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

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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 diffusionbased 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-centeraveraging 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

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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 1. Introduction

Dispersed two-phase flows are widely encountered in chemical engineer-2 ing, energy production, oil and gas industries and biotechnology. Exploring 3 the flow mechanisms of two-phase flows can ensure safety and improve efficiency of industrial facilities. Many of these flow mechanisms are still not 5 well understood due to their high complexity. Experimental investigations 6 on two-phase flows face the difficulty to measure the flow and distribution 7 of two phases. Hence, they are usually costly and time-consuming. In com-8 parison, simulations provide a more accessible way to study such flows, but 9 they invariably rely on models. Among the simulation methods, the Eu-10 lerian two-fluid model shows advantages for simulating bubbly flows up to 11 industrial dimensions with affordable computational cost. 12

For bubbly flows, air is considered to be the dispersed phase and water 13 is considered to be the continuous phase. In the standard Eulerian two-fluid 14 model, the phase-averaging method is used for both phases. Each bubble 15 force is a function of the gas volume fraction. In this way, the coherent 16 motion of each bubble as a whole is not enforced when the bubble diameter 17 is larger than the mesh size. Hence, the gas belonging to a single bubble 18 can accumulate in a region smaller than the bubble dimension. However, 19 a closure model for a bubble force is typically developed by tracking the 20 trajectories of the bubbles' centers of mass and assuming that a force acts 21 on these locations (Hosokawa et al., 2002; Tomiyama et al., 2002; Ziegenhein 22 et al., 2018). Therefore, an inconsistency exists between the development 23 and the usage of closure models for bubble forces in the standard Euler-24 Euler model. Consequently, over-prediction of gas volume fraction peaks can 25 appear in the pipe center or near the wall if the bubble diameter is larger 26 than the mesh size (Lehnigk, 2021; Tomiyama et al., 2003). 27

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

as mass points and a bubble number density is introduced into the solution. 31 In this way, the forces act on the bubbles' centers of mass. Zhang and Pros-32 peretti developed a framework for the Euler-Euler model based on PCAM 33 and proposed closure models for the dilute limit by theoretical analysis and 34 direct numerical simulations (Prosperetti, 1998; Zhang and Prosperetti, 1994, 35 1995, 1997). However, the closure models they developed are for inviscid flow 36 or for rigid interfaces, which cannot be generalized for numerical simulations 37 of bubbly flows. Besides, the calculation of the particle volume fraction from 38 the particle number density in case the particle diameter is larger than the 30 mesh size was not considered. In terms of applications, PCAM was used in 40 the simulation of a wall-bounded bubbly flow by Moraga et al. (2006). How-41 ever, only a one-way coupling of the phases was considered, i.e., the influence 42 of the disperse phase on the flow of the continuous phase was neglected. To 43 recover the consistency of the Euler-Euler model, Tomiyama et al. (2003) 44 proposed to introduce the bubble number density into the disperse phase 45 continuity equation. However, the turbulent dispersion force in the disperse 46 phase momentum equation is still functions of gas volume fraction, which 47 means that the inconsistencies between the development and the usage of 48 force model still exist. In contrast, Lucas et al. (2001, 2007) introduced a 49 bubble number density in the momentum equation so that bubble forces act 50 on the bubbles' centers of mass and the gas volume fraction is obtained from 51 the convolution of the center-of-mass location and the bubble dimension. 52 However, the solver developed by them is only a one-dimensional solver. A 53 three-dimensional solver is needed to study bubbly flows comprehensively, 54 but it has not been developed so far. 55

