

A particle-center-averaged Euler-Euler model for monodisperse bubbly flows

Lyu, H.; Lucas, D.; Rzehak, R.; Schlegel, F.;

Originally published:

October 2022

Chemical Engineering Science 260(2022), 117943

DOI: <https://doi.org/10.1016/j.ces.2022.117943>

Perma-Link to Publication Repository of HZDR:

<https://www.hzdr.de/publications/Publ-32958>

Release of the secondary publication
on the basis of the German Copyright Law § 38 Section 4.

CC BY-NC-ND

A particle-center-averaged Euler-Euler model for monodisperse bubbly flows

Hongmei Lyu*, Dirk Lucas, Roland Rzehak, Fabian Schlegel

*Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner
Landstrasse 400, 01328 Dresden*

Abstract

The standard Euler-Euler model is based on the phase-averaging method. Each bubble force is a function of the local gas volume fraction. As a result, the coherent motion of each bubble as a whole is not enforced when the bubble diameter is larger than the mesh size. However, the bubble force models are typically developed by tracking the bubbles' centers of mass and assuming that the forces act on these locations. In simulations, this inconsistency can lead to a nonphysical gas concentration in the center or near the wall of a pipe when the bubble diameter is larger than the mesh size. Besides, a mesh independent solution may not exist in such cases.

In the present contribution, a particle-center-averaging method is used to average the solution variables for the disperse phase, which allows to represent the bubble forces as forces that act on the bubbles' centers of mass. An approach to simulate bubbly flows is formed by combining the Euler-Euler model framework using the particle-center-averaging method and a diffusion-based method that relates phase-averaged and particle-center-averaged quantities. The remediation of the inconsistency with the standard Euler-Euler model based on phase-averaging method is demonstrated using a simplified two-dimensional test case. The test results illustrate that the particle-center-averaging method can alleviate the over-prediction of the gas volume fraction peak in the channel center and provide mesh independent solutions. Furthermore, a comparison of both approaches is shown for several bubbly pipe flow cases where experimental data are available. The results show that the

*Corresponding author

Email address: h.lyu@hzdr.de (Hongmei Lyu*)

particle-center-averaging method can alleviate the over-prediction of the gas volume fraction peaks in the wall peaking cases as well.

Keywords: particle-center-averaging, phase-averaging, bubble number density, diffusion equation, wall-contact force model, multiphase flow, Euler-Euler model

1. Introduction

Dispersed two-phase flows are widely encountered in chemical engineering, energy production, oil and gas industries and biotechnology. Exploring the flow mechanisms of two-phase flows can ensure safety and improve efficiency of industrial facilities. Many of these flow mechanisms are still not well understood due to their high complexity. Experimental investigations on two-phase flows face the difficulty to measure the flow and distribution of two phases. Hence, they are usually costly and time-consuming. In comparison, simulations provide a more accessible way to study such flows, but they invariably rely on models. Among the simulation methods, the Eulerian two-fluid model shows advantages for simulating bubbly flows up to industrial dimensions with affordable computational cost.

For bubbly flows, air is considered to be the dispersed phase and water is considered to be the continuous phase. In the standard Eulerian two-fluid model, the phase-averaging method is used for both phases. Each bubble force is a function of the gas volume fraction. In this way, the coherent motion of each bubble as a whole is not enforced when the bubble diameter is larger than the mesh size. Hence, the gas belonging to a single bubble can accumulate in a region smaller than the bubble dimension. However, a closure model for a bubble force is typically developed by tracking the trajectories of the bubbles' centers of mass and assuming that a force acts on these locations (Hosokawa et al., 2002; Tomiyama et al., 2002; Ziegenhein et al., 2018). Therefore, an inconsistency exists between the development and the usage of closure models for bubble forces in the standard Euler-Euler model. Consequently, over-prediction of gas volume fraction peaks can appear in the pipe center or near the wall if the bubble diameter is larger than the mesh size (Lehnigk, 2021; Tomiyama et al., 2003).

Applying the particle-center-averaging method (PCAM) has the potential to recover the consistency of the forces in the Euler-Euler model and to form a comprehensive theoretical basis. When using PCAM, bubbles are regarded

31 as mass points and a bubble number density is introduced into the solution.
32 In this way, the forces act on the bubbles' centers of mass. Zhang and Prosperetti
33 developed a framework for the Euler-Euler model based on PCAM
34 and proposed closure models for the dilute limit by theoretical analysis and
35 direct numerical simulations (Prosperetti, 1998; Zhang and Prosperetti, 1994,
36 1995, 1997). However, the closure models they developed are for inviscid flow
37 or for rigid interfaces, which cannot be generalized for numerical simulations
38 of bubbly flows. Besides, the calculation of the particle volume fraction from
39 the particle number density in case the particle diameter is larger than the
40 mesh size was not considered. In terms of applications, PCAM was used in
41 the simulation of a wall-bounded bubbly flow by Moraga et al. (2006). How-
42 ever, only a one-way coupling of the phases was considered, i.e., the influence
43 of the disperse phase on the flow of the continuous phase was neglected. To
44 recover the consistency of the Euler-Euler model, Tomiyama et al. (2003)
45 proposed to introduce the bubble number density into the disperse phase
46 continuity equation. However, the turbulent dispersion force in the disperse
47 phase momentum equation is still functions of gas volume fraction, which
48 means that the inconsistencies between the development and the usage of
49 force model still exist. In contrast, Lucas et al. (2001, 2007) introduced a
50 bubble number density in the momentum equation so that bubble forces act
51 on the bubbles' centers of mass and the gas volume fraction is obtained from
52 the convolution of the center-of-mass location and the bubble dimension.
53 However, the solver developed by them is only a one-dimensional solver. A
54 three-dimensional solver is needed to study bubbly flows comprehensively,
55 but it has not been developed so far.

56 For a PCAM based Euler-Euler model, two different methods are re-
57 quired to average the solution variables for the disperse and the continu-
58 ous phases, namely particle-center-averaging and phase-averaging method,
59 respectively. Hence, a way to relate the particle-center-averaged and the
60 phase-averaged quantities is needed. The interphase coupling methods used
61 in Euler-Lagrange model can be borrowed to deal with this issue. In bubbly
62 flow simulations with an Euler-Lagrange method, a convolution method with
63 a kernel function is used to transfer Lagrangian quantities to the Eulerian
64 fields and vice versa (Bokkers et al., 2006; Darmana et al., 2006; Lau et al.,
65 2014, 2011). The kernel function represents the influence of the Lagrangian
66 quantities defined at the bubbles' centers of mass on the Eulerian quantities
67 in a certain influence region around the bubbles' centers of mass and vice
68 versa (Lau et al., 2014). However, it is complicated to deal with the kernel

69 function near curved boundaries or corners of a domain where the boundaries
70 meet non-orthogonally, and to implement it into a code using unstructured
71 meshes and parallel computation (Sun and Xiao, 2015b). A diffusion-based
72 method proposed by Sun and Xiao (2015b) is theoretically equivalent to a
73 convolution method with a Gaussian kernel function and it can give simi-
74 lar results by selecting a suitable diffusion pseudo-time. More importantly,
75 this method is easy to implement for codes using structured or unstructured
76 meshes and serial or parallel processing. Hence, it is used for the coupling of
77 the quantities between the particle-center-averaged and the phase-averaged
78 fields in this study.

79 In terms of closure models, a baseline model was established at Helmholtz-
80 Zentrum Dresden-Rossendorf (HZDR) for bubbly flows simulations (Rzehak
81 and Krepper, 2015). The baseline model is a set of closure relations for
82 the bubble forces, bubble-induced turbulence and bubble coalescence and
83 breakup. It was validated on a large number of experiments (Fleck and
84 Rzehak, 2019; Hänsch et al., 2021; Krepper et al., 2018; Liao et al., 2016,
85 2019, 2018, 2020; Rzehak et al., 2017a; Rzehak and Krepper, 2015; Rzehak
86 et al., 2017b; Shi and Rzehak, 2018; Zidouni et al., 2015; Ziegenhein et al.,
87 2013). The validation results show that the baseline model can reproduce
88 the experimental data and provide reasonable simulation results. Therefore,
89 in this study, the baseline model is used as the closure in the bubbly flow
90 simulations. One of the previously used validation databases, namely the
91 MTLoop experiment, will also be used here (Lucas et al., 2005).

92 In this work, an approach to simulate bubbly flows using PCAM is es-
93 tablished by combining the Euler-Euler model based on PCAM, the diffusion-
94 based method relating the the particle-center-averaged and the phase-averaged
95 quantities and the HZDR baseline model for the closure models. In this ap-
96 proach, a physically motivated model for the wall-contact force is introduced
97 to avoid the bubbles' centers of mass coming arbitrarily close to the wall. For
98 this purpose, the wall-contact force model of Lucas et al. (2007) is adapted
99 for oblate ellipsoidal bubbles. The entire approach is implemented based on
100 the solver *reactingTwoPhaseEulerFoam* in the OpenFOAM Foundation re-
101 lease (OpenFOAM Foundation, 2020). To evaluate its merits and compare
102 it to the standard approach, a simplified two-dimensional test setup is used
103 first. Laminar and turbulent flows are considered separately. A compari-
104 son between predictions and experimental measurements is then made for
105 selected tests from the MTLoop experimental database.

106 **2. Theory and solution procedure of particle-center-averaged Euler-**
 107 **Euler model**

108 The theory of the applied Euler-Euler model, the averaging methods as
 109 well as the continuity and momentum equations from Prosperetti (1998)
 110 are summarized in this section. The way to relate the phase-averaged and
 111 the particle-center-averaged quantities will be introduced. Besides, the dif-
 112 fusion pseudo-time optimization and the proposed correction terms will be
 113 explained. Finally, the solution procedure will be briefly mentioned. In
 114 this study, both phases are taken as incompressible and a fixed bubble size
 115 (monodisperse) is assumed.

116 *2.1. Phase-averaging and particle-center-averaging method*

The phase-averaging is used to average the solution variables for the con-
 tinuous phase. The phase-averaging of a quantity f of phase k is defined by

$$\overline{f}_k = \frac{1}{\alpha_k} \int_{C^N} f_k X_k P(N, t) dC^N, \quad (1)$$

where X_k is the phase indicator function. It is 1 where the phase k exists,
 otherwise it is 0. In Eq. (1), C^N describes the set of all possible dynamic
 states of the system containing N bubbles and $P(N, t)$ is the probability
 density function of a dynamic state at time t . Note, the indistinguishable
 particle probability is used here, so

$$\int_{C^N} P(N, t) dC^N = 1. \quad (2)$$

Hence, $N!$ does not appear in the definition of the averaged quantities. The
 volume fraction of phase k is defined by

$$\alpha_k = \int_{C^N} X_k P(N, t) dC^N. \quad (3)$$

In this study, “particle” and “bubble” are used interchangeably since the
 formalism is the same, but only applications for bubbly flows are considered.
 PCAM is used to average the solution variables for the disperse phase. It is
 suitable to average quantities that concern the particle as a whole, like the
 center-of-mass velocity. Therefore, the delta function δ indicating the loca-
 tion of the particle center is involved in the average (Biesheuvel and Gorissen,

1990; Moraga et al., 2006; Prosperetti, 1998; Zhang and Prosperetti, 1994). The particle-center-averaging of a quantity f is defined by

$$\langle f \rangle (\mathbf{x}, t) = \frac{1}{n} \int_{C^N} \left[\sum_{i=1}^N \delta (\mathbf{x} - \mathbf{y}^i) f^i (N, t) \right] P (N, t) dC^N, \quad (4)$$

where \mathbf{x} is the spatial location, f^i is the value of the quantity f for bubble i ($i = 1, \dots, N$), and \mathbf{y}^i is the location of its center. The bubble number density is defined by

$$n = \int P (\mathbf{x}, \mathbf{u}, t) d\mathbf{u}. \quad (5)$$

Here $P (\mathbf{x}, \mathbf{u}, t)$ is the one-bubble probability density function, which is related to $P (N, t)$ as

$$P (\mathbf{x}, \mathbf{u}, t) = \int P (N, t) dC^{N-1}. \quad (6)$$

The product of n and $d\mathbf{x}$ represents the probability of finding a bubble center in the vicinity of the location \mathbf{x} at time t .

