimental data.

For the experimental cases of Hibiki et al., the radial distribution of the simulated and the measurement axial gas velocities are shown in Fig. 3.13. Considering that the uncertainty of the measurement gas velocity can be as high as 12% (Table 3.2), the gas velocities simulated with both Euler-Euler models are regarded as agreeing well with the experimental data. For both cases, the gas velocities simulated with both Euler-Euler models are about the same in the pipe-center region with 0 < \(r/R\) < 0.9, but near the wall, the velocity simulated with the standard Euler-Euler model is higher than the one simulated with the Euler-Euler model based on PCAM. This is because the influence region of the wall effects on the particle-center-averaged gas velocity (results for Euler-Euler model based on PCAM) is wider than the region for the phase-averaged gas velocity (standard Euler-Euler simulation results). Near the wall, the axial liquid velocity decreases because of the no-slip boundary on the wall, which introduces the decrease of the axial gas velocity due to the effects of the drag force. The particle-center-averaged gas velocity is determined by the resultant drag force of the bubbles, while the phase-averaged gas velocity is determined by the phase-averaged (local) drag force. Consequently, a difference exists in the influence region for the
wall effects in the standard Euler-Euler simulations and the Euler-Euler simulations based on PCAM.

**Axial liquid velocity**

For the comparisons of the axial liquid velocities, the phase-averaged liquid velocity is used to represent the results of the particle-center-averaged Euler-Euler simulations because it is the local velocity for the continuous phase. Figure 3.14 shows the axial liquid velocity profiles simulated by both Euler-Euler models in comparison with the data obtained in the experiment of Hosokawa et al. The liquid velocities simulated with both Euler-Euler models fit each other. In addition, the simulated liquid velocities are slightly higher than the experimental data, but the shape of the simulated and measurement profiles are similar. The deviation between the simulation results and the experimental data comes from the measurement uncertainty in the experimental data. Although the reported uncertainty of the measurement liquid velocity is around 1% (Table 3.2), for case HO11, the liquid volumetric flow rate calculated from the measurement axial liquid velocity and liquid volume fraction is about 5% lower than the flow rate calculated from the superficial liquid velocity (Table 3.3). Based on this situation, it is speculated that the measurement liquid velocities are slightly lower than the expected values.

For the experimental cases of Shawkat et al., the simulated and measurement axial liquid velocities are presented in Fig. 3.15. For both cases, the axial liquid velocity profiles are flatter than those in the experimental cases of Hosokawa et al. The reason is that the test-section in the experiment of Shawkat et al. is a large pipe with an inner diameter of 200 mm, which is 8 times the pipe diameter in the experiment of Hosokawa et al. For case SH21, the liquid velocities simulated with both Euler-Euler models coincide with each other. In the pipe-center region with $0 < r/R < 0.7$, the simulated liquid velocities are close
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![Graphs showing axial liquid velocity for wall-peaking cases in experiment of Hosokawa et al.](a) HO11 (b) HO12 (c) HO21 (d) HO22

**Figure 3.14** Axial liquid velocity for wall-peaking cases in experiment of Hosokawa et al. (“E-E”: Euler-Euler model; measurement uncertainty: 1%).

![Graphs showing axial liquid velocity for wall-peaking cases in experiment of Shawkat et al.](a) SH21 (b) SH31

**Figure 3.15** Axial liquid velocity for wall-peaking cases in experiment of Shawkat et al. (“E-E”: Euler-Euler model; measurement uncertainty: 3.7%).
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Figure 3.16  Axial liquid velocity for wall-peaking cases in experiment of Hibiki et al. (*E-E*: Euler-Euler model; measurement uncertainty: 3%).

to the experimental data. Near the wall, the simulation results with both Euler-Euler models are over-estimated. The simulated boundary layers are narrower than the boundary layer shown in the measurement data, which indicates that the over-estimation of the liquid velocities is because the near-wall treatments of the turbulent model used in the simulations are not proper for the case.

For case SH31, the simulated liquid velocities by both Euler-Euler models also coincide with each other except that a small difference exists in the pipe-center region with $0 < r/R < 0.5$. In this region, the axial liquid velocity simulated by the Euler-Euler model based on PCAM agrees better with the experimental data. Near the wall, the gradient of the simulated liquid velocities is larger than that of the experimental data, which also results from the near-wall treatments of the turbulent model used in the simulations.

The comparisons of the axial liquid velocities simulated with both Euler-Euler models and the measurement data for the experimental cases of Hibiki et al. are given in Fig. 3.16. For case HI11, the axial liquid velocities simulated with both Euler-Euler models are close to each other and agree with the experimental data. For case HI12, the liquid velocities simulated with both Euler-Euler models are also about the same, but the trends of the simulated profiles are different from the trends of the measurement profile. Moreover, the simulated liquid velocities are over-estimated in the pipe-center region with $0 < r/R < 0.5$. The reason for the deviation is that the turbulent model used in the current simulations is not suitable for the complicated case. For the case, the bulk Reynolds number ($Re = 2\rho c |u_c| R/\mu_c$) is on the order of $10^4$, so it is expected to be a turbulent flow and a turbulent model is used in the simulations. Whereas, the measurement liquid velocity profile is parabolic, which looks like a profile for a laminar flow and cannot be reproduced by the selected turbulent model.
3.4.2 Comparison of center-peaking cases

With the selected models for the bubble shape and the shear-lift force in the current simulations, if the averaged bubble diameter is larger than 5.2 mm, the simulated gas volume fraction profile is center-peaking. This subsection compares the results simulated by the Euler-Euler model based on PCAM and the standard Euler-Euler model with the experimental data for the selected center-peaking cases from the MTLoop experiment. Comparisons are made for the gas volume fractions and the axial gas velocities, respectively.

Figure 3.17 gives the simulated gas volume fraction profiles in comparison with the experimental data. For all cases, the gas volume fractions simulated with both Euler-Euler models are approximately the same. For cases MT35, MT48, and MT107, the simulated gas volume fractions are under-predicted near the wall but over-predicted in the pipe-center region. The deviation comes from two aspects: On the one hand, using the assumption of a monodisperse bubble size in the simulations cannot capture the bubbles’ movements well because the bubble size spectrum of these cases covers a large range. The double
peaks in the experimental data of cases MT35 and MT107 cannot be reproduced by the monodisperse bubble size. On the other hand, in the simulations, the shear-lift force is too strong or the turbulent dispersion force is not strong enough. For the over-estimations in these cases, no improvement is found in the results simulated with the PCAM. A possible explanation is that for these cases, the over-prediction of the gas volume fractions, which is caused by the inconsistency of the bubble force models, may have been smoothed by the turbulent dispersion. The turbulent dispersion is proportional to the turbulence intensity. As shown in Fig. 3.18, the turbulence intensity of the center-peaking cases simulated with the standard Euler-Euler model can be as high as 20, while the turbulence intensity of the wall-peaking cases MT20 and MT42, where the PCAM shows the ability to alleviate the over-predictions of gas volume fractions, is smaller than 0.14.

For case MT142, the cross-section averaged gas volume fraction in the simulation results is higher than that in the experimental data, which is caused by the over-strong drag force in the simulations. This case has a high gas volume fraction (larger than 0.15 in the pipe center), which indicates that the swarm effects are relatively strong. These effects can decrease the drag force but they have not been considered in the current simulations (Simonnet et al., 2007).

The comparisons of the simulated axial gas velocity profiles and the experimental data are given in Fig. 3.19. For all cases, the simulated gas velocities with both Euler-Euler models approximately coincide with each other. For cases MT35 and MT48, the measurement gas velocity profile is relatively flat, while the gas velocity profiles simulated with both Euler-Euler models have a significant center peak and over-estimations of the gas velocity exist in the pipe-center region. The deviation is since the intrusive measurement with the wire-mesh sensor decreases the axial bubble velocity, which is significant when the axial bubble velocity is relatively small. As the axial bubble velocity increases with case MT107, the influence of the wire-mesh sensor on the bubble velocity is less significant, and the gas velocities
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3.4.3 Comparison of finely dispersed flow case

In the MTLoop experiment, when the liquid superficial velocity is as high as 4.047 m s$^{-1}$, a finely dispersed flow regime appears. This subsection selects a finely dispersed flow case (MT22) to compare the results simulated by both Euler-Euler models with the experimental data. The comparisons are shown in Fig. 3.20.