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

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

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

In this work, an approach to simulate bubbly flows using PCAM is es-92 tablished by combining the Euler-Euler model based on PCAM, the diffusion-93 based method relating the the particle-center-averaged and the phase-averaged 94 quantities and the HZDR baseline model for the closure models. In this ap-95 proach, a physically motivated model for the wall-contact force is introduced 96 to avoid the bubbles' centers of mass coming arbitrarily close to the wall. For 97 this purpose, the wall-contact force model of Lucas et al. (2007) is adapted 98 for oblate ellipsoidal bubbles. The entire approach is implemented based on 90 the solver *reactingTwophaseEulerFoam* in the OpenFOAM Foundation re-100 lease (OpenFOAM Foundation, 2020). To evaluate its merits and compare 101 it to the standard approach, a simplified two-dimensional test setup is used 102 first. Laminar and turbulent flows are considered separately. A compari-103 son between predictions and experimental measurements is then made for 104 selected tests from the MTLoop experimental database. 105

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

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

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

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

$$\overline{f_k} = \frac{1}{\alpha_k} \int_{C^N} f_k X_k P\left(N, t\right) dC^N, \qquad (1)$$

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

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

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

$$\alpha_k = \int_{C^N} X_k P\left(N, t\right) dC^N.$$
(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 location 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

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

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

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

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

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

$$\int n d\boldsymbol{x} = N. \tag{7}$$

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)

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

where ρ is the density and \boldsymbol{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

$$\frac{\partial n\rho_d}{\partial t} + \boldsymbol{\nabla} \cdot \left(n\rho_d \left\langle \boldsymbol{u}_d \right\rangle \right) = 0. \tag{9}$$

The momentum equation for the continuous phase is

$$\frac{\partial \alpha_c \rho_c \overline{\boldsymbol{u}_c}}{\partial t} + \boldsymbol{\nabla} \cdot \left(\alpha_c \rho_c \, \overline{\boldsymbol{u}_c} \, \overline{\boldsymbol{u}_c}\right)
= -\alpha_c \nabla \overline{p_c} + \alpha_c \boldsymbol{\nabla} \cdot \overline{\mathbf{S}_c} + \boldsymbol{\nabla} \cdot \left(\alpha_c \overline{\mathbf{T}_c}\right) + \overline{\boldsymbol{f}_c} + \alpha_c \rho_c \boldsymbol{g},$$
(10)

where p, **S**, **T**, f and 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

$$\frac{\partial \beta_d \rho_d \langle \boldsymbol{u}_d \rangle}{\partial t} + \boldsymbol{\nabla} \cdot \left(\beta_d \rho_d \langle \boldsymbol{u}_d \rangle \langle \boldsymbol{u}_d \rangle\right)
= -\beta_d \nabla \overline{p_c} + \beta_d \boldsymbol{\nabla} \cdot \langle \mathbf{S}_c \rangle + \boldsymbol{\nabla} \cdot \left(\beta_d \langle \mathbf{T}_d \rangle\right) + \langle \boldsymbol{f}_d \rangle + \beta_d \rho_d \boldsymbol{g},$$
(11)

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

$$\beta_d = nV_d,\tag{12}$$

¹¹⁹ where V_d is the bubble volume.

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

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

 The phase volume fraction in the viscous stress term of Eq. (10) is outside of the divergence since the part of the viscous stress term related to the gradient of the phase volume fraction is cancelled by the interfacial contributions, which is similar to the pressure term (Prosperetti and Jones, 1984). 2. Equation (11) is derived by averaging the equation of motion for bubbles, while the equation in the standard Euler-Euler model is derived
by averaging the local instantaneous momentum equation and by using
the phase indicator function of the disperse phase.

3. The physical meaning of the momentum equation for the disperse phase 142 in the Euler-Euler model based on PCAM is different from that in the 143 standard Euler-Euler model. Equation (11) displays the momentum 144 balance of gas, which belongs to bubbles having their centers located 145 inside the control volume. This gas may only be partially contained 146 within the control volume. In the standard Euler-Euler model, the 147 equation refers to the momentum balance of all gas contained inside 148 the control volume. This gas may belong partially or even completely 149 to bubbles with centers outside of the control volume. Hence, Eq. (11) 150 is related to the bubble number density, while in the standard Euler-151 Euler model, the momentum equation of the disperse phase is related 152 to the volume fraction of the disperse phase. 153

4. Equation (11) 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 the standard Euler-Euler model, the viscous stress tensor 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

Force and turbulence	Selected model
Drag force	Ishii and Zuber (1979)
(Shear-) lift force	Tomiyama 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, $C_{\rm VM} = 0.5$
Turbulence	$k - \omega$ SST
Bubble-induced turbulence	Ma et al. (2017)

Table 1: HZDR baseline model for monodisperse bubbly flows.

