Basic verification of a numerical framework applied to a morphology adaptive multifield two-fluid model considering bubble motions

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Summary
A morphology adaptive modeling framework is derived that is able to handle computationally efficiently dispersed as well as resolved interfacial structures coexisting in the computational domain with the same set of equations. The Eulerian multifield two-fluid model is combined with the compact momentum interpolation method for multiple phases, which has been proposed in the literature as an extension to the Rhie-Chow pressure-velocity coupling. Additionally to the interfacial drag force, the virtual mass force is consistently accounted for in the model. Utilizing a specialized interfacial drag formulation, large interfacial structures can be described with the presented method in a volume-of-fluid-like manner, additionally to the dispersed description. The strong phase coupling due to the drag closure model in interfacial regions is resolved with a partial elimination algorithm, which is adapted to work in an approximate manner for more than two phases via a sum formulation. The presented model is implemented in the C++ library OpenFOAM and solver performance is compared with results obtained with the homogeneous model approach in two cases of a single rising gas bubble for two- and three-dimensional space, respectively. Additionally, for both three-dimensional cases, the results are compared with experimental data. Finally, the presented method's capability of representing dispersed and resolved interfacial structures at the same time is demonstrated with two test cases: a two-dimensional gas bubble, rising in a liquid, which is laden with micro gas bubbles, and a two-dimensional stagnant stratification of water and oil, sharing a large-scale interface, which is penetrated by micro gas bubbles.

KEYWORDS
Eulerian-Eulerian model, finite volume method, momentum interpolation, multifield two-fluid model, multiphase flow, partial elimination algorithm

1 | INTRODUCTION

Two phase flows and especially gas-liquid flows play an important role in applications of many different industrial fields, for example, in the energy section, in chemical, processing, oil and mining industry, in refineries as well as in numerous...
kinds of reactors. In such fields, reliability and safety are of great interest. Flows occurring in the aforementioned applications are characterized by a high level of complexity. Multiple different morphology regimes appear, even in facilities of simplest geometries, such as pipe flows, where segregated, bubbly, annular, or slug flows play a role. The level of complexity is further increasing, if countercurrent flows or wave breaking phenomena are of interest. From that arises a high demand for simulation techniques for predicting gas-liquid flow behaviors with different flow morphologies sufficiently exact, with feasible computational expense and less knowledge about the occurring flow regimes prior to the investigation. One of the biggest challenges in describing multiphase flows is, in analogy to turbulent flows, the wide range of spatial scales, which span a range between the molecular length scale for the thickness of an interface to the dimensions of an industrial facility. There are many situations, in which a large-scale interface (a boundary between two immiscible phases), for example, a free surface, meets disperse interfacial structures, such as bubbles or droplets, or situations, in which disperse interfacial structures of different phases, size or shape interact with each other. For each of those individual flow morphologies, there are multiple modeling approaches to choose from, which are characterized by different levels of accuracy and computational efficiency.

Interfaces, which exist at a scale above grid scale, are resolved on the computational grid. Wörner\(^1\) gave a comprehensive overview over numerous different interface-resolving models that have been proposed in order to capture the physics of large-scale interfaces, for example, Lagrangian methods such as marker and cell\(^2\) or front-tracking\(^3\) as well as Eulerian approaches, for example, level set,\(^4\) conservative level set,\(^5\) volume of fluid (VOF) with\(^6\) or without\(^7\) interface reconstruction, or phase field methods.\(^8\) All of these methods are typically formulated as a homogeneous model, which means that immiscible phases share a common velocity field and physical properties are considered as mixing properties depending on phase fractions.

Interfacial structures, which are smaller than grid scale—the disperse phase—cannot be resolved and have to be described by appropriate models instead. One way to achieve this is the application of an Euler-Lagrange method, where interfacial structures, such as bubbles or droplets, are individually described by point elements and get transported with an equation of motion, which considers all body forces as modeled source terms.\(^9\) Another way is to represent continuous and disperse phases as interpenetrating continua—the Euler-Euler point of view—in an ensemble averaged manner,\(^10\) where interfacial closure models are formulated as continuous forces and include assumptions about element size, number density, and shape. Interfacial forces are accounted for by including volume force terms into the momentum equation.