Figure 3.20 (a) gives the comparisons for the gas volume fractions. The profile simulated with the standard Euler-Euler model has a significant peak near the wall. After using the PCAM in the Euler-Euler simulation, the peak becomes wider and much lower, so the over-
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This section compares the fixed polydisperse simulation results of the Euler-Euler model based on PCAM and the standard Euler-Euler model with the experimental data. Besides, to reveal the effects of using three or four bubble velocity groups for fixed polydisperse simulations, the monodisperse simulation results are also presented. Comparisons are made for gas volume fractions and axial gas velocities, respectively. The cases selected for the comparisons come from the MTLoop experiment. For the cases, the gas volume fraction profiles in the fixed polydisperse simulation results can have double peaks when the volumetric flow rate fractions for the bubble velocity groups which have a shear-lift force pointing to the pipe center and the groups which have a shear-lift force pointing to the wall of a pipe are both high. In contrast, the gas volume fraction profiles have a single peak when the majority of the gas volumetric flow rate is taken up by the bubble velocity

Figure 3.20  Comparison for finely dispersed flow case MT22 (“E-E”: Euler-Euler model).

prediction is alleviated. Nonetheless, in this condition, the difference between the simulated profile and the measure one is still significant. The measurement profile is relatively flat and does not show a significant wall peak. The reason for the difference comes from insufficiencies in the closure models due to some unknown effects in the finely dispersed flow regime (Lucas et al., 2020). For case MT22, the radial gradient of the axial liquid velocity is large and the bubble diameter is small, which introduces a strong shear-lift force near the wall for the simulations. Consequently, a significant wall peak is formed in the simulation results. The comparisons for the axial gas velocities are presented in Fig. 3.20 (b). The gas velocities simulated with both Euler-Euler models are similar and agree well with the experimental data except the pipe-center region with $0 < r/R < 0.1$. In this region, a sudden drop exists in the experimental data, which results from the measurement uncertainty.
groups which have a shear-lift force pointing to the wall of a pipe. In the following, the results for the cases with double peaks and a single peak are shown consecutively.

### Gas volume fraction for cases with double peaks

Figure 3.21 shows the comparisons of the gas volume fraction profiles for the cases with double peaks. In the figure, the gas volume fraction in the fixed polydisperse simulation results is the total gas volume fraction, which is the sum of the gas volume fraction of all bubble velocity groups. In the monodisperse simulation results, the gas volume fractions simulated with both Euler-Euler models almost coincide with each other. Moreover, the simulated profiles with both Euler-Euler models have a single peak and the peak is located further away from the wall than the peak in the experimental data. Whereas, in the fixed
polydisperse simulation results, the gas volume fraction profiles have double peaks. One peak is located close to the wall and the other is located in the pipe center. Compared with the monodisperse simulation results, the wall peak is located closer to the peak in the experimental data. This is because the averaged diameter of the bubbles which form the wall peak for the fixed polydisperse simulations is smaller than that for the monodisperse simulations. As shown in Fig. 3.22, the shear-lift coefficient used in the simulations increases as the bubble diameter decreases. Hence, the shear-lift force for the fixed polydisperse simulations can be stronger and pushes the bubbles to the location that is closer to the wall.

Except for the pipe-center region with $0 < r/R < 0.3$, the gas volume fractions in the fixed polydisperse simulation results agree better with the experimental data than those in the monodisperse simulation results. For the fixed polydisperse results simulated with the standard Euler-Euler model, the gas volume fraction profiles have a significant peak in the pipe center. Except for case MT40, such a peak does not exist in the measurement profiles. The gas volume fractions in the pipe center simulated with the standard Euler-Euler model are about 1.96, 2.64, 1.69, and 1.86 times the experimental data for cases MT38, MT39, MT40, and MT50, respectively. In contrast, using the PCAM in the simulations can alleviate the over-predictions. The gas volume fractions in the pipe center simulated with PCAM are about 1.83, 2.27, 1.45, and 1.76 times the experimental data for these cases, respectively.

The simulated peak in the pipe center is formed by the bubbles of the third velocity group which has a bubble size range as $5.2 \text{ mm} < d_B \leq 7 \text{ mm}$. For the velocity group, the comparisons of the simulated gas volume fraction profiles and the experimental data are given in Fig. 3.23. The experimental data come from summing up the gas volume fraction of the bubble size groups that belong to this velocity group, and the raw data for the gas volume fraction of the bubble size groups are available. The simulated profiles show a significant peak in the pipe center, which does not exist in the measurement profile except case MT40. In addition, the profiles simulated with the Euler-Euler model based on PCAM have a lower peak than those simulated with the standard Euler-Euler model.
Figure 3.23  Gas volume fraction of the third velocity group ($5.2 \text{ mm} < d_B \leq 7 \text{ mm}$; “PCAM poly”: fixed polydisperse simulation with Euler-Euler model based on PCAM; “Standard poly”: fixed polydisperse simulation with standard Euler-Euler model).

The reasons for the deviation between the simulation results and the experimental data are: First, the shear-lift force model used in the simulations is too sensitive to the bubble size. Second, measurement uncertainty exists in the measurement data, and the uncertainty can be higher than 4%. This is speculated from the fact that the difference between the representative bubble diameter of the third bubble velocity group for these cases is smaller than 0.3 mm (Table 3.4), while the difference in the shape of the measurement profiles is significant. Third, the dynamic effects of bubble coalescence can play a role. The radial profile of the total gas volume fraction is fully developed, but the profile of the gas volume fraction for a single velocity group may not be fully developed. After the bubble coalescence appears, the resulting bubble can move from the region near the wall to the pipe center. During this process, the bubble can appear in any radial location instead of only in the pipe center. Therefore, the measurement gas volume fraction profiles can have a different shape from the center-peaking profile. However, bubble coalescence has
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not been included in the simulations. Note, for the radial distribution of the gas volume fraction, the weighting factor for the deviation between the simulation results and the experimental data in the pipe-center region is smaller than the one near the wall because the cross-sectional area of the pipe-center region is smaller than the near-wall region.

Gas volume fraction for cases with a single peak

For the cases with a single peak in the gas volume fraction profile, the comparisons of the simulated gas volume fraction profiles and the experimental data are presented in Fig. 3.24. In this figure, the gas volume fraction in the fixed polydisperse simulation results is also the total gas volume fraction. Compared with the monodisperse simulation results, the peak of the gas volume fraction profiles in the fixed polydisperse simulation results is
located closer to the peak in the experimental data. For cases MT41, MT52, and MT86, the shape of the gas volume fraction profiles in the fixed polydisperse simulation results are similar to the shape of the measurement profiles. From monodisperse simulations to fixed polydisperse simulations, the peak of the simulated gas volume fraction profiles increases. The peak increments in the standard Euler-Euler simulations are higher than those in the Euler-Euler simulations based on PCAM. In the standard Euler-Euler simulations, the peak for cases MT41, MT52, and MT86 increase by 12.3%, 11.8%, and 35.9%, respectively. For the Euler-Euler simulations based on PCAM, the peaks increase by 5.6%, 5.2%, and 16.2%, respectively. The high increments in the standard Euler-Euler simulations originate from the over-predictions of the gas volume fraction peak in the second velocity group which has a bubble size range as $3 \text{mm} < d_B \leq 5.2 \text{mm}$. For this velocity group, the simulated gas volume fraction profiles in comparison with the experimental data are shown in Fig. 3.25. The reason for the over-predictions is that the shear-lift force and the wall-lift force are the functions of the local gas volume fraction, which drive the gas to the peak without considering the bubble dimension.

Figure 3.24 shows that such over-predictions do not exist in the standard Euler-Euler simulations with the monodisperse assumption. The reason is related to the magnitude of the shear-lift force. For the cases, the averaged bubble diameter used for monodisperse simulations (4.86 mm for case MT41, 4.95 mm for case MT52 and 4.99 mm for case MT86) is close to the critical bubble diameter for the shear-lift coefficient to change its sign (about 5.20 mm), so the shear-lift force is relatively small. For fixed polydisperse simulations, the representative diameter of the second velocity group for the cases (4.61 mm for case MT41, 4.60 mm for case MT52 and 4.46 mm for case MT86) is smaller than the averaged diameter used for monodisperse simulations. In this condition, the shear-lift force of the second velocity group can be higher than that for monodisperse simulation because the shear-lift coefficient increases as the bubble diameter decreases. At last, for case MT86, the over-prediction in the second velocity group leads to an over-prediction for the peak of the total gas volume fraction profile. Whereas, for cases MT41 and MT52, the over-predictions contribute to a good agreement with the experimental data for the peak of the total gas volume fraction profile, which should be treated carefully. Figure 3.25 presents that using the PCAM in the Euler-Euler simulations can avoid or alleviate the over-predictions of the gas volume fraction peaks for the second velocity group. The reason is that the PCAM changes the bubble forces to act on the bubbles’ centers of mass. Consequently, in the fixed polydisperse simulation results simulated with the Euler-Euler model based on PCAM, the peak of the total gas volume fraction profile for case MT86 agrees well with the measurement one. However, the peak of the total gas volume fraction profile for cases MT41 and MT52 is under-predicted. The reason for the under-predictions is that the number of bubble velocity groups used in the simulations is still not enough to reproduce the bubble movement in the experiment.