$$\int n d\mathbf{x} = N. \quad (7)$$

117 This relation justifies that n is the bubble number density.

118 2.2. Continuity and momentum equations

The continuity equation for the continuous phase is the same as in the standard Euler-Euler model (Drew and Passman, 1998)

$$\frac{\partial \alpha_c \rho_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c \overline{\mathbf{u}_c}) = 0, \quad (8)$$

where ρ is the density and \mathbf{u} is the velocity. Here and in the following, a subscript c denotes a quantity for the continuous phase while a subscript d denotes a quantity for the disperse phase. For the disperse phase, the continuity equation becomes a transport equation for the bubble number density

$$\frac{\partial n \rho_d}{\partial t} + \nabla \cdot (n \rho_d \langle \mathbf{u}_d \rangle) = 0. \quad (9)$$

The momentum equation for the continuous phase is

$$\begin{aligned} & \frac{\partial \alpha_c \rho_c \overline{\mathbf{u}}_c}{\partial t} + \nabla \cdot (\alpha_c \rho_c \overline{\mathbf{u}}_c \overline{\mathbf{u}}_c) \\ & = -\alpha_c \nabla \overline{p}_c + \alpha_c \nabla \cdot \overline{\mathbf{S}}_c + \nabla \cdot (\alpha_c \overline{\mathbf{T}}_c) + \overline{\mathbf{f}}_c + \alpha_c \rho_c \mathbf{g}, \end{aligned} \quad (10)$$

where p , \mathbf{S} , \mathbf{T} , \mathbf{f} and \mathbf{g} are pressure, viscous stress tensor, Reynolds stress tensor, interfacial force per unit volume and acceleration of gravity, respectively. The momentum equation for the disperse phase is derived by averaging the equation of motion for bubbles (Prosperetti, 1998; Zhang and Prosperetti, 1994). The momentum equation is

$$\begin{aligned} & \frac{\partial \beta_d \rho_d \langle \mathbf{u}_d \rangle}{\partial t} + \nabla \cdot (\beta_d \rho_d \langle \mathbf{u}_d \rangle \langle \mathbf{u}_d \rangle) \\ & = -\beta_d \nabla \overline{p}_c + \beta_d \nabla \cdot \langle \mathbf{S}_c \rangle + \nabla \cdot (\beta_d \langle \mathbf{T}_d \rangle) + \langle \mathbf{f}_d \rangle + \beta_d \rho_d \mathbf{g}, \end{aligned} \quad (11)$$

where β_d is gas volume fraction projecting all the bubble volume to the bubble centers. It is calculated by

$$\beta_d = nV_d, \quad (12)$$

119 where V_d is the bubble volume.

120 It should be mentioned that some assumptions and simplifications have
 121 been used to derive Eqs. (10) and (11) from the original momentum equations
 122 in Prosperetti (1998). First, the collision stress due to direct bubble-bubble
 123 interactions is not considered in Eq. (11). Second, the terms containing
 124 $A[\boldsymbol{\sigma}_c]$ in the momentum equations in Prosperetti (1998) are regarded as the
 125 interfacial momentum interactions and replaced by $\overline{\mathbf{f}}_c$ and $\langle \mathbf{f}_d \rangle$. At last, the
 126 surface stress term $L[\boldsymbol{\sigma}_c]$ in the momentum equation of the continuous phase
 127 in Prosperetti (1998) originates from the non-uniform distribution of pressure
 128 force on the surface of a bubble or a particle (Zhang and Prosperetti, 1994).
 129 It is neglected since no closure model for it is known in a bubbly flow.

130 Compared to the momentum equations and the way to derive the equa-
 131 tions in the standard Euler-Euler model (Drew and Passman, 1998), the
 132 differences lie in:

- 133 1. The phase volume fraction in the viscous stress term of Eq. (10) is out-
 134 side of the divergence since the part of the viscous stress term related
 135 to the gradient of the phase volume fraction is cancelled by the inter-
 136 facial contributions, which is similar to the pressure term (Prosperetti
 137 and Jones, 1984).

- 138 2. Equation (11) is derived by averaging the equation of motion for bub-
139 bles, while the equation in the standard Euler-Euler model is derived
140 by averaging the local instantaneous momentum equation and by using
141 the phase indicator function of the disperse phase.
- 142 3. The physical meaning of the momentum equation for the disperse phase
143 in the Euler-Euler model based on PCAM is different from that in the
144 standard Euler-Euler model. Equation (11) displays the momentum
145 balance of gas, which belongs to bubbles having their centers located
146 inside the control volume. This gas may only be partially contained
147 within the control volume. In the standard Euler-Euler model, the
148 equation refers to the momentum balance of all gas contained inside
149 the control volume. This gas may belong partially or even completely
150 to bubbles with centers outside of the control volume. Hence, Eq. (11)
151 is related to the bubble number density, while in the standard Euler-
152 Euler model, the momentum equation of the disperse phase is related
153 to the volume fraction of the disperse phase.
- 154 4. Equation (11) explicitly shows the response of bubbles to the pressure
155 and the viscous stress tensor of the continuous phase. Hence, no addi-
156 tional closure model for the viscous stress tensor of the disperse phase is
157 required. In the standard Euler-Euler model, the viscous stress tensor
158 of the disperse phase appears and a closure model for it is needed.

159 *2.3. Closure models*

The selected closure models for the interfacial forces according to the HZDR baseline model, which is based on the standard Euler-Euler model, are listed in Table 1. In the standard Euler-Euler model, the interfacial

Table 1: HZDR baseline model for monodisperse bubbly flows.

Force and turbulence	Selected model
Drag force	Ishii and Zuber (1979)
(Shear-) lift force	Tomiya et al. (2002) with cosine wall damping
Turbulent dispersion force	Burns et al. (2004)
Wall (-lift) force	Hosokawa et al. (2002)
Virtual mass force	Constant coefficient, $C_{VM} = 0.5$
Turbulence	$k - \omega$ SST
Bubble-induced turbulence	Ma et al. (2017)

forces are functions of the gas volume fraction. In the Euler-Euler model based on PCAM, the interfacial forces for the disperse phase are changed to be functions of the bubble number density. The necessary conversion is achieved by

$$\mathbf{f}(n) = \frac{nV_d}{\alpha_d} \mathbf{f}(\alpha_d), \quad (13)$$

160 where $\mathbf{f}(n)$ and $\mathbf{f}(\alpha_d)$ are the force per unit volume as a function of the
 161 bubble number density and the gas volume fraction, respectively. For the
 162 turbulent dispersion force model, an additional change is needed for the term
 163 $\nabla\alpha_d/\alpha_d$, which should be changed to $\nabla\beta_d/\beta_d$ based on the derivation proce-
 164 dure in Burns et al. (2004, see appendix).

Moreover, for the PCAM based Euler-Euler model, an additional wall-contact force has to be introduced to prevent the bubbles' centers of mass from coming nonphysically close to the wall. For this purpose, the wall-contact force model proposed by Lucas et al. (2007) is adopted for bubbles with an oblate ellipsoidal shape. The resulting wall-contact force $\mathbf{f}_d^{contact}$ reads

$$\mathbf{f}_d^{contact} = -\pi d_B \sigma n \left\{ -\frac{1}{\tilde{L}^2} + \frac{3\tilde{L}}{2G} \left[\left(\frac{4\sqrt{G}}{3} + \frac{\tilde{L}^3}{\sqrt{G}} \right) \operatorname{arctanh} \sqrt{G} - 1 \right] \right\}, \quad (14)$$

165 where $\tilde{L} = 2L/d_B$ and $G = 1 - \tilde{L}^3$. In these equations, d_B is the bubble
 166 diameter, σ is the surface tension coefficient and L is the distance between
 167 the bubble's center-of-mass and the wall.

168 For turbulent flows, the continuous phase turbulence is simulated by the
 169 turbulence models in Table 1, while the flow of the disperse phase is assumed
 170 to be laminar since $\rho_d \ll \rho_c$.

171 2.4. Coupling between phase-averaged and particle-center-averaged quantities

172 As discussed above, phase-averaging and particle-center-averaging are
 173 used to average the solution variables for the continuous phase and the
 174 disperse phase, respectively. When the bubble diameter is smaller than
 175 the mesh size, the difference between phase-averaged and particle-center-
 176 averaged quantities is not significant. In this condition, it is reasonable
 177 to assume that a phase-averaged quantity approximately equals the corre-
 178 sponding particle-center-averaged quantity (i.e. $\alpha_d \approx \beta_d$). However, when
 179 the bubble diameter is larger than the mesh size, the difference between the

180 averaging methods becomes significant, and this assumption is not appropri-
 181 ate. Therefore, a comprehensive way is needed to couple phase-averaged and
 182 particle-center-averaged quantities, which can be used in both conditions. In
 183 principle this way could be established by a convolution using a kernel func-
 184 tion that represents the spatial extent of a single bubble (Lyu et al., 2020).
 185 However, implementing such a method efficiently in a numerical simulation
 186 using unstructured grids is difficult. Therefore, a diffusion-based method
 187 is used here to relate phase-averaged and particle-center-averaged quanti-
 188 ties. The bubble influence region, over which the diffusion takes place, may
 189 be larger than the actual bubble volume to comprise also effects of bubble
 190 shape and path oscillations.

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

$$\frac{\partial \alpha_d}{\partial \tau} - \nabla \cdot (C_{\text{diff}} \nabla \alpha_d) = 0, \quad (15)$$

191 with an initial condition of $\alpha_d = nV_d$. In this process, the gas volume is
 192 conserved. In the equation, τ is the diffusion pseudo-time and C_{diff} is the
 193 diffusion coefficient, both determining the size of the bubble influence region.
 194 Note, this diffusion process takes place at every time step of the simulation
 195 such that τ is unrelated to the physical time, and, hence, referred to as a
 196 pseudo-time. Without loss of generality, C_{diff} is set to be $1 \text{ m}^2 \text{ s}^{-1}$ for all dif-
 197 fusion processes in the present study, while an optimized value is determined
 198 for τ in section 2.5. To solve Eq. (15), a Neumann boundary condition with
 199 derivative equal to zero is used for all boundaries.

Similarly, to calculate a phase-averaged gas velocity $\overline{\mathbf{u}_d}$, the bubble mo-
 mentum is distributed about its center-of-mass by the following diffusion
 equation

$$\frac{\partial \alpha_d \overline{\mathbf{u}_d}}{\partial \tau} - \nabla \cdot (C_{\text{diff}} \nabla (\alpha_d \overline{\mathbf{u}_d})) = 0, \quad (16)$$

200 with an initial condition of $\alpha_d \overline{\mathbf{u}_d} = n \langle \mathbf{u}_d \rangle V_d$. Other settings are as described
 201 above.

Besides, the forces acting on the bubble centers are distributed to the

bubble influence region by the following diffusion equation

$$\frac{\partial \overline{\mathbf{f}}_d}{\partial \tau} - \nabla \cdot (C_{\text{diff}} \nabla \overline{\mathbf{f}}_d) = 0, \quad (17)$$

with an initial condition of $\overline{\mathbf{f}}_d = \langle \mathbf{f}_d \rangle$. The total force does not change in this process. Finally, the forces acting on the continuous phase can be calculated by

$$\overline{\mathbf{f}}_c = -\overline{\mathbf{f}}_d. \quad (18)$$

On the contrary, the continuous phase velocity at the bubbles' centers of mass $\langle \mathbf{u}_c \rangle$ can be calculated from the corresponding phase-averaged continuous phase velocity $\overline{\mathbf{u}}_c$ by the following weighted average

$$\langle \mathbf{u}_c \rangle (\mathbf{x}, \tau) = \int_{-\infty}^{+\infty} \overline{\mathbf{u}}_c (\mathbf{x}_0, 0) \frac{1}{(4\pi C_{\text{diff}} \tau)^{\frac{3}{2}}} \exp\left\{-\frac{(\mathbf{x} - \mathbf{x}_0)^2}{4C_{\text{diff}} \tau}\right\} d\mathbf{x}_0, \quad (19)$$

which is the solution of

$$\frac{\partial \langle \mathbf{u}_c \rangle}{\partial \tau} - \nabla \cdot (C_{\text{diff}} \nabla \langle \mathbf{u}_c \rangle) = 0, \quad (20)$$

202 with an initial condition of $\langle \mathbf{u}_c \rangle (\mathbf{x}_0, 0) = \overline{\mathbf{u}}_c (\mathbf{x}_0, 0)$, where \mathbf{x}_0 is the spatial
 203 coordinate vector.

204 2.5. Diffusion pseudo-time optimization

205 A key parameter in the conversions using the diffusion-based method is
 206 the diffusion pseudo-time τ . The diffusion pseudo-time is independent of the
 207 physical time. It affects the size of the bubble influence region.