It is desirable to describe both interfacial flow structures, which are smaller than computational grid size, as well as such, which are larger, in a single-computational domain. Therefore, interface resolving and nonresolving models have to be combined in a hybrid model approach and the appropriate individual models are applied, depending on the local flow morphology. Lagrangian point particle methods have been combined with a level-set method,\(^11,12\) as well as with a VOF method.\(^13\) Additionally, there is a large number of attempts to combine Euler-Euler models for dispersed flows with VOF or VOF-like models with or without interface reconstruction (see Bestion et al\(^14\) for a comprehensive classification). VOF-like methods with interface reconstruction and disperse Euler-Euler model were blended in a two-fluid formulation by Boualouache et al\(^15\) and Yan and Che,\(^16\) and with switching between one- and two-fluid formulation by Černe et al.\(^17\) Lopes et al\(^18\) added an additional disperse Eulerian phase to a VOF model without interface reconstruction with all continuous phases sharing a single-velocity field. Special attention was paid to stratified flows and large interfaces with modeling of interface features below grid scale. This has been realized with VOF-like methods without reconstruction in two-fluid formulation.\(^19\)-\(^24\) Contrary to that, a VOF-like approach without interface reconstruction was combined with Euler-Euler modeling for dispersed flows strictly limited to two fields, representing both physical phases, for example, a gas and a liquid phase.\(^25\)-\(^30\) Within the frame of this modeling approach a blending method ensures that the two-fluid model behaves either as a VOF-like model or as disperse Euler-Euler model, depending on the local flow morphology. To achieve this, interfacial momentum exchange terms have to be formulated for all possible regimes, namely continuous liquid with dispersed gas, continuous gas with dispersed liquid, and continuous gas with continuous liquid. The latter combination describes the interaction between both phases in the region of a pronounced, shared interface. For instance, Wardle and Weller\(^30\) combined an artificial interface compression term for phase fraction transport with a residual drag formulation in order to prevent resolved interfaces from smearing by numerical diffusion. With this method, a slip velocity between both phases sharing an interface is still allowed in that region. Finally, model contributions of all three regimes are summed up, weighted by a regime indicator function, which is based on the ratio of gas and liquid volume fraction. This kind of formulation offers a compact solution for a number of different flow regimes but also implies limitations. For instance, interactions between multiple disperse phases or between a disperse phase and two different continuous phases cannot be covered by such a hybrid model, because only two phases with individual velocity fields are considered. To account for more complex flow situations, disperse phases need to be simulated as individual numerical phase, additionally to the numerical phases for regions, where continuous flows occur. One possible combination is continuous
water, continuous air, air bubbles, modeled as disperse air, and water droplets, modeled as disperse water, in the same computational domain. Tomiyama and Shimada\textsuperscript{31} and Tomaselli and Christensen\textsuperscript{32} proposed models, where both gas and liquid continuous phases share a single-velocity field and every disperse phase is considered to have its own velocity field. Such a method is able to handle an arbitrary number of disperse phases, but only one pair of gas and liquid phases. In contrast to that, Meller et al.\textsuperscript{33} and Mimouni et al.\textsuperscript{34} assigned individual velocity fields to all continuous phases, additionally to the velocity field of the disperse phase, in so-called three-fluid models. Hänsch et al.\textsuperscript{35} and Xiang et al.\textsuperscript{36} distributed gas bubbles of different diameters to separate phases and, in that way, are able to model individual motions of differently sized disperse interfacial structures.

Hou et al.\textsuperscript{37} and Štrubelj et al.\textsuperscript{38} paid special attention to an accurate description of resolved interfaces with a two-fluid model, whereby both authors used conservative level-set methods. As stated by Štrubelj et al.\textsuperscript{38} from a mathematical point of view it is convenient to use a two-fluid formulation for both VOF-like and disperse Euler-Euler models in order to solve for a unique set of equations in the whole computational domain. Furthermore, the choice of a two fluid model in principle allows for a nonzero slip velocity between two continuous phases at an interface. Gauss et al.\textsuperscript{39} showed that such an interfacial slip allows for the description of large interface structures, such that the rising velocity of a single bubble can be predicted correctly, even on numerical grids, which are to coarse to fully resolve physical processes on all scales.