For case MT42, the peak of the simulated gas volume fraction profiles is higher than that in the experimental data. From monodisperse simulation to fixed polydisperse simulation, the peak of the gas volume fraction profiles simulated with the standard Euler-Euler model
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Figure 3.25  Gas volume fraction of the second velocity group (3 mm < \(d_B\) ≤ 5.2 mm; “PCAM poly”: fixed polydisperse simulation with Euler-Euler model based on PCAM; “Standard poly”: fixed polydisperse simulation with standard Euler-Euler model).

decreases (Fig. 3.24 (b)). The reason is that the over-prediction caused by the inconsistency in the bubble force models decreases. This comes from two aspects: On the one hand, the representative bubble diameter of the second velocity group (4.00 mm) where the over-prediction of the gas volume fraction peak exists is larger than the averaged diameter used for monodisperse simulation (3.89 mm). Therefore, the shear-lift force for this velocity group can be lower than that for the monodisperse simulation. On the other hand, for the fixed polydisperse simulation, only a part of the gas contributes to the over-prediction of gas volume fraction near the wall. The volumetric flow rate fraction for the gas which has over-prediction is 89.15%, which is smaller than that for monodisperse simulations (100%). In contrast, the gas volume fractions simulated with the Euler-Euler model based on PCAM for monodisperse and fixed polydisperse simulation are similar, and the over-predictions of the gas volume fraction peaks in the simulation results are alleviated.
Figure 3.26  Axial gas velocity in monodisperse and fixed polydisperse simulations (right side of the black dotted line: \( n < 10^{-6} \text{ m}^{-3} \); “PCAM mono”: monodisperse simulation with Euler-Euler model based on PCAM; “Standard mono”: monodisperse simulation with standard Euler-Euler model; “PCAM poly”: fixed polydisperse simulation with Euler-Euler model based on PCAM; “Standard poly”: fixed polydisperse simulation with standard Euler-Euler model).

Axial gas velocity

In the fixed polydisperse simulation results, the gas velocity presented here is the averaged gas velocity calculated from the gas velocity of each bubble velocity group using the gas volume fraction as the weighting factor

\[
 u_d = \frac{\sum_{i=1}^{N_d} \alpha_{d_i} u_{d_i}}{\alpha_d}. \tag{3.8}
\]

In the results for the Euler-Euler simulation based on PCAM, the particle-center-averaged velocity of each bubble velocity group is used to calculate the average gas velocity. The location of the zero bubble number density line is based on the fixed polydisperse simulation.
Figure 3.26 gives the simulated axial gas velocity profiles in comparison with the experimental data. The results of both, monodisperse and fixed polydisperse, simulations are presented. The simulated gas velocities for the monodisperse and the fixed polydisperse simulations are similar. Moreover, the gas velocities simulated with the standard Euler-Euler model and the Euler-Euler model based on PCAM are close to each other. For case MT40, the shape of the simulated profiles is close to that of the measurement profile, but over-prediction also exists in the pipe-center region with $0 < r/R < 0.5$. This also comes from the measurement uncertainty in the experimental data. For cases MT52 and MT86, the simulated gas velocities agree well with the experimental data.

### 3.6 Conclusion

In this chapter, the predictions for bubbly pipe flows with the standard Euler-Euler model and the Euler-Euler model based on PCAM have been compared with the data obtained in different experiments. Before the comparisons, the experimental conditions and the simulation setup have been introduced. Besides, mesh sensitivity analyses have been performed to select proper mesh resolutions for the simulations. For monodisperse simulations, the simulated gas volume fractions, axial gas and liquid velocities have been compared with the experimental data, respectively. The results show that over-prediction of the gas volume fraction peak exists in the center or near the wall of a pipe for the standard Euler-Euler simulations. In contrast, using the PCAM in the Euler-Euler simulations alleviates or avoids the over-prediction of the gas volume fraction peak for wall-peaking cases and for finely dispersed flow case. However, no improvement is found in the prediction of the gas volume fraction using the PCAM for center-peaking cases. For these cases, the over-prediction of the gas volume fraction caused by the inconsistency of bubble force models can have been smoothed by the turbulent dispersion. The validation results also present that the axial gas and liquid velocities simulated with both Euler-Euler models are close to each other, which proves that the closure models for bubble forces and turbulence are correctly applied in the particle-center-averaged Euler-Euler model.

For the fixed polydisperse simulations, the simulated gas volume fractions and axial gas velocities have been compared with the experimental data, respectively. In the simulations, over-prediction of the gas volume fraction peak also appears in the center or near the wall of a pipe for the standard Euler-Euler simulations. Whereas, the over-prediction is alleviated in the results simulated with the Euler-Euler model based on PCAM. Furthermore, comparisons have also been made for the results of the monodisperse and the fixed polydisperse simulations. The comparisons show that in the standard Euler-Euler simulation results, the over-prediction of the gas volume fraction peak can be more significant for fixed polydisperse simulations than for monodisperse simulations. The reason is that the magnitude of the shear-lift force for fixed polydisperse simulations is higher than that
for monodisperse simulations. The over-prediction is also alleviated by using the PCAM in the Euler-Euler simulations. For fixed polydisperse simulations, the gas velocities simulated with both Euler-Euler models are similar.

In summary, the influence of the inconsistency in the bubble force models on the simulation results is significant when the bubble diameter is larger than the cell size, the turbulent dispersion is low and the shear-lift force is strong. It is necessary to recover the consistency for the simulations in general. The particle-center-averaged Euler-Euler model recovers the consistency and provides a physical treatment for the bubble forces and the bubble dimension.
4 Simulation of bubbly flow in a cylindrical bubble column

This chapter considers bubbly flow in a cylindrical bubble column to validate the Euler-Euler model based on PCAM. The experimental conditions and the simulation setup for the bubbly flow are introduced. The simulation results of the standard Euler-Euler model and the Euler-Euler model based on PCAM are compared with experimental data.

4.1 Description of the experiment

The experimental data were obtained in a bubble column with an inner diameter of 0.1 m and a height of 2 m (Kipping et al., 2021). In the experiment, deionized water and nitrogen at room temperature and atmospheric pressure are used as the continuous and the disperse phase, respectively. Gas is injected into the column through 31 nozzles with an inner diameter of 0.22 mm located at the bottom of the column \( z = 0 \) m. The schematic of the test section and the cross-sectional distribution of the nozzles are shown in Fig. 4.1. Before the gas is injected, the height of the stagnant water in the column is 1.4 m. After the gas leaves the column, it is released into the environment.

The data were obtained at the levels of \( z = 0.1 \) m and \( z = 0.7 \) m by ultrafast electron beam X-ray computed tomography, which is a non-invasive measurement technique. The measurement is based on the different X-ray attenuation coefficients between air and water. In the measurement, a moving X-ray fan is formed by the electromagnetic deflection of an electron beam which is generated by a beam gun. When the X-ray passes through the cross-section of the test section, the radiation attenuation is recorded by the detector rings. In the experiment, the axial bubble velocity were determined by the data obtained in two measurement planes with a small axial pitch around 10 mm (Neumann-Kipping et al.,
The measurements were performed with an imaging frequency of 1000 images per second and a spatial resolution of about 1 mm.

The gas volume fraction, the axial gas velocity, and the bubble size distribution were obtained by post-processing the X-ray images. The local data in the measurement plane may change in time and the cross-sectional distribution of the data may not be circumferentially symmetric. In this condition, to obtain statistical convergence for the measurement gas volume fraction and axial gas velocity, time-averaging and azimuthal averaging are used to post-process the local data. For time-averaging, the local data were averaged over 20 s of the measurement time. To perform azimuthal averaging, the cross-section of the cylinder was divided into 10 parts, including 9 concentric rings and 1 inner circle in the center. The cross-sectional area of the 10 parts is almost the same. Afterward, the area-averaged value of each part is calculated from the local data. Moreover, to plot the radial profiles, one representative radial location is needed for each part. For each ring, the representative radial location is the averaged value of the inner and the outer radius, while for the inner circle, the representative radial location is half of its radius.