208 The size of the bubble influence region in the convolution or the diffusion-
 209 based method is still an open question. Deen et al. (2004) and Darmana
 210 et al. (2006) set this size to be 3 times the bubble mean diameter. However,
 211 Bokkers et al. (2006) and Lau et al. (2011) set it to be 6 and 2 times the bubble
 212 mean diameter, respectively. Besides, Sun and Xiao (2015a) argued that this
 213 size should approximately equal the size of the wake of the particles. Since no
 214 agreement on the value for the bubble influence region is found in literature,
 215 this subsection aims to optimize the diffusion pseudo-time by minimizing the
 216 difference between expected and numerically computed gas volume fractions
 217 in a simplified one-dimensional case.

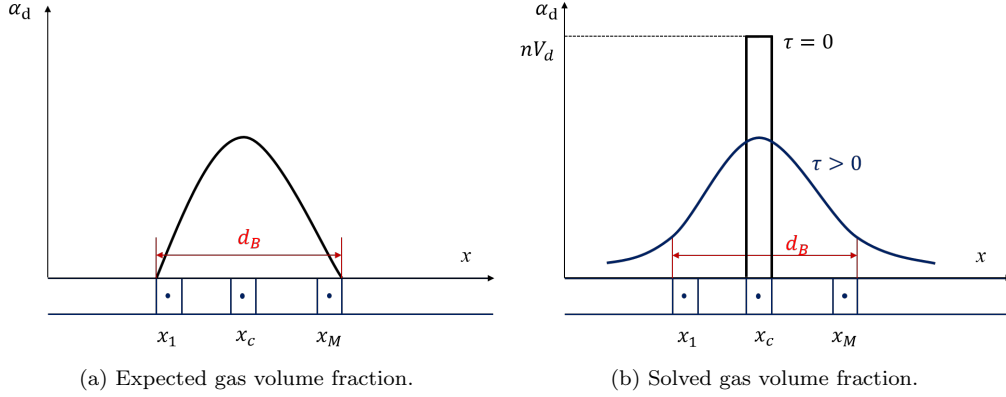


Figure 1: Gas volume fraction for the one-dimensional case

In the condition that 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 perpendicular to the wall. This profile can be used as the expected gas volume fraction in a one-dimensional case where a stream of spherical bubbles is injected at location $x = x_c$. Hence, the expected gas volume fraction reads

$$\alpha_d^{\text{exp}}(x) = \begin{cases} \alpha_{\text{max}} - 4\alpha_{\text{max}}(x - x_c)^2/d_B^2, & |x - x_c| \leq d_B \\ 0, & |x - x_c| > d_B \end{cases}, \quad (21)$$

218 where x is the spatial coordinate and α_{max} is the maximum gas volume
219 fraction.

The gas volume fraction is obtained by solving Eq. (15) in one dimension (Haberman, 2012)

$$\alpha_d(x, \tau) = \int_{-\infty}^{+\infty} n(x_0, 0) V_d \frac{1}{\sqrt{4\pi C_{\text{diff}} \tau}} \exp\left\{-\frac{(x - x_0)^2}{4C_{\text{diff}} \tau}\right\} dx_0. \quad (22)$$

In the one-dimensional case concerned here, the initial bubble number density is concentrated only in one mesh cell. Consequently, the solved gas volume fraction can be discretized as

$$\alpha_d^{\text{sol}}(x, \tau) \approx n(x_c, 0) V_d \frac{1}{\sqrt{4\pi C_{\text{diff}} \tau}} \exp\left\{-\frac{(x - x_c)^2}{4C_{\text{diff}} \tau}\right\} \Delta_x, \quad (23)$$

220 where Δ_x is the size of the grid cell containing the bubble centers.

In the comparison of the expected and the solved gas volume fractions, the gas volume is kept the same by setting

$$n(x_c, 0) = \frac{\sum_{i=1}^M \alpha_d^{\text{exp}}(x_i) V_i}{V_d V_c}, \quad (24)$$

221 where M is the number of cells covered by the bubbles (Fig. 1(a)), while V_i
 222 and V_c are the volumes of the grid cell i and c , respectively.

The optimized diffusion pseudo-time is the time for the error to reach its minimum value

$$E(\tau) = \sum_{i=1}^M [\alpha_d^{\text{exp}}(x_i, \tau) - \alpha_d^{\text{sol}}(x_i, \tau)]^2, \quad (25)$$

223 where $x_i \in (x_c \pm 0.5 d_B)$.

In the last equation, the discretised form of α_d^{sol} is used. The influence of the parameter M , which is used in the discretisation on the optimized diffusion pseudo-time, should be analyzed. Since the optimized diffusion pseudo-time τ_{opt} will depend on C_{diff} as well as d_B , a dimensionless optimized diffusion pseudo-time

$$\tilde{\tau}_{\text{opt}} = \frac{\tau_{\text{opt}} C_{\text{diff}}}{d_B^2} \quad (26)$$

224 will be used in the analysis. The result is shown in Fig. 2.

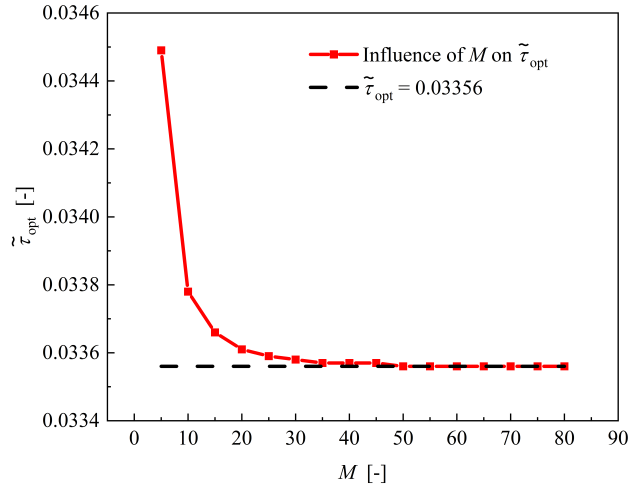


Figure 2: Mesh sensitivity analysis for the dimensionless optimized diffusion pseudo-time.

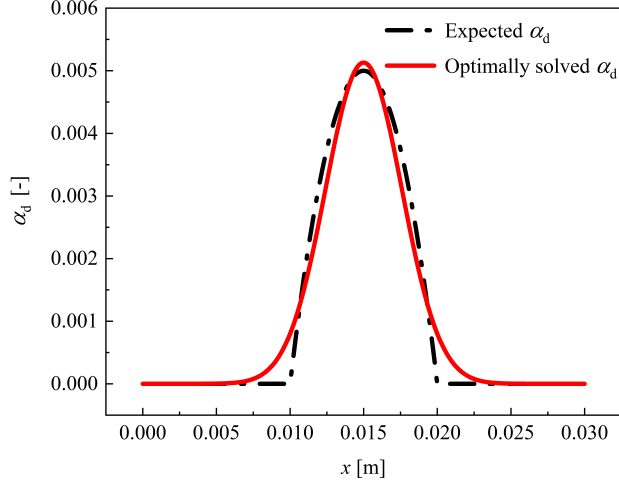


Figure 3: Expected and optimally solved gas volume fraction for the one-dimensional case.

225 As can be seen, $\tilde{\tau}_{\text{opt}}$ is almost a constant when M is larger than 30.
 226 As a result, $\tilde{\tau}_{\text{opt}} = 0.03356$ is used in the following simulations. With the
 227 optimized diffusion pseudo-time, the distributions of the expected and the
 228 solved gas volume fractions for the one-dimensional case can be seen in Fig. 3.
 229 For the solved gas volume fraction, 94.72% of the gas volume is contained
 230 within $x_c \pm 0.5 d_B$.

231 2.6. Correction terms for drag and virtual mass force of continuous phase

In the OpenFOAM multiphase flow solvers for the Euler-Euler model, the drag and virtual mass force are treated semi-implicitly to make the solution stable. After changing the forces to act on the bubble centers based on Eq. (13) and using the particle-center-averaged fields, the drag force and the virtual mass force for the disperse phase are

$$\langle \mathbf{f}_d^{\text{drag}} \rangle = -\frac{3}{4d_B} C_D \rho_c \beta_d |\langle \mathbf{u}_d \rangle - \langle \mathbf{u}_c \rangle| ([\langle \mathbf{u}_d \rangle] - \langle \mathbf{u}_c \rangle) \quad (27)$$

and

$$\langle \mathbf{f}_d^{\text{VM}} \rangle = -C_{\text{VM}} \rho_c \beta_d \left(\frac{D_d [\langle \mathbf{u}_d \rangle]}{Dt} - \frac{D_c \langle \mathbf{u}_c \rangle}{Dt} \right), \quad (28)$$

232 respectively, where C_D and C_{VM} are the coefficients and ρ is the density.
 233 The quantities within the square brackets are the quantities remaining to be
 234 solved. They are treated implicitly. Note, the other term in Eq. (27) involv-
 235 ing $\langle \mathbf{u}_d \rangle$ is treated explicitly, which means the old value from the last time or

236 iteration step will be used. The forces $\langle \mathbf{f}_d^{\text{drag}} \rangle$ and $\langle \mathbf{f}_d^{\text{VM}} \rangle$ can be calculated
 237 directly using the particle-center-averaged fields, and hence, appear directly
 238 on the right hand side of the disperse phase momentum equation.

To keep the forces consistent, these forces, which act on the bubbles' centers of mass are converted to phase-averaged forces acting on the continuous phase using Eqs. (17) and (18). However, this conversion requires an explicit implementation, which will cause numerical stability problems. As a solution, besides the conversion, a correction term

$$\mathbf{f}_c^{\text{drag, correction}} = -\frac{3}{4d_B} C_D \rho_c \beta_d |\langle \mathbf{u}_d \rangle - \langle \mathbf{u}_c \rangle| ([\overline{\mathbf{u}_c}] - \overline{\mathbf{u}_c}) \quad (29)$$

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

$$\mathbf{f}_c^{\text{VM, correction}} = -C_{\text{VM}} \rho_c \beta_d \left(\left[\frac{D_c \overline{\mathbf{u}_c}}{Dt} \right] - \frac{D_c \overline{\mathbf{u}_c}}{Dt} \right) \quad (30)$$

239 is added to the virtual mass force of the continuous phase.

240 These correction terms do not exist in theory. However, once the sim-
 241 ulation has sufficiently converged to a steady state, these terms will be ne-
 242 glectable since the difference between the current and the old values will be
 243 neglectable.

244 2.7. Solution procedure

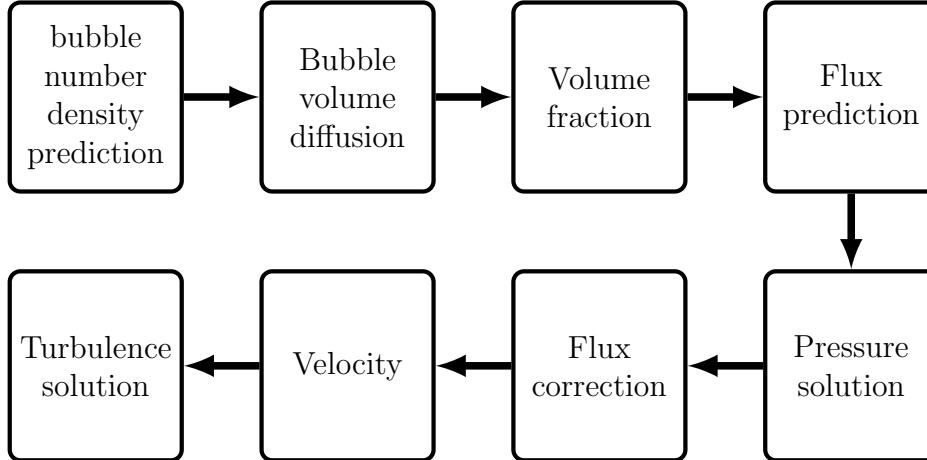


Figure 4: Solution procedure.

245 For the numerical solution, the underlying equations are discretised by
 246 the finite volume method. For the conservation equations in section 2.2, a
 247 first order Euler implicit scheme is used for the temporal discretisation and
 248 a flux-limiter is used for the discretisation of the convection term. For the
 249 pressure and velocity coupling, the PISO (Pressure Implicit with Splitting
 250 of Operator) algorithm is used. Besides, it is assumed that particle-center-
 251 averaged and phase-averaged pressure is the same. Moreover, for the diffusion
 252 equations in section 2.4, which are used to couple the phase-averaged and
 253 particle-center-averaged quantities, an Euler implicit scheme is used in the
 254 temporal discretisation and a Gauss linear scheme is used for the discretisa-
 255 tion of the laplacian term. The solution procedure is shown in Fig. 4.