The present work takes the model of Hänsch et al.\textsuperscript{35} as a conceptual starting point with the goal to describe all continuous and disperse phases as individual numerical phases in a computationally efficient way. A numerical framework is presented, which incorporates a multifield two-fluid model, which is able to account for resolved interfaces. In principle, the two-fluid model allows slip between two phases sharing an interface, for example, in the context of underresolved interfaces. However, within the scope of the present work, a no-slip condition between continuous phases is preserved. The solution procedure is implemented in the OpenFOAM C++ library and the source code is made public by Meller et al. (2020).\textsuperscript{40} To achieve numerical robustness and sufficient accuracy, the compact momentum interpolation method (CMI) for multiphase flows, which was proposed by Cubero et al.,\textsuperscript{41} is extended to consistently take into account the interfacial momentum exchange closure of virtual mass force.

The interfacial drag force of Štrubelj and Tiselj\textsuperscript{42} is applied to pairs of continuous phases, to describe resolved interfaces. The strong phase coupling resulting from that is approximately resolved with a partial elimination algorithm (PEA),\textsuperscript{43} which is formulated for an arbitrary number of phases. In order to show capability of the presented solvers to describe the interplay between large resolved interfaces and finely dispersed flow regimes, interfacial closure models for disperse flows are included, namely drag and virtual mass forces.

Physical modeling and the numerical method are described in Sections 2 and 3, respectively. Subsequently, in Section 4, the capability of the presented method is demonstrated with for a selected set of test cases considering bubble flows. Finally, results are concluded and perspectives are shown in Section 5.

2 | MODELING

The presented model framework consists of the phase specific, ensemble averaged transport equations of the Euler-Euler two-fluid model, a set of closure models for interfacial momentum transfer terms for regimes of dispersed flows, an interfacial drag formulation to represent large, resolved interfaces in the two-fluid model and a morphology adaptive weighting procedure to apply closure models consistently to individual continuous and disperse phases.

2.1 | Basic equations of the two-fluid model

The ensemble averaging procedure results in a set of mass and momentum conservation equations for each individual phase $\alpha$\textsuperscript{44}

$$\partial_t r_\alpha \rho_\alpha + \partial_i r_\alpha \rho_\alpha u_{\alpha,i} = 0,$$

$$\partial_t r_\alpha \rho_\alpha u_{\alpha,i} + \partial_j r_\alpha \rho_\alpha u_{\alpha,j} u_{\alpha,i} = -r_\alpha \partial_i p + \partial_j 2r_\alpha \mu_\alpha S_{\alpha,j} + r_\alpha g_i \rho_\alpha + \sum_{\beta \neq \alpha} r_\alpha \sigma_{\alpha \beta} \rho_\beta n_{\alpha \beta,i} + f_{\alpha,i}. \tag{2}$$

Equation (1) shows the phasic mass conservation equation, which will later be utilized to realize the transport of phase volume fractions $r_\alpha$. Time and spatial partial derivatives are denoted as $\partial_t = \partial/\partial t$ and $\partial_i = \partial/\partial x_i$, respectively, and $u_{\alpha,i}$ as
velocity field of phase \( \alpha \). In the phase momentum conservation Equation (2), \( p \) represents the pressure, which is shared between all phases \( \alpha \). The phase dynamic viscosity is \( \mu_\alpha \), the phase strain rate tensor is

\[
S_{\alpha,ij} = \frac{1}{2} (\partial_i u_{\alpha,j} + \partial_j u_{\alpha,i}) - \delta_{ij} \frac{1}{3} \partial_k u_{\alpha,k},
\]

(3)

the gravitational acceleration is \( g \). Surface tension for resolved interfaces is modeled with the approach of Brackbill et al.,\(^45\) where \( \sigma_{\alpha\beta} \) denotes the surface tension coefficient for the pair of both continuous phases \( \alpha \) and \( \beta \) with according interface curvature \( \kappa_{\alpha\beta} \) and interface normal vector \( n_{\alpha\beta} \). Volume forces are denoted by \( f_{\alpha,i} \), which includes all interfacial momentum exchange closure terms.