According to Banowski et al. (2015), the maximum uncertainty of the determined bubble diameter decreases as the bubble diameter increases. It is smaller than 20% for $d_B \geq 2$ mm, smaller than 10% for $d_B \geq 4$ mm, and smaller than 5% for $d_B \geq 8$ mm. Barthel et al. (2015) reported that the uncertainty of the measurement axial bubble velocity is mainly introduced by the temporal resolution of the X-ray imaging system and the uncertainty decreases as the measurement velocity decreases. Based on their calculation method, the uncertainty of the measurement axial bubble velocity at 0.25 m s$^{-1}$ is around 2.5%.
4.2 Simulation setup

The measurement data at level $z = 0.7$ m are used for comparison with the simulation results. From the available test matrix, the experimental cases with a gas superficial velocity of 0.0055 m s$^{-1}$ and 0.0164 m s$^{-1}$ were simulated. The parameters for the selected cases are listed in Table 4.1. The computational domain used in the simulations is the whole cylinder and the gas nozzles are simulated by 31 inlet patches (Fig. 4.2). Each inlet patch takes up the cross-sectional area of one computational cell. The height of the computational domain is 1.4 m, which is as high as the clear water in the experiment. The free surface is not simulated and a degassing boundary is used on the top of the bubble column instead. The degassing boundary allows the disperse phase to leave the domain, while it works like a free slip wall for the continuous phase and keeps the continuous phase in the domain. On the bottom of the bubble column, an inlet boundary is used for the inlet patches, while a wall boundary is set for the remaining area of the bottom. A wall boundary is also employed for the cylinder wall. The computational domain and the boundary settings are also shown in Fig. 4.2. At the beginning of the simulations, the domain is full of water, and the gas is injected into the domain through the inlet patches.

For monodisperse simulations, the bubble diameters listed in Table 4.1 are used in the simulation setup directly. The gas volume fraction at the inlet patches is 1. The gas volu-
4 Simulation of bubbly flow in a cylindrical bubble column

Table 4.2 Parameters for fixed polydisperse simulations of bubble column cases.

<table>
<thead>
<tr>
<th>Name</th>
<th>(d_B1) [mm]</th>
<th>(d_B2) [mm]</th>
<th>(f_{v1}) % [-]</th>
<th>(f_{v2}) % [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC1</td>
<td>3.63</td>
<td>5.55</td>
<td>86.0</td>
<td>14.0</td>
</tr>
<tr>
<td>BC2</td>
<td>3.84</td>
<td>5.88</td>
<td>54.0</td>
<td>46.0</td>
</tr>
</tbody>
</table>

Metric flow rate in the inlet patches is assumed to be the same and calculated by

\[
q_{v,d} = \frac{1}{31} \pi R^2 J_d, \tag{4.1}
\]

where \(q_{v,d}\) is the gas volumetric flow rate in each inlet patch and \(R\) is the radius of the bubble column.

Restricted by the computational cost, only two bubble velocity groups are used for fixed polydisperse simulations. The bubble size range for these velocity groups is \(d_B > 5.2\) mm and \(0\) mm \(< d_B \leq 5.2\) mm, respectively. For each velocity group, the way to calculate the volumetric flow rate fraction, the representative bubble diameter, and the inlet gas volume fraction is the same as the fixed polydisperse simulations of the MTLoop experimental cases in Section 3.2. The calculated volumetric flow rate fraction and representative bubble diameter for each velocity group are listed in Table 4.2.

The simulations were run in stationary mode. The properties of air are used for the disperse phase. The simulated gas volume fraction and axial gas velocity were also azimuthally averaged in the same post-processing way as the measurement data.

4.3 Mesh sensitivity analysis

For the simulations, a structured grid is used because it has a relatively high mesh quality. To generate the structured grid, the cylindrical computational domain is split into 5 blocks. The block division is marked with the black lines in Fig. 4.2. For the inner block, each side has a curvature of 0.0223. To find a proper mesh resolution for the following simulations, four different mesh resolutions are used to test the influence of the cell numbers on the simulation results of the same case. For the mesh sensitivity analysis, the number of the axial cells is fixed at 280. According to test results (not shown here), continuing to increase the number of the axial cells has little influence on the simulation results at the level of \(z = 0.7\) m. The axial cell spacing is uniform. Moreover, the number of the radial computational cells does not increase with a constant factor. The reason is that it is hard to control such a factor because it has to be ensured that each inlet patch covers only one computational cell. For each mesh resolution, the number of the computational cells in the block side and the total number of the computational cells are listed in Table 4.3. In the following, the mesh sensitivity of the simulated gas volume fraction and axial gas velocity for case BC1 are analyzed.
4.3 Mesh sensitivity analysis

Table 4.3

Mesh resolutions used in the sensitivity analysis ($N_{\text{inner}}$: the number of computational cells for each side of the inner square; $N_{\text{outer}}$: the number of computational cells for the side between the inner square and the outer circle; $N_{\text{axial}}$: the number of computational cells in the axial direction; $N_{\text{total}}$: total number of computational cells).

<table>
<thead>
<tr>
<th>Name</th>
<th>$N_{\text{inner}}$ [-]</th>
<th>$N_{\text{outer}}$ [-]</th>
<th>$N_{\text{axial}}$ [-]</th>
<th>$N_{\text{total}}$ [-]</th>
<th>$\Delta cs$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>BC1-M1</td>
<td>11</td>
<td>9</td>
<td>280</td>
<td>144,760</td>
<td>3.90</td>
</tr>
<tr>
<td>BC1-M2</td>
<td>13</td>
<td>11</td>
<td>280</td>
<td>207,480</td>
<td>3.26</td>
</tr>
<tr>
<td>BC1-M3</td>
<td>19</td>
<td>18</td>
<td>280</td>
<td>484,120</td>
<td>2.13</td>
</tr>
<tr>
<td>BC1-M4</td>
<td>23</td>
<td>21</td>
<td>280</td>
<td>689,080</td>
<td>1.79</td>
</tr>
</tbody>
</table>

(a) Standard Euler-Euler model

(b) Euler-Euler model based on PCAM

Figure 4.3

Mesh sensitivity analysis for gas volume fraction.

For both Euler-Euler models, the mesh sensitivity of the gas volume fractions simulated with the mesh resolutions listed in Table 4.3 for case BC1 is given in Fig. 4.3. In the simulation results of both Euler-Euler models, the gas volume fraction simulated with mesh BC1-M3 coincides with that simulated with mesh BC1-M4. Therefore, the gas volume fractions simulated with mesh BC1-M3 and mesh BC1-M4 are mesh-independent.

Figure 4.4 shows the axial gas velocity profiles simulated by both Euler-Euler models with different mesh resolutions. In the simulation results of both Euler-Euler models, the gas velocity simulated with mesh BC1-M3 is also almost the same as the one simulated with mesh BC1-M4. Therefore, the gas velocities simulated with mesh BC1-M3 and mesh BC1-M4 are mesh-independent as well.

For the following simulations of the bubble column cases, mesh BC1-M4 is used because the ratio between the bubble diameter and the radial cell spacing given by this mesh resolution, which is listed in Table 4.1, is higher than that given by mesh BC1-M3. Note, the cross-section averaged cell spacing is used to calculate the ratio because the cross-sectional distribution of the cell size is non-uniform. The ratio for cases BC1 and BC2 is
2.3 and 2.6, respectively, which is smaller than the ratio used in the simulations in the last chapter. However, it is not necessary to further decrease the cell size because the mesh-independent solutions have been obtained with mesh BC1-M4.

### 4.4 Monodisperse simulation

This section compares the monodisperse simulation results of the Euler-Euler model based on PCAM and the standard Euler-Euler model with the experimental data. The comparisons for the gas volume fractions are shown in Fig. 4.5. Here and in the following, the simulated profiles are not smooth because the presented simulation results are azimuthally averaged values for the 10 parts of the cross-section regions mentioned in Subsection 4.1. For case BC1, the gas volume fractions simulated with both Euler-Euler models are close to each other and good agreements are obtained between the simulation results and the experimental data. For case BC2, the gas volume fractions simulated with both Euler-Euler models are also about the same. They agree well with the experimental data in the pipe-center region with $0 < r/R < 0.8$, but near the wall, they are under-estimated. The cross-section averaged gas volume fractions in the simulation results are lower than the averaged value of the experimental data. This indicates that the drag force used in the simulations is not strong enough. The bubble interactions, which increase the drag coefficient, have not been considered in the simulations. Moreover, the wall peak of the simulated profiles is not as significant as the peak in the experimental data. This is because the bubble diameter, which is determined from the experimental data, can be over-estimated by around 10%. Whereas the shear-lift force used in the simulations is sensitive to the bubble diameter, and the 10% over-estimation can change the shape of the wall peak for the simulated profiles.