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

$$\boldsymbol{f}(n) = \frac{nV_d}{\alpha_d} \boldsymbol{f}(\alpha_d), \qquad (13)$$

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

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

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

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

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

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

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

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

To calculate a phase-averaged quantity from the corresponding particlecenter-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 centerof-mass by solving the following diffusion equation

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

with an initial condition of $\alpha_d = nV_d$. In this process, the gas volume is 191 conserved. In the equation, τ is the diffusion pseudo-time and C_{diff} is the 192 diffusion coefficient, both determining the size of the bubble influence region. 193 Note, this diffusion process takes place at every time step of the simulation 194 such that τ is unrelated to the physical time, and, hence, referred to as a 195 pseudo-time. Without loss of generality, C_{diff} is set to be 1 m² s⁻¹ for all dif-196 fusion processes in the present study, while an optimized value is determined 197 for τ in section 2.5. To solve Eq. (15), a Neumann boundary condition with 198 derivative equal to zero is used for all boundaries. 199

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

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

with an initial condition of $\alpha_d \overline{u_d} = n \langle u_d \rangle V_d$. Other settings are as described above.

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

bubble influence region by the following diffusion equation

$$\frac{\partial \overline{\boldsymbol{f}_d}}{\partial \tau} - \boldsymbol{\nabla} \cdot \left(C_{\text{diff}} \nabla \overline{\boldsymbol{f}_d} \right) = 0, \qquad (17)$$

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

$$\overline{\boldsymbol{f}_c} = -\overline{\boldsymbol{f}_d}.\tag{18}$$

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

$$\langle \boldsymbol{u}_c \rangle \left(\boldsymbol{x}, \tau \right) = \int_{-\infty}^{+\infty} \overline{\boldsymbol{u}_c} \left(\boldsymbol{x_0}, 0 \right) \frac{1}{\left(4\pi C_{\text{diff}} \tau \right)^{\frac{3}{2}}} \exp\left\{ -\frac{\left(\boldsymbol{x} - \boldsymbol{x_0} \right)^2}{4C_{\text{diff}} \tau} \right\} d\boldsymbol{x_0}, \quad (19)$$

which is the solution of

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

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

204 2.5. Diffusion pseudo-time optimization

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

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



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

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

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

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

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

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

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

$$n(x_{c},0) = \frac{\sum_{i=1}^{M} \alpha_{d}^{\exp}(x_{i}) V_{i}}{V_{d} V_{c}},$$
(24)

where M is the number of cells covered by the bubbles (Fig. 1(a)), while V_i 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

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

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

In the last equation, the discretised form of $\alpha_d^{\rm sol}$ 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 $\tau_{\rm opt}$ will depend on $C_{\rm diff}$ as well as d_B , a dimensionless optimized diffusion pseudo-time

$$\widetilde{\tau}_{\rm opt} = \frac{\tau_{\rm opt} C_{\rm diff}}{d_B^2} \tag{26}$$

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.