### 2.2 Interfacial momentum exchange for dispersed and resolved interfacial structures in the two-fluid model

In the disperse two-fluid model, all information about interfacial structures and interactions between different phases is lost due to the applied averaging procedure. Hence, interfacial momentum exchange mechanisms between both phases of each continuous-disperse phase pair have to be modeled. The following interfacial forces are usually considered in modeling of dispersed flows:\(^46\) drag, lift, virtual mass, turbulent dispersion, and wall lubrication. In bubbly flows, drag and virtual mass forces are of great importance\(^9\) and their consideration is required to achieve a solution procedure that is numerically stable. Therefore, only interfacial drag and virtual mass forces are accounted for, together with related closure models, which are selected according to Liao et al.\(^46\) Nevertheless, the algorithm is capable of handling all other interfacial momentum exchange forces. For drag forces, the closure model of Ishii and Zuber\(^47\) is applied without any correction terms considering swarm effects. The closure term by Crowe et al.\(^48\) is applied to model the virtual mass force between a disperse phase \( d \) and a continuous phase \( c \)

\[
\mathbf{f}_{\text{VM}}^{cd} = -f_{\text{VM}}^{dc} = r_d \rho_c C_{\text{VM}}^{cd} (D_{t,c} \mathbf{u}_c - D_{t,d} \mathbf{u}_d).
\]

(4)

The substantial derivative of a quantity is denoted as \( D_{t,\alpha} \), considering phase velocity \( \mathbf{u}_\alpha \). The model constant \( C_{\text{VM}}^{cd} \) is set to 0.5. For a pair of two continuous phases \( cc \), a virtual mass force is not defined and, therefore, \( C_{\text{VM}}^{cc} \) is set to zero.

Whenever large-scale interfaces occur, such flow structures have to be resolved within the computational grid. In order to keep the thickness of an interface finite, local velocity components normal to the interface have to be identical for both continuous phases, which share the interface. This requirement is often referred to as the interface normal condition. In a one-fluid model, which is also known as homogeneous model, both continuous phases share a single-velocity field, or in other words, all velocity components are identical, which is a more restrictive constraint than only ensuring the equality of interface normal components. Such a no-slip interface condition is reasonable, if the resolution of the computational grid is fine enough to resolve interfacial structures.\(^9\) In contrast to a homogeneous model, the two-fluid model is able to allow for a tangential slip velocity between both phases, which is an appropriate approach to model interfaces in an underresolved manner.\(^39\) For the sake of simplicity in the present work, the model framework is setup, such that all relative velocity components between multiple phases are identical in the region of a shared interface. In the future, the interfacial drag modeling in resolved interface regions will be made capable to properly handle a free-slip condition. In this way, the capability of the present model is demonstrated to reproduce the behavior of a homogeneous model, which has been shown theoretically by Yan and Che.\(^16\) This can be achieved by application of an interfacial drag model, which is designed to ensure that both phases have identical velocities in the interface region.

Štrubelj and Tiselj\(^42\) proposed a drag closure, which is formulated for a pair of two phases \( \alpha \) and \( \beta \)

\[
\mathbf{f}_{\alpha\beta}^D = K_{\alpha\beta}^D (\mathbf{u}_\beta - \mathbf{u}_\alpha) \quad \text{with} \quad K_{\alpha\beta}^D = r_\alpha r_\beta \rho_{\alpha\beta} \frac{1}{\tau_r}.
\]

(5)

The mixture density is formulated as

\[
\rho_{\alpha\beta} = \frac{\rho_\alpha r_\alpha + \rho_\beta r_\beta}{r_\alpha + r_\beta}.
\]

(6)

The drag coefficient \( K_{\alpha\beta}^D \) is formulated in terms of relaxation time \( \tau_r \), which has to be chosen much smaller than the physical time step.\(^42\) The model is applied to the present framework with a small value for the relaxation time.
τ_r = 10^{-8} \Delta_t in order couple continuous phases in an interfacial region, even if dispersed phases are present at the same location.