256 **3. Basic verification of the improvement of Euler-Euler model based** 257 **on the particle-center-averaging method**

258 In this section, a simplified two-dimensional test case is used to reveal
 259 the numerical problems and nonphysical results of the standard Euler-Euler
 260 model caused by the inconsistency in the bubble force models. Besides, the
 261 improvement by changing the bubble forces to act on the bubbles' centers of
 262 mass by PCAM is shown.

263 *3.1. Geometry and simulation setups*

264 A two-dimensional test case similar to that used in Tomiyama et al. (2003)
 265 is employed. The domain and boundary settings are shown in Fig. 5 (a).
 266 It is a rectangle with a size of 0.03 m \times 0.5 m. A stream of air bubbles is
 267 injected at $x = 0$ and $y = 0$ into the domain that contains only water at
 268 the beginning. The inlet liquid velocity is a parabolic profile (Fig. 5 (b))
 269 to introduce a shear flow field, while the inlet gas velocity is uniform with a
 270 value of 0.1 m s⁻¹. Besides, the inlet gas volume fraction distribution for the
 271 simulations with the standard Euler-Euler model is shown in Fig. 5 (c). In
 272 this profile, the lateral length over which the gas volume fraction is non-zero
 273 equals the bubble diameter.

For the PCAM Euler-Euler simulations, bubble number density at the
 inlet is non-zero only in the center cell of the mesh. To keep the inlet gas
 flow rate the same as in the standard Euler-Euler simulation, the inlet bubble
 number density is calculated by

$$n = \frac{1}{V_d} \sum_{j=1}^M \alpha_{d,j}, \quad (31)$$

274 where $\alpha_{d,j}$ is the gas volume fraction in mesh cell j , M is the number of
 275 mesh cells in the first layer near the inlet containing non-zero gas volume
 276 fraction, and the mesh aspect ratio is kept at a value of 1 (i.e. grid spacing
 277 $\Delta = \Delta_x = \Delta_y$).

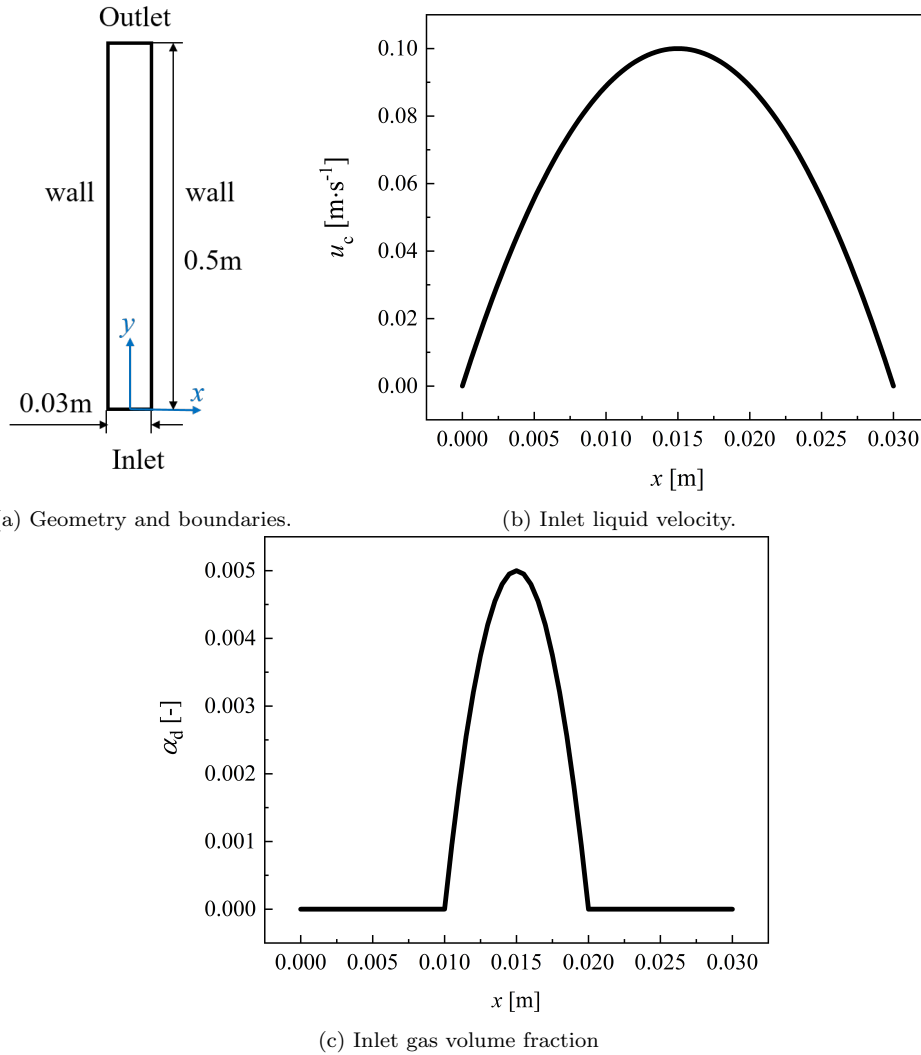


Figure 5: Geometry and boundary conditions

Table 2: Boundary settings.

Variable	Inlet	Wall	Outlet
α_d/α_c	fixedValue	zeroGradient	zeroGradient
n/β_d	fixedValue	fixedValue (0)	zeroGradient
U_d	fixedValue	slip	pressureInletOutletVelocity
U_c	fixedValue	noSlip	pressureInletOutletVelocity
p_{rgh}	fixedFluxPressure	fixedFluxPressure	prghPressure
p	calculated	calculated	calculated

Table 3: Physical properties of the fluids (μ : dynamic viscosity).

ρ_c [kg m ⁻³]	ρ_d [kg m ⁻³]	μ_c [kg m ⁻¹ s ⁻¹]	μ_d [kg m ⁻¹ s ⁻¹]
995.6	1.165	7.97e-4	1.86e-05

The detailed boundary settings are listed in Table 2. Note, OpenFOAM solver works with a pseudo pressure p_{rgh} instead of p to treat the machine precision issues. Their relation is

$$p = p_{\text{rgh}} + \rho_m g h, \quad (32)$$

where ρ_m is the mixture density. It is calculated by

$$\rho_m = \alpha_d \rho_d + \alpha_c \rho_c. \quad (33)$$

278 In all simulations, the Courant number is 0.002. Besides, the temperature of
 279 air and water is 25 °C and the pressure is 101325 Pa. The physical properties
 280 of the fluids are shown in Table 3.

281 3.2. Mesh sensitivity analysis

282 A mesh sensitivity is carried out for the standard Euler-Euler model and
 283 the PCAM Euler-Euler simulation. In this analysis, the ratio between the
 284 bubble diameter and the size of the mesh cells ranges from 2.5 to 20. Since
 285 the simulations of the standard Euler-Euler model do not reach a steady
 286 state, the results for the gas volume fraction α_d are averaged between 5 s
 287 and 20 s of simulation time at an axial height of $y = 0.4$ m. Laminar and
 288 turbulent flow cases are considered separately.

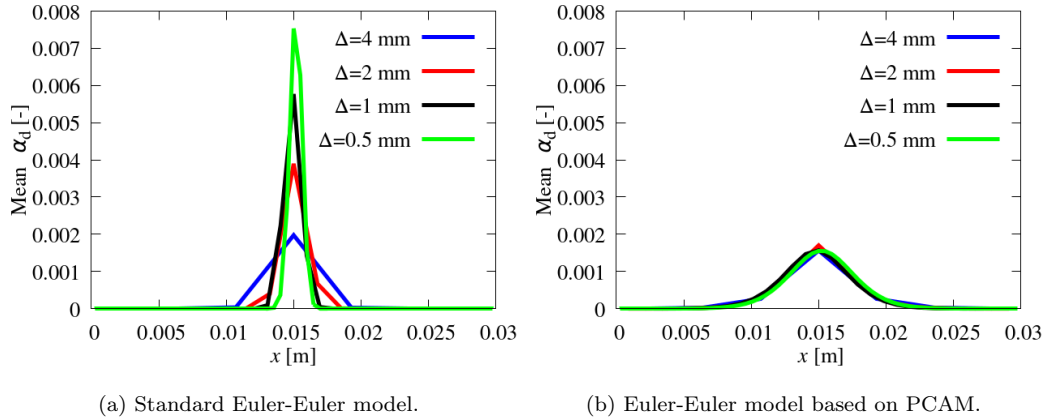


Figure 6: Mesh sensitivity analysis for the laminar flow case (Δ : grid spacing)

289 For a laminar flow, the results of the mesh sensitivity analysis are shown
 290 in Fig. 6. For the standard Euler-Euler model, the peak of the gas volume
 291 fraction increases continuously with decreasing mesh size. This results from
 292 the fact that the lift force acts on the distributed gas and drives it to the
 293 mesh cells in the channel center. The resulting concentration of gas in the
 294 channel center becomes higher when the mesh is refined and mesh indepen-
 295 dent results cannot be found. In contrast, in the results of the Euler-Euler
 296 simulation based on PCAM, the gas volume fraction distributions are similar
 297 upon refining the mesh. The reason is that in this method, the bubble
 298 forces are changed to act on the bubbles' centers of mass and these centers
 299 are located at the centreline of the channel, where the shear gradient
 300 vanishes. Therefore, the PCAM remedies the numerical deficiency in the
 301 standard Euler-Euler approach and provides a mesh independent solution
 302 for laminar flow.

303 For a turbulent flow, the results of the mesh sensitivity analysis are shown
 304 in Fig. 7 and show overall similar results as for the laminar flow. In the
 305 results of the standard Euler-Euler model, the gas volume fraction peak for
 306 a mesh size of 0.5 mm is slightly lower than the peak in the laminar flow.
 307 The reason is that the turbulent dispersion force flattens the gas volume
 308 fraction peak. For other mesh sizes, the gas volume fraction peaks in the
 309 laminar and the turbulent flow case are almost the same. As a result, the
 310 phenomenon that the gas volume fraction peak grows with decreasing mesh
 311 size is still significant. After using PCAM, the gas volume fractions remain

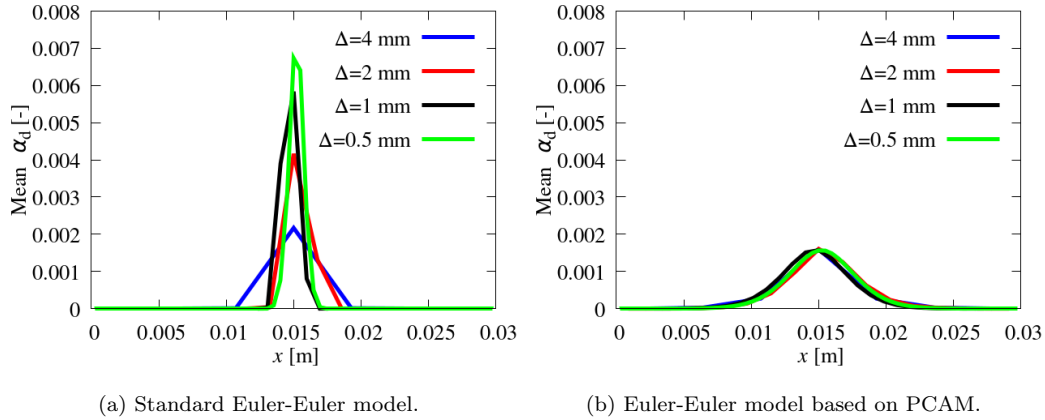


Figure 7: Mesh sensitivity analysis for the turbulent flow case (Δ : grid spacing)

312 similar upon refining the mesh.

313 In summary, using PCAM in the Euler-Euler model yields a mesh inde-
 314 pendent solution, where the standard Euler-Euler model does not. However,
 315 these test cases are simplified. It is conceivable that mesh independent solu-
 316 tions may exist also for the standard Euler-Euler model when the turbulent
 317 dispersion force is strong enough.

318 3.3. Axial development of gas volume fraction

319 In this subsection, the axial development of the gas volume fractions is
 320 analyzed. The grid spacing for all simulations in this subsection is 2 mm. At
 321 the inlet, the lateral region between $x = 0.01$ and $x = 0.02$ has non-zero gas
 322 volume fractions, which is equal to the bubble diameter.