As can be seen, $\tilde{\tau}_{opt}$ is almost a constant when M is larger than 30. As a result, $\tilde{\tau}_{opt} = 0.03356$ 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. 3. For the solved gas volume fraction, 94.72% of the gas volume is contained 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

$$\left\langle \boldsymbol{f}_{d}^{\mathrm{drag}} \right\rangle = -\frac{3}{4d_{B}}C_{D}\rho_{c}\beta_{d} |\langle \boldsymbol{u}_{d} \rangle - \langle \boldsymbol{u}_{c} \rangle|\left([\langle \boldsymbol{u}_{d} \rangle] - \langle \boldsymbol{u}_{c} \rangle\right)$$
(27)

and

$$\left\langle \boldsymbol{f}_{d}^{\mathrm{VM}} \right\rangle = -C_{\mathrm{VM}}\rho_{c}\beta_{d} \left(\frac{D_{d} \left[\left\langle \boldsymbol{u}_{d} \right\rangle \right]}{Dt} - \frac{D_{c} \left\langle \boldsymbol{u}_{c} \right\rangle}{Dt} \right), \tag{28}$$

respectively, where C_D and $C_{\rm VM}$ are the coefficients and ρ is the density. The quantities within the square brackets are the quantities remaining to be solved. They are treated implicitly. Note, the other term in Eq. (27) involving $\langle \boldsymbol{u}_d \rangle$ is treated explicitly, which means the old value from the last time or iteration step will be used. The forces $\langle \boldsymbol{f}_{d}^{\text{drag}} \rangle$ and $\langle \boldsymbol{f}_{d}^{\text{VM}} \rangle$ can be calculated directly using the particle-center-averaged fields, and hence, appear directly 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

$$\boldsymbol{f}_{c}^{\text{drag, correction}} = -\frac{3}{4d_{B}}C_{D}\rho_{c}\beta_{d}|\langle\boldsymbol{u}_{d}\rangle - \langle\boldsymbol{u}_{c}\rangle|\left([\overline{\boldsymbol{u}_{c}}] - \overline{\boldsymbol{u}_{c}}\right)$$
(29)

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

$$\boldsymbol{f}_{c}^{\text{VM, correction}} = -C_{\text{VM}}\rho_{c}\beta_{d}\left(\left[\frac{D_{c}\overline{\boldsymbol{u}_{c}}}{Dt}\right] - \frac{D_{c}\overline{\boldsymbol{u}_{c}}}{Dt}\right)$$
(30)

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

These correction terms do not exist in theory. However, once the simulation has sufficiently converged to a steady state, these terms will be neglectable since the difference between the current and the old values will be neglectable.

244 2.7. Solution procedure



Figure 4: Solution procedure.

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

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

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

263 3.1. Geometry and simulation setups

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

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

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

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



Figure 5: Geometry and boundary conditions

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

Table 2: Boundary settings.

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

$\rho_c [\mathrm{kg} \mathrm{m}^{-3}]$	$\rho_d \; [\mathrm{kg} \mathrm{m}^{-3}]$	$\mu_c [\mathrm{kg} \mathrm{m}^{-1} \mathrm{s}^{-1}]$	$\mu_d [\mathrm{kg} \mathrm{m}^{-1} \mathrm{s}^{-1}]$
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

$$p = p_{\rm rgh} + \rho_m gh, \tag{32}$$

where ρ_m is the mixture density. It is calculated by

$$\rho_m = \alpha_d \rho_d + \alpha_c \rho_c. \tag{33}$$

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

281 3.2. Mesh sensitivity analysis

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



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

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

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



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

³¹² similar upon refining the mesh.

In summary, using PCAM in the Euler-Euler model yields a mesh independent solution, where the standard Euler-Euler model does not. However, these 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.

318 3.3. 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 2 mm. At the inlet, the lateral region between x = 0.01 and x = 0.02 has non-zero gas volume fractions, which is equal to the bubble diameter.