### 2.3 Morphology adaptive weighting of closure models

The present model framework utilizes an arbitrary number of continuous and disperse phases and each of those is dedicated to a physical phase, for example, air, oil, or water, and to an individual flow morphology, for example, continuum, bubbles, or droplets. Hence, special care has to be taken of interfacial momentum transfer modeling, whenever three or more phases occur in the same location. To account for such situations, a weighting factor $F_{\alpha\beta}$ is inserted into the formulation of all individual momentum exchange terms between two phases $\alpha$ and $\beta$

$$f_{\alpha\beta} = F_{\alpha\beta} \tilde{f}_{\alpha\beta},$$

where $\tilde{f}_{\alpha\beta}$ denotes the original closure formulation. It is worth noting that this type of regime adaption is purely related to the fact that the presented hybrid model distinguishes between continuous and disperse phases. The weighting factor between any pair of continuous phases $F_{cc}$ is set to unity. In that way, the strong velocity coupling between velocity fields of different continuous phases via the drag model formulation of Štrubelj and Tiselj\textsuperscript{42} is maintained in order to fulfill the no-slip interface condition. Between two disperse phases (dd), no momentum exchange terms are defined and, therefore, $F_{dd}$ is set to zero. For all momentum exchange terms of a pair of disperse and continuous phases (cd), the following weighting factor

$$F_{cd} = \frac{r_c}{\sum_{i \in C} r_i}$$

is applied, where C denotes the set of all continuous phases. As $F_{cd}$ equals unity, wherever exactly one continuous phase is present, the original closure model is recovered, even if there are two or more disperse phases, resulting in the intended behavior of the original closure model. In an interfacial region, where multiple continuous phases are existent, the prefactors $F_{cd}$ for all pairs of one and the same disperse phase d and any of the continuous phases c sum up unity. In that way, all momentum exchange closures, for example, the drag force, are accounted for in the right amount and the disperse phase is able to pass the interface, which will be demonstrated in Section 4.

### 3 Numerical Method

#### 3.1 Equations

Equation (2) results in a set of partial differential equations that is solved numerically on a collocated grid. The coupled system of equations is solved in a segregated manner by linearization and subsequent application of the Jacobi method. Thereby, the resulting equational system is solved iteratively. In the following, the notation of Cubero et al\textsuperscript{41} is adopted, so variables at cell centers and faces are denoted with $[.]_p$ and $[.]_f$, respectively, and the linear interpolation operation from cell centers to cell faces is depicted with $\lfloor\cdot\rfloor$. The linear system of equations is expressed in matrix form

$$[a]_p [u]_p = [H]_p + [G]_p. \quad (9)$$

The implicit diagonal matrix coefficients are referred to as $a$, explicit off-diagonal contributions, momentum exchange closures and volume force contributions as $H$, and the contribution due to pressure force is denoted as $G \propto -\nabla p$. At this point, implicit and explicit contributions of the transient term are included in coefficients $a$ and $H$, respectively. In order to suppress decoupling of pressure and velocity fields (checker boarding) due to the stencil structure of the discretization scheme for pressure gradient forces, Rhie and Chow\textsuperscript{49} proposed a face-based momentum interpolation algorithm. The numerical flux $[\phi]_f$ is calculated by formulation of Equation (9) on cell faces $f$ and division by the implicit coefficient $a$:

$$[\phi]_f = \left[\frac{H}{a}\right]_f \cdot n_f + \left[\frac{1}{a}\right]_f [G]_f. \quad (10)$$
Wherever \( r_\alpha \) takes a value of zero, residual contributions are added to both coefficients, \( a \) and \( H \), in order to obtain a numerical solution from Equation (10).

### 3.2 Compact momentum interpolation (CMI)

For the multifluid model Cubero and Fueyo\(^5\) and Cubero et al\(^4\) showed that the above face-based formulation does not satisfy the four requirements of consistency: A solution procedure is considered consistent, if it fulfills the following requirements:\(^4\)

1. If ever achieved, a steady-state solution has to be independent from the size of the time step,
2. Wherever only a single phase is present, the single-phase CMI formulation needs to be recovered inherently,
3. All interfacial drag forces in the momentum equations need to cancel out,
4. The pressure forces acting on individual phases have to proportional to the forces resulting from the shared pressure.