323 For a laminar flow, the simulation results are shown in Fig. 8. In the
 324 results for the standard Euler-Euler model, the gas volume fraction profiles
 325 are narrow with high peak, which means that gas concentrates in the channel
 326 center following the flow downstream. Besides, the lateral region covered by
 327 the gas becomes smaller than the bubble diameter, which is nonphysical.
 328 This phenomenon is caused again by the lift force, which transports the
 329 distributed gas to the channel center even though it really belongs to the
 330 same bubble. In contrast, by using PCAM in the Euler-Euler model, the
 331 distribution of the gas volume fraction remains almost unchanged after the
 332 inlet (Fig. 8 (b)). Besides, the width of the region covered by the gas has
 333 a size close to the bubble diameter. Therefore, the gas volume fractions
 334 predicted by PCAM are considered to be more reasonable.

335 In turbulent flow, the simulation results are shown in Fig. 9. In the results
 336 of the standard Euler-Euler model, the gas over-concentration in the channel
 337 center downstream of the inlet is still significant although it does not change
 338 anymore. After changing the forces to act on the bubbles' centers of mass by
 339 PCAM, the over-concentration of the gas in the channel center disappears
 340 from the simulation results.

341 In conclusion, gas over-concentration can appear in the channel center
 342 in the standard Euler-Euler model since lift force is a function of the gas
 343 volume fraction. This gas over-concentration is avoided by changing the
 344 bubble forces to act on the bubbles' centers of mass as done by PCAM.

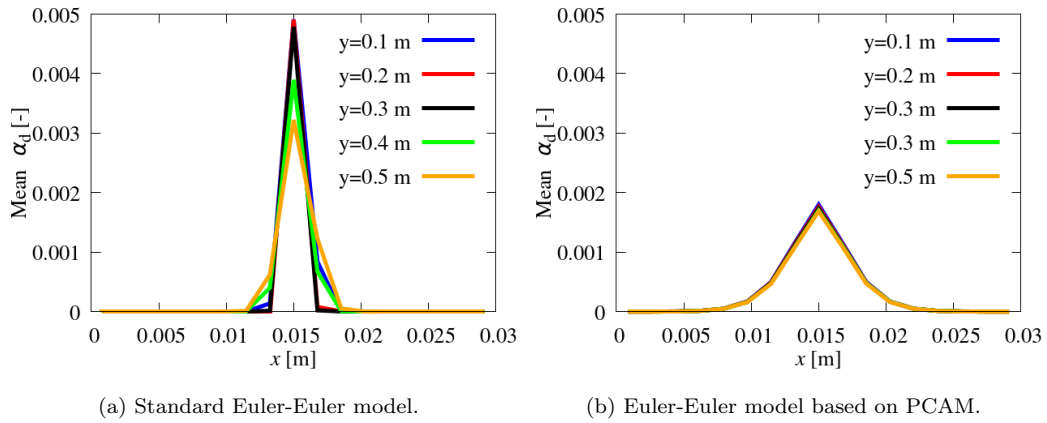


Figure 8: Gas volume fraction for laminar flow at different downstream positions

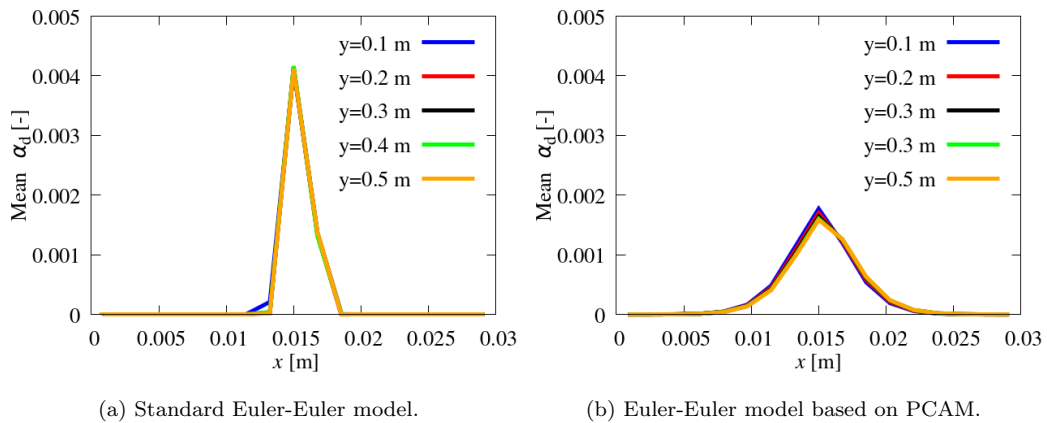


Figure 9: Gas volume fraction for turbulent flow at different downstream positions

345 4. Comparisons of simulation results and experimental data in 346 bubbly pipe flows

347 4.1. Experimental conditions

348 To evaluate PCAM in the Euler-Euler model, the results of the stan-
349 dard Euler-Euler model and the Euler-Euler simulations based on PCAM are
350 compared with the measurement data from the MTLoop experiment (Lucas
351 et al., 2005). The test section in the experiment is a vertical pipe. Its inner
352 diameter is 51.2 mm. The temperature of air and water in the experiment
353 is 30 °C and the pressure is 101325 Pa. The data used for comparison are
354 measured at a distance of 3.03 m from the gas injection. At this level, the
355 ratio between the distance from the gas inlet and the pipe diameter is about
356 59. Therefore, a fully-developed flow is expected.

357 4.2. Simulation setup

358 To reduce the computational cost, the geometry in the simulations is a
359 wedge with a center angle of 1.0 degree. The axial length of the wedge is
360 3.5 m. A wedge boundary condition is used in the circumference direction.
361 The numbers of mesh cells in the radial and the axial directions are 50 and
362 800, respectively. The mesh spacing is uniform in both directions. At the
363 inlet, a uniform profile for the velocity and the phase fraction of each phase is
364 used. The values are calculated from the superficial air and water velocities
365 by assuming that the relative velocity between the disperse and continuous
366 phases is zero at the inlet. The detailed boundary settings are listed in
367 Table 2. Besides, the parameters for the selected cases are listed in Table
368 4. The selected cases comprise different flow regimes, namely flows with
369 wall peaking and center peaking gas volume fraction profiles as well as finely
370 dispersed bubbly flows.

371 4.3. Comparison of wall peaking cases

372 If the gas volume fraction peaks are located near the wall and the bubble
373 diameters are larger than the mesh size, the gas volume fraction peaks sim-
374 ulated by the standard Euler-Euler model can be over-predicted. In Fig. 10,
375 the gas volume fraction peaks of the cases 43, 20, 98, 42 and 109 simulated by
376 the standard Euler-Euler model are about 590%, 170%, 170%, 70% and 70%
377 higher than the peaks in the experimental data, respectively. The extent of
378 over-prediction is influenced by the magnitude of the radial resultant force

Table 4: Parameters for the selected MTLoop cases (J : superficial velocity; Δ : radial grid spacing).

Name	J_c [m s ⁻¹]	J_d [m s ⁻¹]	α_d %	d_B [mm]	d_B/Δ
19	1.0170	0.0040	0.43	4.697	9.2
20	1.6110	0.0040	0.30	3.610	7.1
30	1.0170	0.0062	0.63	4.962	9.7
35	0.0641	0.0096	3.78	6.619	12.9
41	1.0170	0.0096	0.95	5.114	10.0
42	1.6110	0.0096	0.68	4.151	8.1
43	2.5540	0.0096	0.47	2.918	5.7
47	0.1020	0.0151	5.08	7.442	14.5
48	0.1610	0.0151	4.23	6.486	12.7
52	1.0170	0.0151	1.46	4.951	9.7
58	0.1020	0.0235	8.23	7.154	14.0
66	4.0470	0.0235	0.75	2.631	5.1
88	4.0470	0.0574	1.89	2.997	5.9
98	2.5540	0.0898	3.94	4.273	8.3
109	2.5540	0.1400	5.87	4.642	9.1
110	4.0470	0.1400	4.46	3.455	6.7

379 (the sum of the radial component of drag, virtual mass, turbulent disper-
380 sion and wall force) and the ratio between bubble diameter and radial grid
381 spacing. Compared to cases 20 and 42, case 43 has a small ratio between
382 bubble diameter and radial grid spacing (Table 4), but the magnitude of the
383 radial resultant force is relatively high (Fig. 11). Hence, the over-prediction
384 in case 43 is the highest. After employing PCAM in the simulations, these
385 gas volume fraction peaks compared to the experimental data decrease to
386 250%, 20%, 70%, 10% and 30%, respectively (Fig. 10). This proves that the
387 over-prediction of the gas volume fraction peak near the wall in the results
388 of the Euler-Euler model can be alleviated by changing the bubble forces to
389 act on the bubbles' centers of mass as done by PCAM.

390 However, not all wall peaking cases show the trend that the gas volume
391 fraction peak simulated by using PCAM fits the peak in the experimental
392 data better. For the wall peaking cases in Fig. 12, the gas volume fraction
393 peaks simulated by PCAM are under-predicted. The under-prediction in
394 cases 30, 19, 41 and 52 are about 27%, 25%, 25% and 9% of the peaks

395 in the experimental data, respectively. Nevertheless, the previous analysis
 396 shows that the standard Euler-Euler can have high gas concentration in the
 397 peak because of the inconsistency between the development and usage of the
 398 bubble force models. Therefore, it is possible that the agreement between the
 399 standard Euler-Euler model results and experimental data in cases 19 and 52
 400 includes the contribution of this inconsistency. Besides, the under-prediction
 401 of the gas volume fraction peaks also exist in the results of the standard
 402 Euler-Euler simulations in cases 30 and 41. Hence, the under-prediction
 403 may results from the insufficiency in the interfacial force models or errors in
 404 the experimental data. Furthermore, the gas volume fractions in the near
 405 wall region where $0.95 < r/R < 1$ predicted by both Euler-Euler models
 406 are under-predicted. In addition, the gas volume fraction peaks in some
 407 simulation results are located further away from the wall than the locations
 408 of the peaks in the experimental data. There are two possible reasons for
 409 these results: The first reason is using the assumption of a monodisperse flow
 410 in the simulations. If bubbles smaller than the mean diameter slide on the
 411 wall or flow near the wall, the gas volume fraction peak can be located closer
 412 to the wall. The second reason is that the spatial resolution of the wire-mesh
 413 sensors in the experimental measurement is limited. As a result, they can
 414 give high gas volume fraction measurement in the measurement cell nearest
 415 to the wall if there are a lot of small bubbles flowing near the wall.

416 *4.4. Comparison of cases with center peaks*

417 If the gas volume fraction peaks are located in the pipe center and the
 418 bubble diameters are larger than the mesh size, an over-prediction of the gas
 419 volume fraction peaks can appear in the pipe center for standard Euler-Euler
 420 simulations. In Fig. 13, the over-prediction of the gas volume fraction peaks
 421 for standard Euler-Euler simulations is significant. Nevertheless, no improve-
 422 ment is found in the results of Euler-Euler model based on PCAM. Figure 14
 423 shows that the turbulent intensity in these center peaking cases is higher
 424 than that in the wall peaking cases. A possible explanation is that the over-
 425 prediction of the gas volume fractions, which is caused by the inconsistency
 426 in the interfacial forces has been smoothed by the high turbulent dispersion.
 427 The over-prediction by both Euler-Euler models for the cases in Fig. 13 may
 428 result from using monodisperse assumption in the simulations, insufficiencies
 429 in the interfacial force models and errors in the experimental data. Besides,
 430 similar to the results in the wall peaking cases, the under-prediction of the
 431 gas volume fraction exists near the wall ($0.95 < r/R < 1$).

432 *4.5. Comparison of cases in finely dispersed flow*

433 In a pipe flow, a finely disperse flow regime can appear when the liquid
434 superficial velocity is relatively high. The over-prediction of the gas volume
435 fraction peaks in the results of the standard Euler-Euler model is significant
436 (Fig. 15). The reason is that the magnitudes of the lift and the wall force
437 can be as high as 10^3 N m^{-3} in the near-wall region (Fig. 16) since the liquid
438 velocity gradient is high and the bubble diameter is small. For case 66, the
439 gas volume fraction peak is located on the wall. This is nonphysical since the
440 smallest distance between the peak of the gas volume fraction and the wall
441 should be about one bubble radius in pipe flow if the bubble deformation is
442 ignored (Lubchenko et al., 2018).