For a laminar flow, the simulation results are shown in Fig. 8. In the 323 results for the standard Euler-Euler model, the gas volume fraction profiles 324 are narrow with high peak, which means that gas concentrates in the channel 325 center following the flow downstream. Besides, the lateral region covered by 326 the gas becomes smaller than the bubble diameter, which is nonphysical. 327 This phenomenon is caused again by the lift force, which transports the 328 distributed gas to the channel center even though it really belongs to the 320 same bubble. In contrast, by using PCAM in the Euler-Euler model, the 330 distribution of the gas volume fraction remains almost unchanged after the 331 inlet (Fig. 8 (b)). Besides, the width of the region covered by the gas has 332 a size close to the bubble diameter. Therefore, the gas volume fractions 333 predicted by PCAM are considered to be more reasonable. 334

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

In conclusion, gas over-concentration can appear in the channel center in the standard Euler-Euler model since lift force is a function of the gas volume fraction. This gas over-concentration is avoided by changing the 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

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

347 4.1. Experimental conditions

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

357 4.2. Simulation setup

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

371 4.3. Comparison of wall peaking cases

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

Name	$J_c \; [\mathrm{ms^{-1}}]$	$J_d \; [\mathrm{ms^{-1}}]$	$lpha_d$ %	$d_B \; [\mathrm{mm}]$	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

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

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

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

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

416 4.4. Comparison of cases with center peaks

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

432 4.5. Comparison of cases in finely dispersed flow

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

After employing PCAM, the over-prediction is alleviated (Fig. 15). Fur-443 thermore, combining PCAM with the wall-contact force avoids the gas vol-444 ume fraction peak being located on the wall. Note, if the wall-contact force 445 is a function of the gas volume fraction, it can drive too much gas away from 446 the wall. That is the reason why it is not suggested to use it in the standard 447 Euler-Euler model. Nevertheless, no matter which Euler-Euler model is used, 448 the trends of the simulation results do not agree well with the trends of the 440 experimental data even if PCAM is used. The reason can be insufficiencies 450 in the HZDR baseline model due to some unknown effects in finely dispersed 451 flow (Lucas et al., 2020). 452



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 disperse 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).

5. Summary and Conclusions

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

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

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

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

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488 7. Nomenclature

C^N	a set of all possible dynamic states	-
$C_{\rm diff}$	diffusion coefficient	$\mathrm{m}^2\mathrm{s}^{-1}$
C_D	drag coefficient	-
$C_{\rm VM}$	virtual mass coefficient	-
d	diameter	m
E	error	-
f	force per unit volume	${ m N}{ m m}^{-3}$
g	acceleration of gravity	${ m ms^{-2}}$
J	superficial velocity	${ m ms^{-1}}$
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	-
$P(\boldsymbol{x}, \boldsymbol{u}, t)$	one-bubble probability density function	${\rm m}^{-4}{\rm s}$
p	pressure	${ m Nm^{-2}}$
r	radial coordinate	m
R	pipe radius	m
\boldsymbol{S}	viscous stress tensor	${ m N}{ m m}^{-2}$
T	Reynold stress tensor	${ m N}{ m m}^{-2}$
t	time	S
\boldsymbol{u}	velocity vector	${ m ms^{-1}}$
V_d	bubble volume	m^3
X_k	phase indicator function for phase k	-
x, y, z	spatial coordinates	m
$oldsymbol{x}, oldsymbol{x}_{oldsymbol{0}}$	spatial coordinate vector	m
x_c, \boldsymbol{y}	bubble center location	m
α	phase volume fraction	-
ß,	gas volume fraction projecting	_
Pd	all bubble volume to bubble centers	
$\delta(x)$	Dirac delta function	-
μ	dynamic viscosity	$\mathrm{kg}\mathrm{m}^{-1}\mathrm{s}^{-1}$
ρ	density	${ m kg}{ m m}^{-3}$
au	diffusion pseudo-time	S
σ	surface tension coefficient	${ m N}{ m m}^{-1}$

B	bubble
С	continuous
d	disperse
k	phase index
m	mixture
\exp	expected
max	maximum
opt	optimized
sol	solved
VM	virtual mass force
$\overline{\cdot}$	phase-average
$<\cdot>$	particle-center-average
$\widetilde{\cdot}$	dimensionless