Hence, they proposed the so-called compact momentum interpolation

\[
\left( 1 + \left[ \frac{1}{a_\alpha} \right]_f \left[ a_\alpha^T \right]_f + \sum_{\beta \neq \alpha} \left[ \frac{1}{a_\alpha} \right]_f \left[ a_\alpha^D \right]_f \right) \phi_\alpha |_f \\
= \phi_\alpha |_f + \left[ \frac{1}{a_\alpha} \right]_f \left[ a_\alpha^T \right]_f \phi_\alpha |_f + \left[ r_\alpha \right]_f \left[ \frac{1}{a_\alpha} \right]_f \left[ G \right]_f \\
+ \sum_{\beta \neq \alpha} \left[ \frac{1}{a_\alpha} \right]_f \left[ a_\alpha^D \right]_f \phi_\beta |_f 
\]

with the pseudo-flux

\[
\phi_\alpha |_f = [\hat{u}a]_f \cdot n_f \quad \text{with} \quad [\hat{u}a]_p = \left[ \frac{H_a}{a_\alpha} \right]_p .
\]

where \( n_f \) is the normal vector of face \( f \). The basic idea of CMI is to split the implicit and explicit coefficients \( a \) and \( H \) for the individual phases into separate parts for convective-diffusive (without superscript), temporal (T), and interfacial drag (D) contributions, which are separately interpolated to the faces. Temporal coefficients are defined as \( a_\alpha^T = r_\alpha \rho \nu / \Delta_t \) with volume \( \nu \) of a grid cell and time step width \( \Delta_t \). Time integration is formulated with first-order Euler backward scheme, where \( n \) denotes quantities from the recent time step. The extension to second order time integration scheme is described by Shen et al.\(^5\) As the system of equations is solved iteratively in a segregated manner, the numerical flux \( \phi_\beta |_f \) of another phase is taken from the recent Jacobi iteration. In contrast to Cubero et al.,\(^4\) interfacial drag is formulated for an arbitrary number of phases by using a sum formulation in the present work. The drag coefficient is defined as \( a_\alpha^D = F_{\alpha \beta} K_{\alpha \beta} \), including weighting factor \( F_{\alpha \beta} \), according to Section 2.

### 3.3 Consistent formulation of virtual mass

The formulation of the virtual mass force needs to be included into the solution procedure in a way that the requirements for consistency from Section 1 are met. Therefore, the virtual mass coefficient is

\[
a_{vd}^{\text{VM}} = F_{cd} r_\alpha \rho_c C^{\text{VM}} .
\]

The model of Crowe et al.\(^4\), which is shown in Equation (4), contains material derivatives and, therefore, convective and temporal contributions. The convective contribution is

\[
\mathbf{f}^{\text{VM},c}_{\alpha \beta} = a_{\alpha \beta}^{\text{VM}} \left( \phi_\beta \cdot \nabla \right) \mathbf{u}_\beta - \left( \phi_\alpha \cdot \nabla \right) \mathbf{u}_\alpha
\]
Approximate resolution of phase coupling