443 After employing PCAM, the over-prediction is alleviated (Fig. 15). Fur-
444 thermore, combining PCAM with the wall-contact force avoids the gas vol-
445 ume fraction peak being located on the wall. Note, if the wall-contact force
446 is a function of the gas volume fraction, it can drive too much gas away from
447 the wall. That is the reason why it is not suggested to use it in the standard
448 Euler-Euler model. Nevertheless, no matter which Euler-Euler model is used,
449 the trends of the simulation results do not agree well with the trends of the
450 experimental data even if PCAM is used. The reason can be insufficiencies
451 in the HZDR baseline model due to some unknown effects in finely dispersed
452 flow (Lucas et al., 2020).

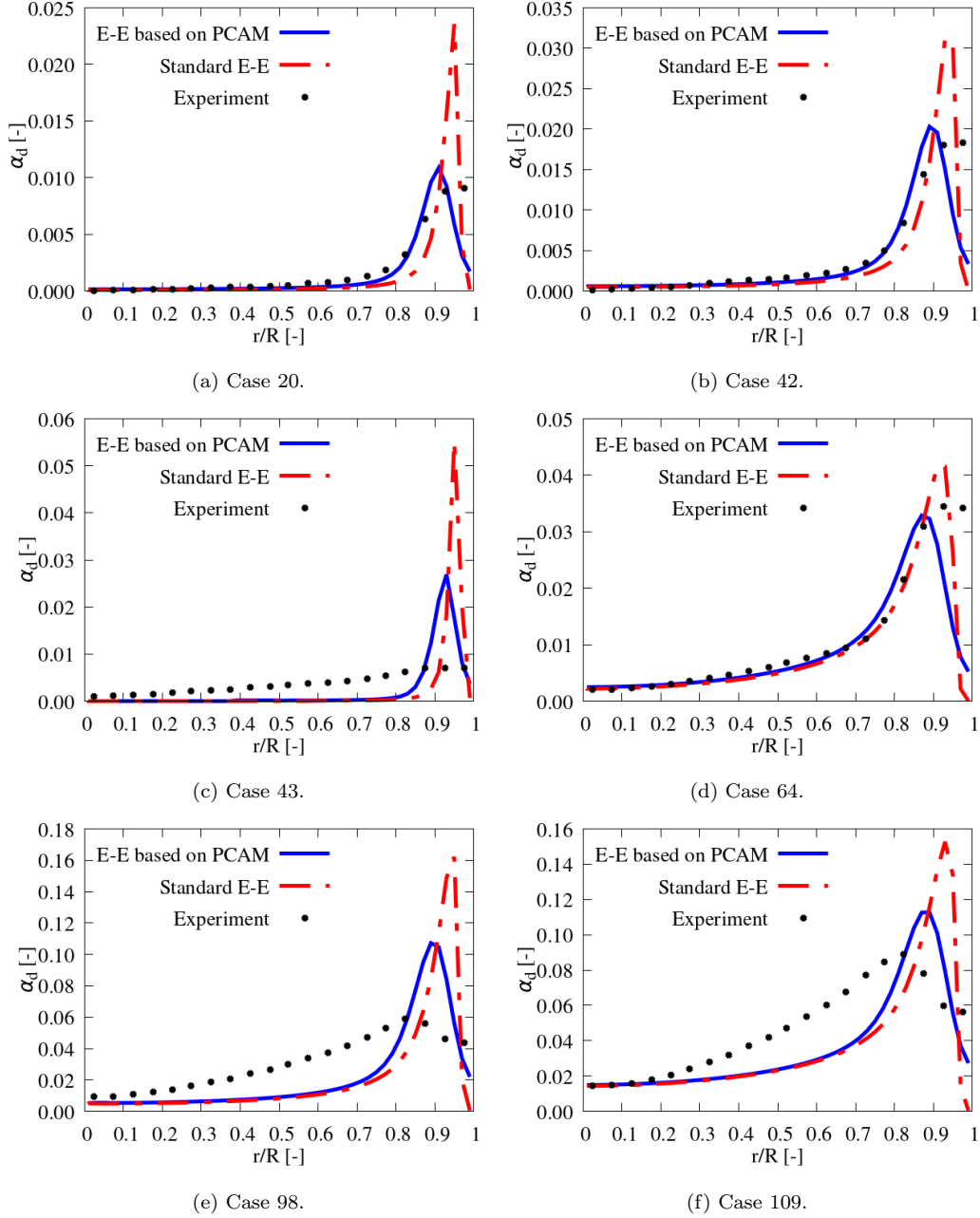


Figure 10: Comparison of the gas volume fraction between standard Euler-Euler (E-E) and Euler-Euler based on PCAM (r : radial location; R : pipe radius).

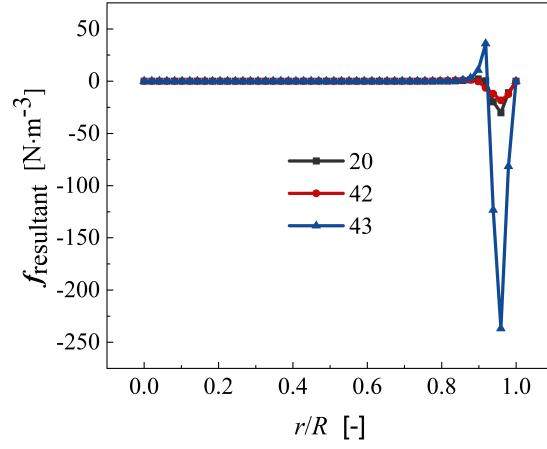


Figure 11: Radial resultant force for continuous phase in standard Euler-Euler simulations.

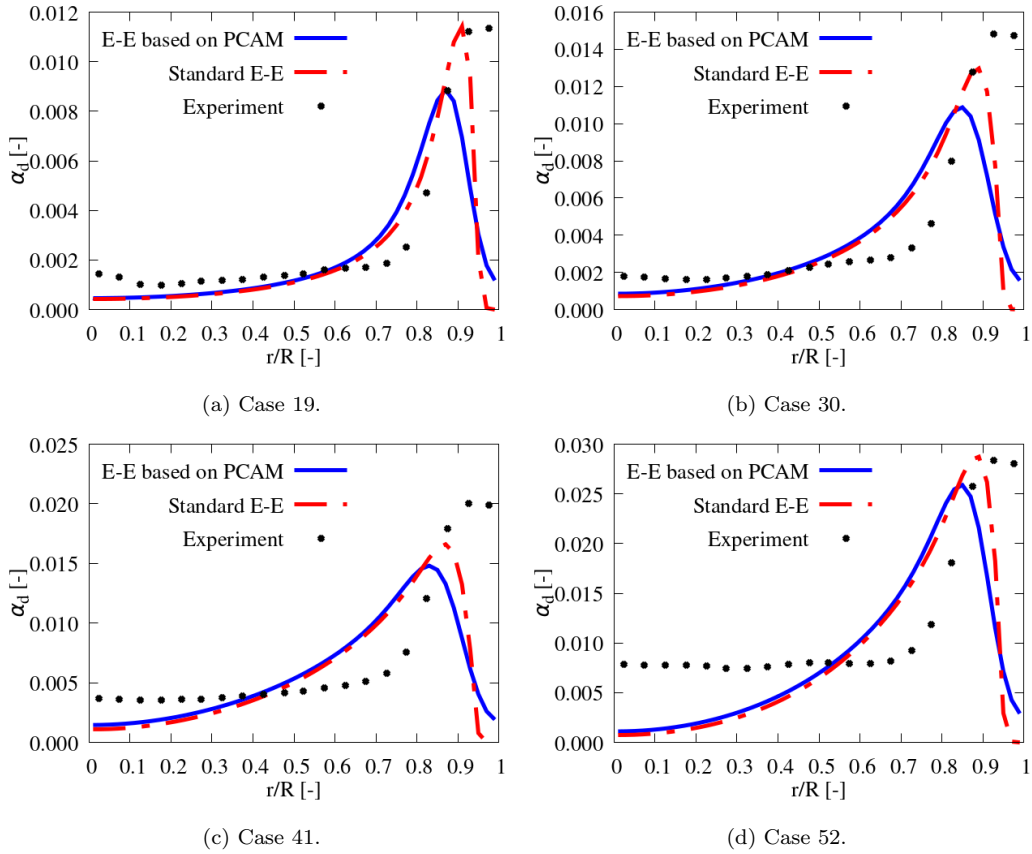


Figure 12: Gas volume fraction for wall peaking cases with under-prediction.

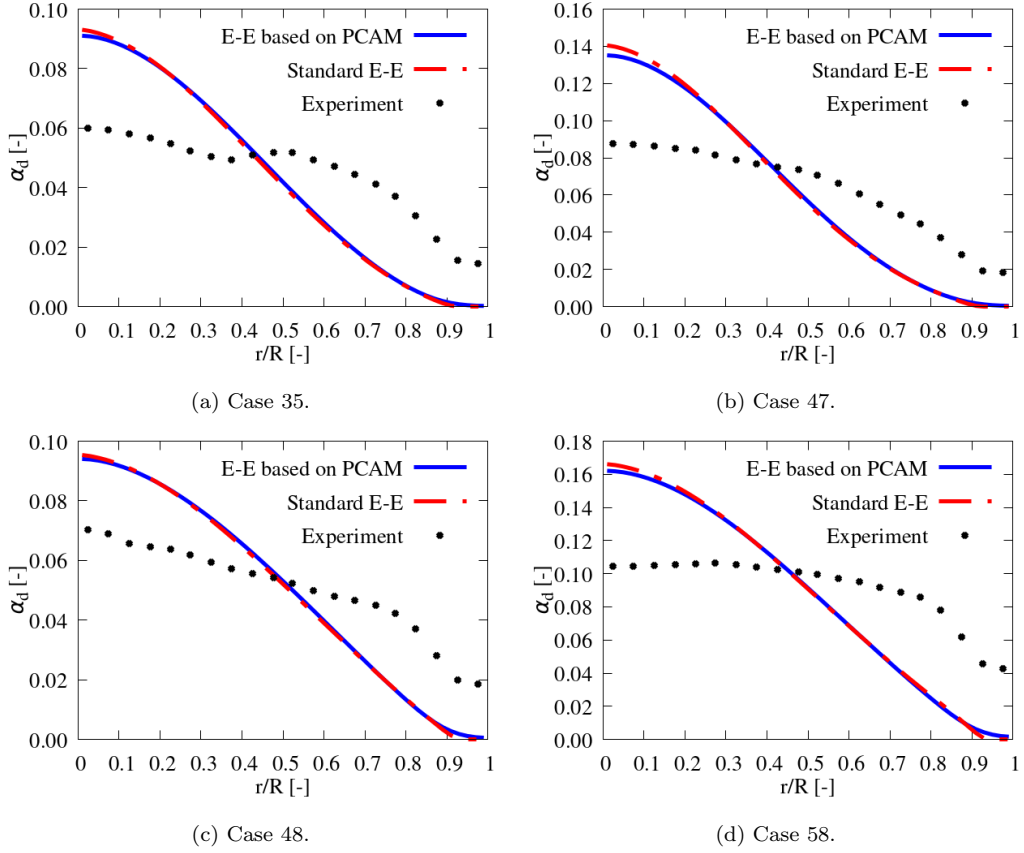


Figure 13: Gas volume fraction for center peaking cases.

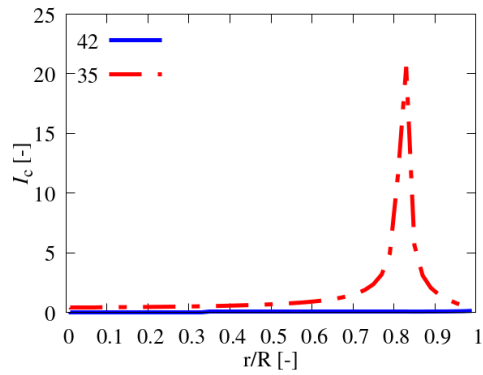


Figure 14: Turbulent intensity.