489 Appendix

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

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

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

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

into Eq. (1), we obtain

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

A single dash (') here denotes the fluctuating quantity relative to the timeaveraged quantity. Replacing $\langle \phi_d \rangle$ in the last equation with $\langle u_d \rangle$, we obtain

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

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

$$\overline{\overline{\boldsymbol{u}}_{c}}^{t} = \overline{\overline{\boldsymbol{u}}_{c}}^{F} - \frac{\overline{\alpha_{c}'\overline{\boldsymbol{u}_{c}'}}^{t}}{\overline{\alpha_{c}}^{t}}.$$
(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

$$\left\langle \boldsymbol{f}_{d}^{\mathrm{drag}} \right\rangle = -D_{\mathrm{cd, p}} A_{\mathrm{cd}} \left(\left\langle \boldsymbol{u}_{d} \right\rangle - \overline{\boldsymbol{u}_{c}} \right),$$
 (6)

where

$$D_{\rm cd,\,p} = \frac{1}{8} C_D \rho_c \left| \left\langle \boldsymbol{u}_d \right\rangle - \overline{\boldsymbol{u}_c} \right|,\tag{7}$$

and

$$A_{\rm cd} = n\pi d_B^2. \tag{8}$$

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 $D_{\rm cd,p}$ does not change with time. Applying time average to Eq.(6) yields

$$\overline{\left\langle \boldsymbol{f}_{d}^{\mathrm{drag}} \right\rangle}^{t} = -D_{\mathrm{cd,p}} \left[\overline{A_{\mathrm{cd}}}^{t} \left(\overline{\left\langle \boldsymbol{u}_{d} \right\rangle}^{t} - \overline{\boldsymbol{u}_{c}}^{t} \right) + \overline{A_{\mathrm{cd}}' \left(\left\langle \boldsymbol{u}_{d} \right\rangle' - \overline{\boldsymbol{u}_{c}'} \right)}^{t} \right].$$
(9)

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

$$\overline{\left\langle \boldsymbol{f}_{d}^{\mathrm{drag}} \right\rangle}^{t} = -D_{\mathrm{cd,p}} \overline{A_{\mathrm{cd}}}^{t} \left[\left(\overline{\left\langle \boldsymbol{u}_{d} \right\rangle}^{F} - \frac{\overline{n' \left\langle \boldsymbol{u}_{d} \right\rangle'}^{t}}{\overline{n}^{t}} \right) - \left(\overline{\overline{\boldsymbol{u}_{c}}}^{F} - \frac{\overline{\alpha_{c}' \overline{\boldsymbol{u}_{c}}'}^{t}}{\overline{\alpha_{c}}^{t}} \right) \right] \quad (10)$$
$$- D_{\mathrm{cd,p}} \overline{A_{\mathrm{cd}}' \left(\left\langle \boldsymbol{u}_{d} \right\rangle' - \overline{\boldsymbol{u}_{c}}' \right)}^{t}$$

The last equation can be simplified to

$$\overline{\left\langle \boldsymbol{f}_{d}^{\mathrm{drag}} \right\rangle}^{t} = -D_{\mathrm{cd, p}} \overline{A_{\mathrm{cd}}}^{t} \left(\overline{\left\langle \boldsymbol{u}_{d} \right\rangle}^{F} - \overline{\overline{\boldsymbol{u}}_{c}}^{F} \right) + \boldsymbol{f}_{d}^{\mathrm{TD}}, \tag{11}$$

where

$$\boldsymbol{f}_{d}^{\mathrm{TD}} = D_{\mathrm{cd, p}} \overline{A_{\mathrm{cd}}}^{t} \left(\frac{\overline{n' \langle \boldsymbol{u}_{d} \rangle}^{t}}{\overline{n}^{t}} - \frac{\overline{\alpha_{c}' \overline{\boldsymbol{u}_{c}'}}^{t}}{\overline{\alpha_{c}}^{t}} \right) - D_{\mathrm{cd, p}} \overline{A_{\mathrm{cd}}' \left(\langle \boldsymbol{u}_{d} \rangle' - \overline{\boldsymbol{u}_{c}'} \right)}^{t}.$$
(12)