For both cases, over-estimation of the gas volume fraction peak does not appear in the simulation results. The reason is that the turbulent dispersion for both cases is strong
4.4 Monodisperse simulation

Figure 4.5 Gas volume fraction for monodisperse simulations ("E-E": Euler-Euler model).

and the over-prediction of the gas volume fraction peak caused by the inconsistency of the bubble force models used in the standard Euler-Euler simulation has been smoothed by the turbulent dispersion. The turbulent dispersion is stronger when the turbulence intensity is higher. The turbulence intensity for both cases simulated with the standard Euler-Euler model can be higher than 12 near the wall (Fig. 4.6). This turbulence intensity is much higher than the one in the wall-peaking MTLoop cases (< 0.14) where the over-prediction of the gas volume fraction peak exists.

Figure 4.7 presents the simulated axial gas velocity profiles in comparison with the experimental data. For both cases, the gas velocities simulated with both Euler-Euler models fit each other except in the near-wall region with $0.95 < r/R < 1$. Near the wall, the gas velocity simulated with the Euler-Euler model based on PCAM is smaller than that simulated with the standard Euler-Euler model. The reason is that the influence region of the wall effects on the particle-center-averaged gas velocity (results for the Euler-Euler model based on PCAM) is wider than the region for the phase-averaged gas velocity (results for the standard Euler-Euler model), because the particle-center-averaged and the phase-averaged
4. Simulation of bubbly flow in a cylindrical bubble column

Figure 4.7  Axial gas velocity for monodisperse simulations ("E-E": Euler-Euler model; right side of the black dotted line: $n < 10^{-6}$ $m^{-3}$; measurement uncertainty: 2.5%).

gas velocity are determined by the resultant drag force and the local drag force, respectively. For case BC1, the shape of the gas velocity profiles simulated with both Euler-Euler models is similar to the measurement one, but over-estimations exist in the pipe-center region. For case BC2, the simulated gas velocities in the pipe-center region with $0 < r/R < 0.4$ are also over-estimated, while near the wall, they are under-estimated. The gas superficial velocity increases from case BC1 to case BC2, but the measurement gas velocity for case BC2 is slightly lower than that for case BC1, which indicates that the bubble motions are influenced by the bubble interactions. For both cases, the deviation between the simulation results and the experimental data is because the drag force model used in the simulations is the model for a single bubble. The bubble interactions, including the wake characteristic of the turbulent eddies and motions of the other bubbles in the system, increase the drag force. These interactions have not been included in the simulations.

4.5 Fixed polydisperse simulation

This section compares the fixed polydisperse simulation results of the Euler-Euler model based on PCAM and the standard Euler-Euler model with the experimental data. Figure 4.8 shows the comparisons for the simulated and the measurement gas volume fractions. For case BC1, the gas volume fractions simulated with both Euler-Euler models are close to each other. Compared with the monodisperse simulation results, the peak of the simulated gas volume fraction profiles slightly decreases. Good agreements are still obtained between the simulation results and the experimental data except that the peak of the simulated profiles is slightly lower than the peak in the experimental data. The under-prediction results from the measurement uncertainty of the bubble diameter. For case BC2, the simulated gas volume fractions with both Euler-Euler models are approximately the same. Compared with the monodisperse simulation results, the simulated gas volume
fractions slightly increase in the pipe-center region with $0 < r/R < 0.4$, while they decrease a little near the wall with $0.7 < r/R < 0.8$. For both cases, no improvement is found after using two bubble velocity groups in the simulations. This indicates that facilitating the bubbles to move in different directions cannot decrease the deviation between the simulation results and the experimental data, so the direction of bubble motions is not the main reason for the deviation.

The comparisons for the simulated and measurement axial gas velocities are presented in Fig. 4.9. For both cases, the gas velocities simulated with both Euler-Euler models approximately coincide with each other except in the near-wall region with $0.95 < r/R < 1$, which also results from the difference in the influence region of the wall effects. Near the wall, the difference in the simulated velocities is smaller than that in the monodisperse simulation.
results. This originates from the fact that the diameter of the bubbles moving near the wall for fixed polydisperse simulations is smaller than that for the monodisperse simulations. For case BC1, the gas velocities are almost the same as the monodisperse simulation results. For case BC2, compared with the monodisperse simulation results, the simulated gas velocities slightly increase in the pipe-center region with $0 < r/R < 0.4$, while they decrease a little in the region with $0.7 < r/R < 0.8$. As a result, the agreement between the simulated gas velocities and the experimental data becomes slightly worse. This phenomenon also supports that the deviation between the simulation results and the experimental data is not introduced by using not enough bubble velocity groups in the simulations.

### 4.6 Conclusion

In this chapter, the results simulated by the Euler-Euler model based on PCAM and the standard Euler-Euler model have been compared with the data obtained in the bubbly flow experiment in a cylindrical bubble column. The gas volume fractions and the axial gas velocities for monodisperse and fixed polydisperse simulations are compared, respectively. The comparisons show that in the monodisperse and the fixed polydisperse simulation results, the gas volume fractions simulated with both Euler-Euler models are similar. The axial gas velocities simulated with both Euler-Euler models are also close to each other. The results indicate that the sink and source terms used for the continuity equations and the degassing boundary in the Euler-Euler model based on PCAM are correct. Furthermore, the results of the fixed polydisperse simulations using two bubble velocity groups are close to those of monodisperse simulations.

Using the PCAM in the Euler-Euler simulations does not improve the simulation results for the cases in this chapter because over-prediction of the gas volume fraction peak does not exist in the standard Euler-Euler simulation results. The reason can be that the turbulent dispersion has smoothed the over-prediction caused by the inconsistency in the bubble force models used in the standard Euler-Euler simulations. In the future, a bubble column case with a low turbulent dispersion should be used in the validation.
5 Simulations considering bubble deformation

In the Euler-Euler model based on PCAM, the conversions between phase-averaged and particle-center-averaged quantities are realized by a Gaussian convolution method. During quantity conversion, bubble deformation can be considered. In the previous chapters, the bubble shape was assumed to be spherical for quantity conversion. However, bubble deformation usually occurs when the bubble diameter is larger than 1.3 mm. A way to consider an oblate ellipsoidal bubble shape for quantity conversion has been described in Subsection 2.4.5. In this chapter, the influence of bubble shape on the results of the Euler-Euler simulations based on PCAM is discussed.

5.1 Verification

A simplified two-dimensional test case is used to verify the method of considering an oblate ellipsoidal bubble shape in simulations. The fluid domain of the test case is a square with a size of $0.02 \, \text{m} \times 0.02 \, \text{m}$. An empty boundary is used for all boundaries of the domain. In the empty boundary condition, quantities have no variability in the direction perpendicular to the boundary face (Damián et al., 2012). Air and water are the disperse and the continuous phase, respectively. In the simulation, both air and water are at rest. Only the process of diffusing the bubble volume from the bubbles' centers of mass was simulated. The initial value for the $\alpha_d$ is zero for all locations. Furthermore, the initial value for $\beta_d$ in the center cell is 1, and it is 0 in the other cells. The bubble diameter is 10 mm. The number of cells at each side of the fluid domain is 81, and the cell spacing is uniform. Under this condition, the ratio between the bubble diameter and the cell spacing is 40.5. In this test case, the gas volume fractions for the bubble with a spherical and an oblate ellipsoidal shape are solved, respectively.
Simulations considering bubble deformation

(a) Spherical shape  (b) Oblate ellipsoidal shape

Figure 5.1  Gas volume fraction distribution simulated with different bubble shapes.

The gas volume fraction distributions simulated with a spherical and an oblate ellipsoidal bubble shape are shown in Fig. 5.1. For the spherical bubble shape, each isoline of the simulated gas volume fraction forms a circle. Whereas, for the oblate ellipsoidal bubble shape, each isoline forms an ellipse. Moreover, the orientation of the ellipse is as expected. These results prove that the method of considering the oblate ellipsoidal bubble shape in the simulations works as expected.

5.2 Monodisperse simulation

This section compares the monodisperse simulation results for a spherical and an oblate ellipsoidal bubble shape with the experimental data. The selected cases for the comparison are the MTLoop cases. The parameters and the simulation setup for the cases have been explained in Chapter 3. The radial distribution of the gas volume fraction for the selected cases is wall-peaking or center-peaking. The simulated gas volume fractions and axial gas velocities are compared with the experimental data, respectively.