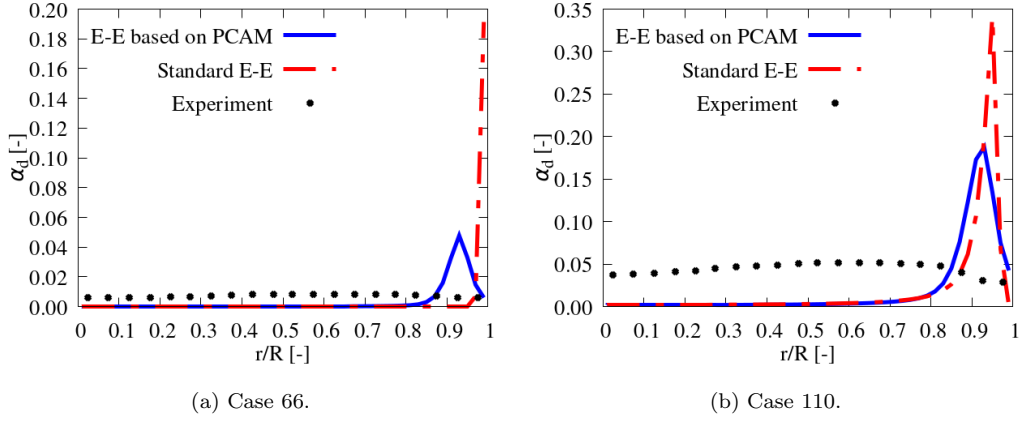


Figure 15: Gas volume fraction for finely dispersed cases.

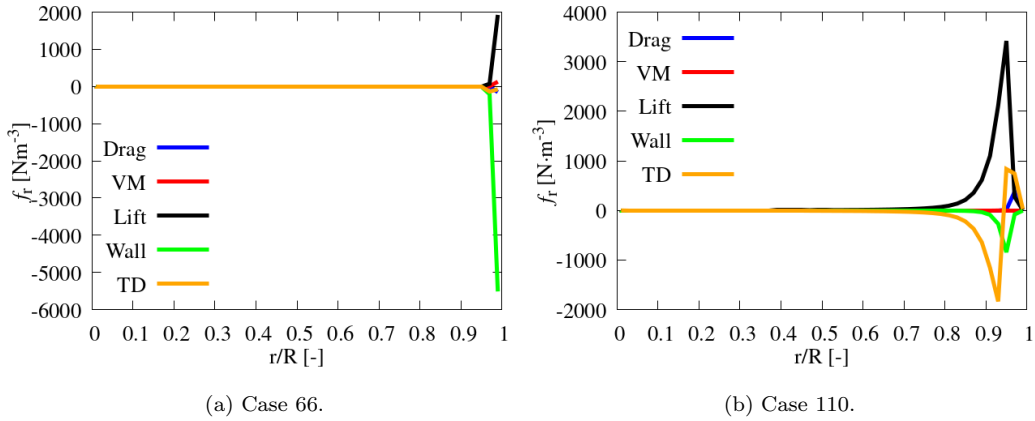


Figure 16: Radial force component in disperse phase for finely dispersed cases (Drag: drag force; VM: virtual mass force; Lift: lift force; Wall: wall force; TD: turbulent dispersion force).

453 5. Summary and Conclusions

454 In the present study, a particle-center-averaging method is employed to
455 recover the consistency of the interfacial forces in the Euler-Euler model. The
456 results of a simplified two-dimensional case reveal that the inconsistency of
457 the interfacial forces in the standard Euler-Euler model can cause the over-
458 prediction of the gas volume fraction peaks in the channel center. Besides,
459 a mesh independent solutions may not exist. The results show the potential
460 of using the particle-center-averaging method to remedy these issues.

461 In the present bubbly pipe flows, when the ratio of bubble diameter and
462 mesh radial spacing is between 5.1 and 14.5, the over-prediction of the gas
463 volume fraction peak exists in a near-wall region or a pipe center for the
464 standard Euler-Euler model. Using the particle-center-averaging method in
465 the Euler-Euler model shows the ability to alleviate the over-prediction of the
466 gas volume fraction peaks for some wall peaking and finely disperse cases.
467 Moreover, it can also avoid the gas volume fraction peak being nonphysically
468 located on the wall by introducing a wall-contact force.

469 Nevertheless, no improvement in the prediction of the gas volume frac-
470 tion in the center peaking cases with the particle-center-averaging method
471 is found. A possible explanation is the over-prediction of the gas volume
472 fraction caused by the inconsistency of interfacial forces has been smoothed
473 by the high turbulent dispersion. Besides, in majority of the simulations,
474 some differences still exist between the measured and the simulated gas vol-
475 ume fractions although the particle-center-averaging method is used. The
476 reasons may come from several aspects: First, some open questions still exist
477 in the HZDR baseline model. Second, monodisperse simulations may not
478 reproduce the flow phenomena in the experiments well. At last, some errors
479 may exist in the experimental data due to the limited spatial resolution of
480 the wire-mesh sensors and the challenges in measuring and discriminating
481 the two phases.

482 In further studies, using more than one bubble velocity groups is needed.
483 Besides, bubble coalescence and breakup are remained to be considered.

484 6. Acknowledgment

485 This work was supported by the Chinese Scholarship Council (CSC) and
486 partly supported by the Helmholtz European Partnering Program in the
487 project “Crossing borders and scales (Crossing)”.

488 **7. Nomenclature**

C^N	a set of all possible dynamic states	-
C_{diff}	diffusion coefficient	$\text{m}^2 \text{s}^{-1}$
C_D	drag coefficient	-
C_{VM}	virtual mass coefficient	-
d	diameter	m
E	error	-
\mathbf{f}	force per unit volume	N m^{-3}
\mathbf{g}	acceleration of gravity	m s^{-2}
J	superficial velocity	m s^{-1}
L	distance between bubble center and wall	m
M	number of mesh cells covered by a bubble	-
n	number density of bubble centers	m^{-3}
N	the number of bubbles in the system	-
$P(N; t)$	probability density function	-
$P(\mathbf{x}, \mathbf{u}, t)$	one-bubble probability density function	$\text{m}^{-4} \text{s}$
p	pressure	N m^{-2}
r	radial coordinate	m
R	pipe radius	m
\mathbf{S}	viscous stress tensor	N m^{-2}
\mathbf{T}	Reynold stress tensor	N m^{-2}
t	time	s
\mathbf{u}	velocity vector	m s^{-1}
V_d	bubble volume	m^3
X_k	phase indicator function for phase k	-
x, y, z	spatial coordinates	m
\mathbf{x}, \mathbf{x}_0	spatial coordinate vector	m
x_c, \mathbf{y}	bubble center location	m
α	phase volume fraction	-
β_d	gas volume fraction projecting all bubble volume to bubble centers	-
$\delta(x)$	Dirac delta function	-
μ	dynamic viscosity	$\text{kg m}^{-1} \text{s}^{-1}$
ρ	density	kg m^{-3}
τ	diffusion pseudo-time	s
σ	surface tension coefficient	N m^{-1}

B	bubble
c	continuous
d	disperse
k	phase index
m	mixture
exp	expected
max	maximum
opt	optimized
sol	solved
VM	virtual mass force
$\bar{\cdot}$	phase-average
$\langle \cdot \rangle$	particle-center-average
$\tilde{\cdot}$	dimensionless

489 Appendix

490 In this appendix, the derivation of turbulent dispersion force for the Euler-
 491 Euler model based on PCAM will be introduced. This derivation procedure
 492 here is similar to the procedure in Burns et al. (2004) which is used to derive
 493 the turbulent dispersion force for the standard Euler-Euler model.

494 *Relations between time average and Favre average*

For incompressible flow, the Favre average of a particle-center-averaged variable $\langle \phi_d \rangle$ is defined by

$$\overline{\langle \phi_d \rangle}^F = \frac{\overline{n \langle \phi_d \rangle}^t}{\overline{n}^t}, \quad (1)$$

where the tilde denotes Favre average, while the overbar and the index t represent time average. Substituting

$$\overline{n \langle \phi_d \rangle}^t = \overline{n}^t \overline{\langle \phi_d \rangle}^t + \overline{n' \langle \phi_d \rangle}'^t \quad (2)$$

into Eq. (1), we obtain

$$\overline{\langle \phi_d \rangle}^t = \overline{\langle \phi_d \rangle}^F - \frac{\overline{n' \langle \phi_d \rangle}'^t}{\overline{n}^t}. \quad (3)$$

A single dash (') here denotes the fluctuating quantity relative to the time-averaged quantity. Replacing $\langle\phi_d\rangle$ in the last equation with $\langle\mathbf{u}_d\rangle$, we obtain

$$\overline{\langle\mathbf{u}_d\rangle}^t = \overline{\langle\mathbf{u}_d\rangle}^F - \frac{\overline{n'\langle\mathbf{u}_d\rangle'}^t}{\overline{n}^t}. \quad (4)$$

For phase-averaged velocity of the continuous phase $\overline{\mathbf{u}_c}$, the relation between time-averaged and Favre-averaged velocities is (Burns et al., 2004)

$$\overline{\mathbf{u}_c}^t = \overline{\mathbf{u}_c}^F - \frac{\overline{\alpha_c'\overline{\mathbf{u}_c}'}^t}{\overline{\alpha_c}^t}. \quad (5)$$

495 *Derivation of turbulent dispersion force for the disperse phase*

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

$$\langle\mathbf{f}_d^{\text{drag}}\rangle = -D_{\text{cd,p}}A_{\text{cd}}(\langle\mathbf{u}_d\rangle - \overline{\mathbf{u}_c}), \quad (6)$$

where

$$D_{\text{cd,p}} = \frac{1}{8}C_D\rho_c|\langle\mathbf{u}_d\rangle - \overline{\mathbf{u}_c}|, \quad (7)$$

and

$$A_{\text{cd}} = n\pi d_B^2. \quad (8)$$

Note, the phase-averaged velocity of the continuous phase is used in the drag force here to keep the original definition of this quantity. It is assumed that $D_{\text{cd,p}}$ does not change with time. Applying time average to Eq.(6) yields

$$\overline{\langle\mathbf{f}_d^{\text{drag}}\rangle}^t = -D_{\text{cd,p}}\left[\overline{A_{\text{cd}}^t}\left(\overline{\langle\mathbf{u}_d\rangle}^t - \overline{\mathbf{u}_c}^t\right) + \overline{A_{\text{cd}}'}\left(\overline{\langle\mathbf{u}_d\rangle'} - \overline{\mathbf{u}_c}'\right)^t\right]. \quad (9)$$

496 Substituting Eqs. (4) and (5) into Eq. (9), we obtain

$$\begin{aligned} \overline{\langle\mathbf{f}_d^{\text{drag}}\rangle}^t = & -D_{\text{cd,p}}\overline{A_{\text{cd}}^t}\left[\left(\overline{\langle\mathbf{u}_d\rangle}^F - \frac{\overline{n'\langle\mathbf{u}_d\rangle'}^t}{\overline{n}^t}\right) - \left(\overline{\mathbf{u}_c}^F - \frac{\overline{\alpha_c'\overline{\mathbf{u}_c}'}^t}{\overline{\alpha_c}^t}\right)\right] \\ & - D_{\text{cd,p}}\overline{A_{\text{cd}}'}\left(\overline{\langle\mathbf{u}_d\rangle'} - \overline{\mathbf{u}_c}'\right)^t \end{aligned} \quad (10)$$

The last equation can be simplified to

$$\overline{\langle\mathbf{f}_d^{\text{drag}}\rangle}^t = -D_{\text{cd,p}}\overline{A_{\text{cd}}^t}\left(\overline{\langle\mathbf{u}_d\rangle}^F - \overline{\mathbf{u}_c}^F\right) + \mathbf{f}_d^{\text{TD}}, \quad (11)$$

where

$$\mathbf{f}_d^{\text{TD}} = D_{\text{cd,p}} \overline{A_{\text{cd}}}^t \left(\frac{\overline{n' \langle \mathbf{u}_d \rangle}^t}{\overline{n}^t} - \frac{\overline{\alpha_c' \overline{\mathbf{u}}_c}^t}{\overline{\alpha_c}^t} \right) - D_{\text{cd,p}} \overline{A_{\text{cd}}'}^t (\langle \mathbf{u}_d \rangle' - \overline{\mathbf{u}}_c')^t. \quad (12)$$

Substituting

$$\overline{C_{\text{cd,p}}}^t = D_{\text{cd,p}} \overline{A_{\text{cd}}}^t \quad (13)$$

into Eq. (12) results in

$$\mathbf{f}_d^{\text{TD}} = \overline{C_{\text{cd,p}}}^t \left(\frac{\overline{n' \langle \mathbf{u}_d \rangle}^t}{\overline{n}^t} - \frac{\overline{\alpha_c' \overline{\mathbf{u}}_c}^t}{\overline{\alpha_c}^t} \right) - \overline{C_{\text{cd,p}}}^t \frac{\overline{A_{\text{cd}}'}^t (\langle \mathbf{u}_d \rangle' - \overline{\mathbf{u}}_c')^t}{\overline{A_{\text{cd}}}^t}. \quad (14)$$