Substituting

$$\overline{C_{\rm cd,p}}^t = D_{\rm cd,p} \overline{A_{\rm cd}}^t \tag{13}$$

into Eq. (12) results in

$$\boldsymbol{f}_{d}^{\mathrm{TD}} = \overline{C_{\mathrm{cd,p}}}^{t} \left(\frac{\overline{n' \langle \boldsymbol{u}_{d} \rangle'}^{t}}{\overline{n}^{t}} - \frac{\overline{\alpha_{c}' \overline{\boldsymbol{u}_{c}'}}^{t}}{\overline{\alpha_{c}}^{t}} \right) - \overline{C_{\mathrm{cd,p}}}^{t} \frac{\overline{A_{\mathrm{cd}}' \left(\langle \boldsymbol{u}_{d} \rangle' - \overline{\boldsymbol{u}_{c}'} \right)^{t}}}{\overline{A_{\mathrm{cd}}}^{t}}.$$
 (14)

Bubble diameter is a constant. Therefore

$$A_{\rm cd}' = n' \pi d_B^2, \tag{15}$$

and

$$\overline{A_{\rm cd}}^t = \overline{n}^t \pi d_B^2. \tag{16}$$

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

$$\frac{\overline{A_{\rm cd}'\left(\langle \boldsymbol{u}_d \rangle' - \overline{\boldsymbol{u}_c'}\right)^t}}{\overline{A_{\rm cd}}^t} = \frac{\overline{n'\left(\langle \boldsymbol{u}_d \rangle' - \overline{\boldsymbol{u}_c'}\right)^t}}{\overline{n}^t}.$$
(17)

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

$$\boldsymbol{f}_{d}^{\mathrm{TD}} = \overline{C_{\mathrm{cd,p}}}^{t} \left(\frac{\overline{n' \boldsymbol{\overline{u_{c}}}'}^{t}}{\overline{n}^{t}} - \frac{\overline{\alpha_{c}' \boldsymbol{\overline{u_{c}}}'}^{t}}{\overline{\alpha_{c}}^{t}} \right).$$
(18)

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

$$\overline{n' \boldsymbol{u}_c'}^t = -\frac{\upsilon_c^{\text{turb}}}{\sigma_{\text{nc}}} \nabla \overline{n}^t, \qquad (19)$$

and

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

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

$$\boldsymbol{f}_{d}^{\mathrm{TD}} = -\overline{C_{\mathrm{cd,p}}}^{t} \left(\frac{v_{c}^{\mathrm{turb}}}{\sigma_{\mathrm{nc}}} \frac{\nabla \overline{n}^{t}}{\overline{n}^{t}} - \frac{v_{c}^{\mathrm{turb}}}{\sigma_{\mathrm{\alpha c}}} \frac{\nabla \overline{\alpha_{c}}^{t}}{\overline{\alpha_{c}}^{t}} \right).$$
(21)

Here, we assumed that

$$\sigma_{\rm nc} = \sigma_{\alpha c}.\tag{22}$$

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

$$\frac{\nabla \overline{n}^t}{\overline{n}^t} = \frac{\nabla \overline{\beta_d}^t}{\overline{\beta_d}^t}.$$
(23)

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

$$\boldsymbol{f}_{d}^{\mathrm{TD}} = -\overline{C_{\mathrm{cd,p}}} \frac{t}{\sigma_{\mathrm{cc}}} \frac{v_{c}^{\mathrm{turb}}}{\sigma_{\mathrm{ac}}} \left(\frac{\nabla \overline{\beta_{d}}^{t}}{\overline{\beta_{d}}^{t}} - \frac{\nabla \overline{\alpha_{c}}^{t}}{\overline{\alpha_{c}}^{t}} \right).$$
(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.

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