5.2.1 Comparison of wall-peaking cases

Figure 5.2 gives the comparisons for the gas volume fractions. The peak of the gas volume fraction profiles simulated with the oblate ellipsoidal bubble shape is lower than that simulated with the spherical bubble shape. The reason is that compared with the spherical bubble shape, the oblate ellipsoidal bubble shape spreads more gas to the radial direction from the bubbles’ centers of mass. As a result, for all cases except for case MT19, the over-predictions of the gas volume fraction peaks are alleviated. As mentioned in Subsection 3.4.1, the peak of the gas volume fraction profiles simulated with the spherical
5.2 Monodisperse simulation

Figure 5.2  Gas volume fraction simulated with different bubble shapes for wall-peaking cases.
Figure 5.3  Axial gas velocity simulated with different bubble shapes for wall-peaking cases (right side of the black dotted line: \( n < 10^{-6} \) m\(^{-3}\)).
bubble shape is about 1.07, 2.12, 1.99, 1.55, and 1.65 times the peak in the experimental data for cases MT17, MT20, MT42, MT64, and MT120, respectively. In contrast, the peak of the gas volume fraction profiles simulated with the oblate ellipsoidal bubble shape is around 0.99, 1.59, 1.59, 1.30, and 1.50 times the peak in the experimental data. For case MT19, the peak of the gas volume fraction profile simulated with the oblate ellipsoidal bubble shape is under-estimated. It is about 0.89 times the peak in the experimental data. This results from assuming a monodisperse bubble size in the simulation and the measurement uncertainty in the experimental data.

Near the wall with \(0.92 < r/R < 1\), the gas volume fractions simulated with the oblate ellipsoidal bubble shape are higher than those simulated with the spherical bubble shape. This contributes to a better agreement between the simulation results and the experimental data except for case MT120. For case MT120, near the wall, the gas volume fraction is over-estimated. This is because the drag force used in the simulations is too strong.

The comparisons of the simulated and measurement axial gas velocities are shown in Fig. 5.3. The gas velocities simulated with both bubble shapes are approximately the same. The reason is that the effects of bubble deformation have been included in the drag force model used in the simulations for both bubble shapes.

### 5.2.2 Comparison of center-peaking cases

For center-peaking cases, the comparison of the gas volume fractions for the spherical and the oblate ellipsoidal bubble shape and the experimental data is presented in Fig. 5.4. The simulation results for both bubble shapes are almost the same, except that a small difference exists near the wall with \(0.92 < r/R < 1\) for cases MT107 and MT142. The bubble diameter for the center-peaking cases is larger than the diameter for the wall-peaking cases. However, the influence of the bubble shape on the gas volume fraction for the center-peaking cases is less significant than that for the wall-peaking cases. The reason is that the influence for the center-peaking cases is canceled because the bubble number density profiles are relatively flat.

As shown in Fig. 5.5, the peak of the bubble number density profiles for the wall-peaking cases is more significant than the peak for the center-peaking cases. The relation between the bubble shape effects and the bubble number density profile is explained as follows: in the mathematical limit that all bubbles’ centers of mass are located at the same location, the effects of the bubble shape on the gas volume fraction distribution will be accumulated. Consequently, the effects will be the most significant. In contrast, if the bubbles’ centers of mass are uniformly distributed in the radial direction, the effect of a bubble that decreases the gas volume fraction can be canceled by the effect of a nearby bubble that increases the gas volume fraction. Furthermore, for cases MT107 and MT142, the effects of the bubble shape on the gas volume fraction distribution appear near the wall with \(0.92 < r/R < 1\) because, in this region, the slope of the bubble number density profiles for both cases is higher than that for cases MT35 and MT48.
5 Simulations considering bubble deformation

Figure 5.4 Gas volume fraction simulated with different bubble shapes for center-peaking cases.

Figure 5.5 Bubble number density simulated with an oblate ellipsoidal bubble shape.
5.3 Fixed polydisperse simulation

This section compares the fixed polydisperse simulation results simulated with a spherical and an oblate ellipsoidal bubble shape with the experimental data. The cases selected for comparisons are also taken from the MTLoop experiment. The parameters and the simulation setup for the cases have been introduced in Chapter 3.

Figure 5.6 shows the gas volume fraction profiles simulated with both bubble shapes in comparison with the experimental data. For case MT38, the gas volume fractions simulated with both bubble shapes almost coincide with each other. This also originates from the fact that the bubble number density profile of case MT38 is relatively flat. For case MT86, the peak of the profile simulated with the oblate ellipsoidal bubble shape is lower than that simulated with the spherical bubble shape. Near the wall with $0.92 < r/R < 1$, the gas volume fraction simulated with the oblate ellipsoidal bubble shape is higher than that simulated with the spherical bubble shape. The difference in the simulated gas volume
fractions is introduced by the results of the second bubble velocity group which has a bubble size range as $3 \text{ mm} < d_B \leq 5.2 \text{ mm}$. For this velocity group, the peak of the gas volume fraction profile simulated with the spherical bubble shape is 1.36 times the peak in the experimental data. In contrast, the peak simulated with the oblate ellipsoidal bubble shape is 1.18 times the peak in the experimental data. This proves that the over-prediction of the gas volume fraction peak is alleviated by using the oblate ellipsoidal bubble shape in the simulations.

### 5.4 Conclusion

In this chapter, the simulation results of bubbly pipe flows for the Euler-Euler model based on PCAM using an oblate ellipsoidal and a spherical bubble shape have been compared. For monodisperse simulations, it is found that using the oblate ellipsoidal bubble shape can alleviate the over-prediction of the gas volume fraction peak for wall-peaking cases. Whereas, the gas volume fractions simulated with both bubble shapes for the center-peaking cases are similar because the bubble number density profiles for the cases are relatively flat. Moreover, The axial gas velocities simulated with both bubble shapes are about the same because the effects of the bubble deformation have been included in the drag force model. For the fixed polydisperse simulations, using the oblate ellipsoidal bubble shape can also decrease the over-prediction of gas volume fraction peak near the wall. Overall, the oblate ellipsoidal bubble shape spreads more gas in the radial direction than the spherical bubble shape.
6 Conclusion and outlook

6.1 Summary and conclusion

In this thesis, a particle-center-averaged Euler-Euler approach for bubbly flow simulations has been developed by combining the particle-center-averaged Euler-Euler framework with a Gaussian convolution method. For the implementation of this approach, correction terms have been proposed for the drag and the virtual mass force of the continuous phase to keep the simulations stable and the forces consistent. For the simulations with this approach, a wall contact force model has been derived for oblate ellipsoidal bubbles to avoid the bubbles’ centers of mass being located nonphysically close to the wall. This approach has been tested and validated carefully. A simplified two-dimensional case has been used to test this approach. The test results illustrate that the particle-center-averaging method alleviates the over-prediction of the gas volume fraction peak in the channel center and provides a mesh-independent solution.

Experimental data from bubbly flows in different vertical pipes have been used to validate this approach. The simulation results of this approach and the standard Euler-Euler model have been compared with the experimental data. For monodisperse simulations, the particle-center-averaging method alleviates the over-predictions of the gas volume fraction peaks for wall-peaking cases and finely dispersed flow case. Whereas, no improvement in the prediction of the gas volume fraction for the center peaking cases with the particle-center-averaging method is found. The reason is that the over-prediction of the gas volume fraction caused by the inconsistency of bubble force models used in the standard Euler-Euler simulations has been smoothed by the turbulent dispersion. The axial gas and liquid velocities simulated with the particle-center-averaged approach and the standard Euler-Euler model are close to each other, which indicates that the closure models for bubble forces and turbulence are correctly applied in the particle-center-averaged Euler-Euler approach.
In the standard Euler-Euler simulation results, the over-prediction of the gas volume fraction peak can be more significant for fixed polydisperse simulations than that for monodisperse simulations. This is because the magnitude of the shear-lift force for the fixed polydisperse simulations is higher than that for the monodisperse simulations. For the fixed polydisperse simulations, the particle-center-averaged Euler-Euler model can alleviate the over-prediction of the gas volume fraction peak in the center or near the wall of a pipe. The axial gas velocities simulated with the particle-center-averaged Euler-Euler model and the standard Euler-Euler model are also similar.

Experimental data from bubbly flows in a cylindrical bubble column have also been used in the validation. An over-prediction of the gas volume fraction peak does not appear in the results simulated with the standard Euler-Euler model, which is also due to the high turbulent dispersion. For monodisperse and fixed polydisperse simulations, the gas volume fractions and the axial gas velocities simulated with both Euler-Euler models are close to each other, which proves that the settings of the sink and source terms for the continuity equations and the degassing boundary in the particle-center-averaged Euler-Euler model are correct.

Eventually, anisotropic diffusion has been introduced for the conversion between phase-averaged and particle-center-averaged quantities to consider bubble deformation for the particle-center-averaged Euler-Euler simulations. The theory of the diffusion tensor imaging method has been applied to determine the diffusion tensor for an oblate ellipsoidal bubble shape. The effects of the bubble shape on the bubbly pipe flow simulation results have been investigated. The results show that using the oblate ellipsoidal bubble shape in simulations can further alleviate the over-predictions of gas volume fraction peaks for wall-peaking cases. However, the bubble shape has little influence on the simulated gas volume fractions for the center-peaking cases because the bubble number density profiles of the cases are relatively flat. It also has little influence on the simulated axial gas velocities since the bubble deformation effects have been included in the drag force model.