Bubble diameter is a constant. Therefore

$$A_{\text{cd}}' = n' \pi d_B^2, \quad (15)$$

and

$$\overline{A_{\text{cd}}}^t = \overline{n}^t \pi d_B^2. \quad (16)$$

Based on Eqs. (15) and (16), we have

$$\frac{\overline{A_{\text{cd}}'}^t (\langle \mathbf{u}_d \rangle' - \overline{\mathbf{u}}_c')^t}{\overline{A_{\text{cd}}}^t} = \frac{\overline{n'}^t (\langle \mathbf{u}_d \rangle' - \overline{\mathbf{u}}_c')^t}{\overline{n}^t}. \quad (17)$$

Substituting Eq. (17) into Eq. (14) and simplifying it, we obtain

$$\mathbf{f}_d^{\text{TD}} = \overline{C_{\text{cd,p}}}^t \left(\frac{\overline{n' \overline{\mathbf{u}}_c}^t}{\overline{n}^t} - \frac{\overline{\alpha_c' \overline{\mathbf{u}}_c}^t}{\overline{\alpha_c}^t} \right). \quad (18)$$

Using the eddy diffusivity hypothesis in the modeling of the turbulence related terms, we have

$$\overline{n' \overline{\mathbf{u}}_c}^t = -\frac{v_c^{\text{turb}}}{\sigma_{\text{nc}}} \nabla \overline{n}^t, \quad (19)$$

and

$$\overline{\alpha_c' \overline{\mathbf{u}}_c}^t = -\frac{v_c^{\text{turb}}}{\sigma_{\alpha c}} \nabla \overline{\alpha_c}^t, \quad (20)$$

After substituting Eqs. (19) and (20) into Eq. (18), we have

$$\mathbf{f}_d^{\text{TD}} = -\overline{C_{\text{cd,p}}}^t \left(\frac{v_c^{\text{turb}}}{\sigma_{\text{nc}}} \frac{\nabla \overline{n}^t}{\overline{n}^t} - \frac{v_c^{\text{turb}}}{\sigma_{\alpha c}} \frac{\nabla \overline{\alpha_c}^t}{\overline{\alpha_c}^t} \right). \quad (21)$$

Here, we assumed that

$$\sigma_{nc} = \sigma_{\alpha c}. \quad (22)$$

Since $\beta_d = nV_d$ and the bubble volume V_d is a constant, we have

$$\frac{\nabla \bar{n}^t}{\bar{n}^t} = \frac{\nabla \bar{\beta}_d^t}{\bar{\beta}_d^t}. \quad (23)$$

Substituting Eqs. (22) and (23) into Eq. (21), we obtain

$$\mathbf{f}_d^{\text{TD}} = -\overline{C_{cd,p}}^t \frac{v_c^{\text{turb}}}{\sigma_{\alpha c}} \left(\frac{\nabla \bar{\beta}_d^t}{\bar{\beta}_d^t} - \frac{\nabla \bar{\alpha}_c^t}{\bar{\alpha}_c^t} \right). \quad (24)$$

497 Comparing the last equation with the turbulent dispersion force model in
 498 Burns et al. (2004), we can find that $\nabla \alpha_d / \alpha_d$ is changed to $\nabla \beta_d / \beta_d$ here.

References

- Biesheuvel, A., Gorissen, W., 1990. Void fraction disturbances in a uniform bubbly fluid. *International Journal of Multiphase Flow* 16, 211–231.
- Bokkers, G., Laverman, J., van Sint Annaland, M., Kuipers, J., 2006. Modelling of large-scale dense gas–solid bubbling fluidised beds using a novel discrete bubble model. *Chemical Engineering Science* 61, 5590–5602.
- Burns, A.D., Frank, T., Hamill, I., Shi, J.M., et al., 2004. The Favre averaged drag model for turbulent dispersion in Eulerian multi-phase flows, in: 5th International Conference on Multiphase Flow, International Conference on Multiphase Flow. pp. 1–17.
- Darmana, D., Deen, N.G., Kuipers, J., 2006. Parallelization of an Euler–Lagrange model using mixed domain decomposition and a mirror domain technique: Application to dispersed gas–liquid two-phase flow. *Journal of Computational Physics* 220, 216–248.
- Deen, N.G., van Sint Annaland, M., Kuipers, J., 2004. Multi-scale modeling of dispersed gas–liquid two-phase flow. *Chemical Engineering Science* 59, 1853–1861.
- Drew, D.A., Passman, S.L., 1998. *Theory Multicomponent Fluids*. volume 135. Springer-Verlag.

- Fleck, S., Rzehak, R., 2019. Investigation of bubble plume oscillations by euler-euler simulation. *Chemical Engineering Science* 207, 853–861.
- Haberman, R., 2012. Applied partial differential equations with Fourier series and boundary value problems. Pearson Higher Ed.
- Hänsch, S., Evdokimov, I., Schlegel, F., Lucas, D., 2021. A workflow for the sustainable development of closure models for bubbly flows. *Chemical Engineering Science* , 116807.
- Hosokawa, S., Tomiyama, A., Misaki, S., Hamada, T., 2002. Lateral migration of single bubbles due to the presence of wall, in: *Fluids Engineering Division Summer Meeting*, pp. 855–860.
- Ishii, M., Zuber, N., 1979. Drag coefficient and relative velocity in bubbly, droplet or particulate flows. *AIChE journal* 25, 843–855.
- Krepper, E., Rzehak, R., Lucas, D., 2018. Validation of a closure model framework for turbulent bubbly two-phase flow in different flow situations. *Nuclear Engineering and Design* 340, 388–404.
- Lau, Y., Bai, W., Deen, N., Kuipers, J., 2014. Numerical study of bubble break-up in bubbly flows using a deterministic Euler–Lagrange framework. *Chemical Engineering Science* 108, 9–22.
- Lau, Y., Roghair, I., Deen, N., van Sint Annaland, M., Kuipers, J., 2011. Numerical investigation of the drag closure for bubbles in bubble swarms. *Chemical Engineering Science* 66, 3309–3316.
- Lehnigk, R., 2021. A generalized population balance model for the simulation of polydisperse multiphase flows within the Euler-Euler framework. Ph.D. thesis. Technische Universität Dresden. Dresden, Germany.
- Liao, J., Ziegenhein, T., Rzehak, R., 2016. Bubbly flow in an airlift column: a cfd study. *Journal of Chemical Technology & Biotechnology* 91, 2904–2915.
- Liao, Y., Ma, T., Krepper, E., Lucas, D., Fröhlich, J., 2019. Application of a novel model for bubble-induced turbulence to bubbly flows in containers and vertical pipes. *Chemical Engineering Science* 202, 55–69.

- Liao, Y., Ma, T., Liu, L., Ziegenhein, T., Krepper, E., Lucas, D., 2018. Eulerian modelling of turbulent bubbly flow based on a baseline closure concept. *Nuclear Engineering and Design* 337, 450–459.
- Liao, Y., Upadhyay, K., Schlegel, F., 2020. Eulerian-Eulerian two-fluid model for laminar bubbly pipe flows: Validation of the baseline model. *Computers & Fluids* 202, 104496.
- Lubchenko, N., Magolan, B., Sugrue, R., Baglietto, E., 2018. A more fundamental wall lubrication force from turbulent dispersion regularization for multiphase cfd applications. *International Journal of Multiphase Flow* 98, 36–44.
- Lucas, D., Krepper, E., Liao, Y., Rzehak, R., Ziegenhein, T., 2020. General guideline for closure model development for gas-liquid flows in the multi-fluid framework. *Nuclear Engineering and Design* 357, 110396.
- Lucas, D., Krepper, E., Prasser, H.M., 2001. Prediction of radial gas profiles in vertical pipe flow on the basis of bubble size distribution. *International Journal of Thermal Sciences* 40, 217–225.
- Lucas, D., Krepper, E., Prasser, H.M., 2005. Development of co-current air-water flow in a vertical pipe. *International Journal of Multiphase Flow* 31, 1304–1328.
- Lucas, D., Krepper, E., Prasser, H.M., 2007. Use of models for lift, wall and turbulent dispersion forces acting on bubbles for poly-disperse flows. *Chemical Engineering Science* 62, 4146–4157.
- Lyu, H., Schlegel, F., Rzehak, R., Lucas, D., 2020. Improvement of euler-euler simulation of two-phase flow by particle-center-averaged method, in: 14th International Conference on CFD in 6 Oil & Gas, Metallurgical and Process Industries SINTEF, Trondheim, Norway, October 12–14, 2020, SINTEF Academic Press.
- Ma, T., Santarelli, C., Ziegenhein, T., Lucas, D., Fröhlich, J., 2017. Direct numerical simulation-based reynolds-averaged closure for bubble-induced turbulence. *Physical Review Fluids* 2, 034301.

- Moraga, F., Larreteguy, A., Drew, D., Lahey Jr, R., 2006. A center-averaged two-fluid model for wall-bounded bubbly flows. *Computers & Fluids* 35, 429–461.
- OpenFOAM Foundation, 2020. OpenFOAM-dev. URL: <https://github.com/OpenFOAM/OpenFOAM-dev/tree/7dd592ff4013fc6e444f27b12ff8729774cb5e0f/applications/solvers/multiphase/reactingEulerFoam/reactingTwoPhaseEulerFoam>.
- Prosperetti, A., 1998. Ensemble averaging techniques for disperse flows, in: *Particulate Flows*. Springer, pp. 99–136.
- Prosperetti, A., Jones, A., 1984. Pressure forces in disperse two-phase flow. *International Journal of Multiphase Flow* 10, 425–440.
- Rzehak, R., Krauß, M., Kováts, P., Zähringer, K., 2017a. Fluid dynamics in a bubble column: New experiments and simulations. *International Journal of Multiphase Flow* 89, 299–312.
- Rzehak, R., Krepper, E., 2015. Bubbly flows with fixed polydispersity: validation of a baseline closure model. *Nuclear Engineering and Design* 287, 108–118.
- Rzehak, R., Ziegenhein, T., Kriebitzsch, S., Krepper, E., Lucas, D., 2017b. Unified modeling of bubbly flows in pipes, bubble columns, and airlift columns. *Chemical Engineering Science* 157, 147–158.
- Shi, P., Rzehak, R., 2018. Bubbly flow in stirred tanks: Euler-Euler/RANS modeling. *Chemical Engineering Science* 190, 419–435.
- Sun, R., Xiao, H., 2015a. Diffusion-based coarse graining in hybrid continuum–discrete solvers: Applications in CFD–DEM. *International Journal of Multiphase Flow* 72, 233–247.
- Sun, R., Xiao, H., 2015b. Diffusion-based coarse graining in hybrid continuum–discrete solvers: theoretical formulation and a priori tests. *International Journal of Multiphase Flow* 77, 142–157.
- Tomiya, A., Shimada, N., Asano, H., 2003. Application of number density transport equation for the recovery of consistency in multi-field model, in: *Fluids Engineering Division Summer Meeting*, pp. 501–508.

- Tomiyama, A., Tamai, H., Zun, I., Hosokawa, S., 2002. Transverse migration of single bubbles in simple shear flows. *Chemical Engineering Science* 57, 1849–1858.
- Zhang, D., Prosperetti, A., 1994. Averaged equations for inviscid disperse two-phase flow. *Journal of Fluid Mechanics* 267, 185–219.
- Zhang, D., Prosperetti, A., 1995. Energy and momentum equations for disperse two-phase flows and their closure for dilute suspensions. *Journal of Fluid Mechanics* .
- Zhang, D., Prosperetti, A., 1997. Momentum and energy equations for disperse two-phase flows and their closure for dilute suspensions. *International Journal of Multiphase Flow* 23, 425–453.
- Zidouni, F., Krepper, E., Rzehak, R., Rabha, S., Schubert, M., Hampel, U., 2015. Simulation of gas–liquid flow in a helical static mixer. *Chemical Engineering Science* 137, 476–486.
- Ziegenhein, T., Rzehak, R., Krepper, E., Lucas, D., 2013. Numerical simulation of polydispersed flow in bubble columns with the inhomogeneous multi-size-group model. *Chemie Ingenieur Technik* 85, 1080–1091.
- Ziegenhein, T., Tomiyama, A., Lucas, D., 2018. A new measuring concept to determine the lift force for distorted bubbles in low morton number system: Results for air/water. *International Journal of Multiphase Flow* 108, 11–24.