In summary, the simulation results for the standard Euler-Euler model show that the inconsistency of the bubble force models can have a considerable influence on the simulation results when the bubble diameter is larger than the computational cell size, the turbulent dispersion is relatively low and the shear-lift force is strong. The consistency of the bubble force models should be recovered because it better reveals the physics. The test and validation results illustrate that the consistency of the bubble force models is recovered with the particle-center-averaged Euler-Euler approach. Based on this approach, the bubble dimension and deformation can be fully considered in simulations. Besides, this approach serves as a better Euler-Euler framework for improving or validating the closure models for future study. This approach also provides a possible way to consider a zig-zag or a helical bubble path in the simulations by setting a proper diffusion domain and a diffusion pseudo-time.

However, it should not be expected that the particle-center-averaged Euler-Euler approach leads to better agreements for all bubbly flow cases because this approach solves only
one problem for the bubbly flow modeling. In the validations, some results simulated with the particle-center-averaged Euler-Euler model do not agree better with the experimental data than the results of the standard Euler-Euler model, which comes from inconsistencies in the bubble force models and the measurement uncertainty in the experimental data. Further research to decrease the deviation between the simulation results and the experimental data is beyond the scope of the thesis work.

6.2 Outlook

The particle-center-averaged Euler-Euler approach has been implemented correctly and reasonable simulation results have been obtained in the validations. To apply this approach in further research, the following directions are worth trying:

1. The implementation of the particle-center-averaged Euler-Euler approach can be optimized to reduce the computational time.

2. Developing a new solution procedure for the particle-center-averaged Euler-Euler approach without using the assumption of shared pressure between phase-averaged and particle-center-averaged fields will be an interesting and challenging research topic.

3. The bubbly flows used for validations in this thesis have high bubble Reynolds numbers (around $10^3$). Further validations can try to focus on bubbly flows with lower bubble Reynolds numbers. In addition, a case with a low turbulence intensity will be suitable to investigate the effects of using the particle-center-averaging method in the simulations of bubbly flows in a bubble column.

4. The particle-center-averaged Euler-Euler model can be coupled with the population balance model to consider the bubble coalescence and breakup in simulations.
A.1 Turbulent dispersion force for the particle-center-averaged Euler-Euler model

In this appendix, the derivation of turbulent dispersion force for the particle-center-averaged Euler-Euler model will be introduced. The derivation procedure is according to the procedure in Burns et al. (2004) which is used to derive the turbulent dispersion force for the standard Euler-Euler model.

A.1.1 Relation between time-averaging and Favre-averaging

For incompressible flows, the Favre-averaging of a particle-center-averaged variable \( \langle \varphi_d \rangle \) is defined by

\[
\langle \varphi_d \rangle^F = \frac{n\langle \varphi_d \rangle^t}{\bar{n}}, \tag{A.1.1}
\]

where the overbar and the superscript F denote Favre-averaging, while the overbar and the superscript t represent time-averaging. Substituting

\[
\bar{n}\langle \varphi_d \rangle^t = \overline{n} \langle \varphi_d \rangle^t + \overline{n}' \langle \varphi_d \rangle'^t \tag{A.1.2}
\]

into Eq. (A.1.1), we obtain

\[
\langle \varphi_d \rangle^t = \langle \varphi_d \rangle^F - \frac{\overline{n}' \langle \varphi_d \rangle'^t}{\bar{n}}. \tag{A.1.3}
\]
A single dash (′) here denotes the fluctuating quantity relative to the time-averaged quantity. Replacing \( \langle \varphi_d \rangle \) in the last equation with \( \langle u_d \rangle \), we obtain

\[
\langle u_d \rangle_t = \langle u_d \rangle^F - \frac{n'\langle u_d \rangle_t}{n}.
\]  
(A.1.4)

This is the relation between time-averaging and Favre-averaging for the particle-center-averaged quantities. According to Burns et al. (2004), for phase-averaged liquid velocity \( \langle u_c \rangle \), the relation between time-averaged and Favre-averaged velocities is

\[
\overline{u_c} = \overline{u_c}^F - \frac{\alpha_c \overline{u_c}^t}{\overline{\alpha_c}}.
\]  
(A.1.5)

Herein, the double overbars and the superscript t denote the double averaging with the phase-averaging as the first averaging method and the time averaging as the second averaging method. Similarly, the double overbars and the superscript F denote the double averaging with the phase-averaging as the first averaging method and the Favre-averaging as the second averaging method.

### A.1.2 Formulation of turbulent dispersion force

The drag force for the disperse phase for the Euler-Euler model based on PCAM is

\[
\bigg\langle f_d^0 \bigg\rangle = -D_{cd,p} A_{cd} (\langle u_d \rangle - \langle u_c \rangle),
\]  
(A.1.6)

where

\[
D_{cd,p} = \frac{1}{8} C_D \rho_c |\langle u_d \rangle - \langle u_c \rangle|,
\]  
(A.1.7)

and

\[
A_{cd} = \pi n d_B^2.
\]  
(A.1.8)

Herein, the phase-averaged liquid velocity is used for the drag force. The reason is that as shown in Section A.1.1, the original definition of the velocity is required to derive the relation between the time-averaged and the Favre-averaged velocity. Using Eq. (2.7) to define a particle-center-averaged quantity is physical only for the disperse phase. A particle-center-averaged liquid velocity should be interpreted as the liquid velocity in the bubbles’ centers of mass that considers the contribution of the phase-averaged liquid velocity in a certain influence region around the bubbles’ centers of mass. It is a weighted averaged liquid velocity calculated using a Gaussian function as the weighting factor. The simplification of using a phase-averaged liquid velocity to calculate the resultant drag force of a single bubble acting on the bubbles’ centers of mass was also used by Xue et al. (2017).

It is assumed that \( D_{cd,p} \) does not change with time. Applying time-averaging to Eq. (A.1.6)
A.1.2 Formulation of turbulent dispersion force

yields
\[
\langle f_d^D \rangle = -D_{cd,p} \left[ A_{cd} \left( \langle u_d^i \rangle - \bar{u}_c^i \right) + A_{cd}' \left( \langle u_d' \rangle - \bar{u}_c' \right) \right].
\] (A.1.9)

Substituting Eqs. (A.1.4) and (A.1.5) into Eq. (A.1.9), we obtain
\[
\langle f_d^D \rangle = -D_{cd,p} A_{cd} \left[ \left( \frac{n'(u_d^i)}{\bar{n}^i} - \frac{\alpha_c u_c^i}{\bar{u}_c^i} \right) - \left( \frac{n'(u_d')}{\bar{n}^i} - \frac{\alpha_c u_c'}{\bar{u}_c'} \right) \right] - D_{cd,p} A_{cd}' \left( \langle u_d' \rangle - \bar{u}_c' \right). \] (A.1.10)

Equation (A.1.10) can be simplified to
\[
\langle f_d^D \rangle = -D_{cd,p} A_{cd} \left[ \left( \frac{n'(u_d^i)}{\bar{n}^i} - \frac{\alpha_c u_c^i}{\bar{u}_c^i} \right) - \left( \frac{n'(u_d')}{\bar{n}^i} - \frac{\alpha_c u_c'}{\bar{u}_c'} \right) \right] + f_d^{TD}, \] (A.1.11)

where
\[
f_d^{TD} = D_{cd,p} A_{cd} \left( \frac{n'(u_d^i)}{\bar{n}^i} - \frac{\alpha_c u_c^i}{\bar{u}_c^i} \right) - D_{cd,p} A_{cd}' \left( \langle u_d' \rangle - \bar{u}_c' \right). \] (A.1.12)

Substituting
\[
\tau_{cd,p} = D_{cd,p} A_{cd} \] (A.1.13)

into Eq. (A.1.12) leads to
\[
f_d^{TD} = \tau_{cd,p} \left( \frac{n'(u_d^i)}{\bar{n}^i} - \frac{\alpha_c u_c^i}{\bar{u}_c^i} \right) - \tau_{cd,p} A_{cd}' \left( \langle u_d' \rangle - \bar{u}_c' \right). \] (A.1.14)

The bubble diameter is a constant. Therefore
\[
A_{cd}' = n' \pi d_B^2, \] (A.1.15)

and
\[
A_{cd}^i = n' \pi d_B^2. \] (A.1.16)

Based on Eqs. (A.1.15) and (A.1.16), we have
\[
\frac{A_{cd}'}{A_{cd}^i} \left( \langle u_d' \rangle - \bar{u}_c' \right) = \frac{n'}{\bar{n}^i} \left( \langle u_d^i \rangle - \bar{u}_c^i \right). \] (A.1.17)

Substituting Eq. (A.1.17) into Eq. (A.1.14) and simplifying it, we obtain
\[
f_d^{TD} = \tau_{cd,p} \left( \frac{n u_c^i}{\bar{n}^i} - \frac{\alpha_c u_c^i}{\bar{u}_c^i} \right). \] (A.1.18)

Using the eddy diffusivity hypothesis in the modeling of the turbulence related terms, we
have
\[ n' \overline{\nabla n} = - \frac{\nu_{\text{turb}}}{\sigma_{\text{nc}}} \overline{\nabla n}, \] (A.1.19)
and
\[ \alpha' \overline{\nabla \alpha} = \frac{\nu_{\text{turb}}}{\sigma_{\alpha}} \overline{\nabla \alpha}. \] (A.1.20)

Herein, \( \nu_{\text{turb}} \) is the turbulent eddy viscosity, while \( \sigma_{\text{nc}} \) and \( \sigma_{\alpha} \) are the Schmidt number for the dispersion of bubble number density and volume fraction, respectively. After substituting Eqs. (A.1.19) and (A.1.20) into Eq. (A.1.18), we have
\[ f_{\text{TD}} = -C_{\text{cd}, p} \left( \frac{\nu_{\text{turb}}}{\sigma_{\text{nc}}} \overline{\nabla n} \overline{n} - \frac{\nu_{\text{turb}}}{\sigma_{\alpha}} \overline{\nabla \alpha} \right). \] (A.1.21)

Here, we assumed that
\[ \sigma_{\text{nc}} = \sigma_{\alpha}. \] (A.1.22)

Since \( \beta = nV \) and the bubble volume \( V \) is a constant, we have
\[ \overline{\nabla n} = \frac{\overline{\nabla \beta}}{\overline{\beta}}. \] (A.1.23)

Substituting Eqs. (A.1.22) and (A.1.23) into Eq. (A.1.21), we obtain
\[ f_{\text{TD}} = -C_{\text{cd}, p} \frac{\nu_{\text{turb}}}{\sigma_{\alpha}} \left( \frac{\overline{\nabla \beta}}{\overline{\beta}} - \frac{\overline{\nabla \alpha}}{\overline{\alpha}} \right). \] (A.1.24)

For Eq. (A.1.24), after omitting the time-averaging symbol and applying the particle-center-averaging quantities to express the terms, we obtain
\[ \langle f_{\text{TD}} \rangle = \frac{3\beta d}{4d^3} C_{\text{D}} \rho c \left( u_d - \langle u_c \rangle \right) \left( \frac{\nu_{\text{turb}}}{\sigma_{\alpha}} \right) \left( \frac{\overline{\nabla \beta}}{\overline{\beta}} - \frac{\overline{\nabla \alpha}}{\overline{\alpha}} \right). \] (A.1.25)

The differences between Eq. (A.1.25) and the turbulent dispersion force model of Burns et al. (2004) are that \( \alpha_d \) is changed to \( \beta_d \) and \( \nabla \alpha_d \) is also changed to \( \nabla \beta_d \).
A.2 Wall-contact force for oblate ellipsoidal bubbles

The wall-contact force proposed by Lucas et al. (2007) is based on the prolate ellipsoidal bubble shape. However, an oblate ellipsoidal bubble shape is encountered more often in bubbly flows. In this appendix, the wall-contact force for oblate ellipsoidal bubbles is derived based on the way used in Lucas et al. (2007).

In the process of a bubble hitting the wall, the bubble usually deforms after it has contacted the wall and its surface area increases. It is assumed that the energy required to enlarge this bubble's surface area equals the work done by the wall-contact force. In the following, the relation between the bubble surface area and the distance between the bubble's center-of-mass and the wall is established. Afterward, the formulation of the wall-contact force for oblate ellipsoidal bubbles is derived.

A.2.1 Relation between bubble surface area and wall distance

The surface area of an oblate ellipsoid is calculated by

\[ S_{\text{oblate}} = 2\pi a^2 \left[ 1 + \frac{c^2}{ea^2} \arctanh(e) \right], \quad (A.2.1) \]

where

\[ e = \sqrt{1 - \frac{c^2}{a^2}}. \quad (A.2.2) \]

Herein, \( S_{\text{oblate}} \) is the surface area, \( a \) is the semi-major axis of the oblate ellipsoid, while \( c \) is the semi-minor axis of the ellipsoid.
The bubble shape is assumed to be oblate ellipsoidal with its semi-minor axis equal to the distance between this bubble’s center-of-mass and the wall (Fig. A.2.1). That is,

\[ c = L, \]  

(A.2.3)

where \( L \) is the distance between the bubble’s center-of-mass and the wall.

Since the bubble radius \( r_B \) is more common than \( a \), it is used to replace \( a \) in Eq. (A.2.1). The relation between \( r_B \) and \( a \) is established based on the assumption that the volume of the oblate ellipsoidal bubble equals that of the spherical bubble

\[ \frac{4}{3} \pi a^2 c = \frac{4}{3} \pi r_B^3. \]  

(A.2.4)

After substituting Eq. (A.2.3) into Eq. (A.2.4) and simplifying the equation, we obtain

\[ a^2 = \frac{r_B^3}{L}. \]  

(A.2.5)

Substituting Eqs. (A.2.3) and (A.2.5) into Eq. (A.2.2) and simplifying the resulting equation, we have

\[ e = \sqrt{1 - \left( \frac{L}{r_B} \right)^3}. \]  

(A.2.6)

Substituting Eqs. (A.2.3), (A.2.5) and (A.2.6) into Eq. (A.2.1), we obtain

\[ S_{oblate}(L) = 2 \pi \left[ \frac{r_B^3}{L} + \frac{L^2}{\sqrt{1 - \left( \frac{L}{r_B} \right)^3}} \arctanh \left( \sqrt{1 - \left( \frac{L}{r_B} \right)^3} \right) \right]. \]  

(A.2.7)

To simplify the equation, a dimensionless variable \( \tilde{L} \) is defined as \( \tilde{L} = L/r_B \). After using it to
A.2.2 Formulation of wall-contact force

When the wall-contact force acts, the bubble shape is assumed to be oblate ellipsoidal. Under this condition, if the center-of-mass of the bubble which contacts the wall moves a tiny distance from \( L \) to \( L + dL \) towards the wall, the increment of bubble surface area is

\[
\frac{dS}{dL} = S_{\text{oblate}}(L + dL) - S_{\text{oblate}}(L). \tag{A.2.9}
\]

In this process, the energy needed to enlarge this surface area can be computed by

\[
dW = \sigma \frac{dS}{dL}. \tag{A.2.10}
\]

As mentioned before, this energy is assumed to equal the work done by the wall-contact force. Since \( dL \) is a tiny distance, it is reasonable to assume that the wall-contact force is constant within the distance. Therefore, we have

\[
dW = -F_{\text{WC}} n_w dL, \tag{A.2.11}
\]

where \( F_{\text{WC}} \) is the resultant wall-contact force that acts on the bubble's center-of-mass. The wall-contact force is a wall repulsive force, and it is perpendicular to the wall. Therefore, Eq. (A.2.11) can be simplified to be

\[
F_{\text{WC}} = -\frac{dW}{dL} n_w. \tag{A.2.12}
\]

Substituting Eq. (A.2.10) into Eq. (A.2.12) and simplifying the equation, we have

\[
F_{\text{WC}} = -\sigma \frac{dS_{\text{oblate}}(L)}{dL} n_w. \tag{A.2.13}
\]

Since \( L = r_B \tilde{L} \) and \( r_B \) is a constant,

\[
dL = r_B d\tilde{L}. \tag{A.2.14}
\]

Therefore,

\[
\frac{dS_{\text{oblate}}(L)}{dL} = \frac{1}{r_B} \frac{dS_{\text{oblate}}(\tilde{L})}{d\tilde{L}}. \tag{A.2.15}
\]

From Eq. (A.2.8), we can derive the following equation

\[
\frac{dS_{\text{oblate}}(\tilde{L})}{d\tilde{L}} = -2\pi r_B^2 \left[ \frac{1}{L^2} - \frac{3}{2G} \left( \frac{4\sqrt{G}}{3} + \frac{\tilde{L}^3}{\sqrt{G}} \right) \right], \tag{A.2.16}
\]
where $G = 1 - \bar{L}^3$. Substituting Eqs. (A.2.15) and (A.2.16) into Eq. (A.2.13), we have

$$F_{WC}^B = 2\pi r_B \sigma \left[ \frac{1}{L^2} \left( \frac{4\sqrt{G}}{3} + \frac{\bar{L}^3}{\sqrt{G}} \right) \arctanh \left( \sqrt{G} \right) - 1 \right] \cdot n_w. \quad (A.2.17)$$
Reference