3.4 Approximate resolution of phase coupling

As stated in Section 2, drag coefficient $a_{a\beta}^D$ is chosen to be very large in order to ensure stability of resolved interfaces, even in the presence of more than two phases at the same location. In the limit of an infinitely large $a_{a\beta}^D$, this coefficient dominates Equation (15) and both phase velocities $u_\alpha$ and $u_\beta$ become identical. This results in underrelaxation of phase velocities and phase fluxes and the system of equations becomes stiff. Multiple approaches have been proposed in the literature to resolve such situations of stiff phase coupling. For an arbitrary number of phases the coupling can be fully canceled by solving the phase momentum Equation (2) for all phases in a coupled manner, as proposed by Karema and Lo. A solution procedure utilizing full-block coupling of all phase velocities as well as shared pressure in combination with CMI was presented by Ferreira et al., who proved the phase coupling to be resolved for a number of up to four phases for dispersed flow regimes. A different approach is the partial elimination algorithm (PEA) of Spalding, which is algebraically formulated for the quantity of exactly two phases. Compared with coupled approaches, PEA can be included into any segregated solution procedure, which is available in OpenFOAM-dev. The basic idea is to eliminate terms in the phasic momentum Equation (2), which contain the phase velocity or the phase flux of the other phase $\beta$ by substitution and rearranging of those equations. A full cancelation of phase coupling can only be achieved for exactly two phases. Nevertheless, an arbitrary number of phases occurs at the same location and, therefore, phase coupling becomes resolved in an approximate manner. The steps of the derivation are applied to Equation (15) in the following way:

1. sum up Equation (15) over all phases $\alpha$,
2. apply constraint $\sum_\alpha r_\alpha = 1$,
3. by applying the interface condition in terms of phase fluxes $[\phi_\alpha]_f = [\phi_\beta]_f$ to drag and temporal virtual mass terms those cancel out,
4. rearrange equation in terms phase flux $[\phi_\beta]_f$,
5. substitute $[\phi_\beta]_f$ back into Equation (15).

For the whole procedure, the sum formulation needs to be maintained considering all phases $\alpha, \xi, \beta \neq \alpha, \gamma \neq \{\alpha, \beta\}$. This results in CMI equations with approximately resolved phase coupling

\[
\begin{align*}
&\left(1 + \frac{1}{a_\alpha} [a_\alpha^T]_f + \frac{1}{a_\alpha} [a_\alpha^D]_f + \frac{1}{a_\alpha} \sum_{\beta \neq \alpha} [a_{a\beta}^\text{VM,T}]_f \right) [\phi_\alpha]_f \\
&= [\phi_\alpha]_f + \frac{1}{a_\alpha} [a_\alpha^T]_f [\phi_\beta]_f + \frac{1}{a_\alpha} (r_\alpha)_f + [r_\alpha]_f [G]_f \\
&+ [S_\alpha^D]_f + \frac{1}{a_\alpha} \sum_{\beta \neq \alpha} [a_{a\beta}^\text{VM,T}]_f ([\phi_\alpha]_f + [\phi_\beta]_f - [\phi_\beta]_f). \quad (16)
\end{align*}
\]
with implicit drag coefficient

\[ [a^D_{\beta \alpha} f] = \sum_{\beta \neq \alpha} \left[ \frac{|\alpha|}{\alpha f} \left( 1 + \frac{|\alpha|}{\alpha f} \right) \right]. \]

drag pressure coefficient

\[ [c^D_{\alpha} f] = \sum_{\beta \neq \alpha} \left[ \frac{|a^D_{\beta \alpha}| f}{|\alpha f| + |\beta f|} \right]. \]

and explicit drag contribution

\[ [S^D_{\alpha} f] = \sum_{\beta \neq \alpha} \left( \left[ \frac{|a^D_{\beta \alpha}| f}{|\beta f|} \left( \left[ \frac{1}{\alpha f} \right] f + \left[ c^D_{\beta \alpha} f \right] f \right) \left[ \frac{1}{\alpha f} \right] f + \left[ \frac{1}{\beta f} \right] f + \left[ c^T_{\alpha} f \right] f \right) \left( \left[ \frac{1}{\beta f} \right] f + \left[ c^T_{\beta} f \right] f \right) \right]. \]

It is obvious that there are still contributions \( \phi_\gamma \) and \( \phi_\xi \) from third phases \( (\xi, \gamma \neq \{ \alpha, \beta \}) \) in the explicit drag contribution. This means that phase coupling is not fully resolved, whenever there are more than two phases present. The original PEA algorithm is recovered in the presence of exactly two phases. It was found that number of phases that equivalently dominate the momentum equation in terms of mass has to be limited, which is clearly the case, for example, for a single liquid phase and multiple gas phases. It is expected that typical gas liquid flow applications are within the limit of this multiphase formulation of the PEA algorithm.

In the limit of infinitely high drag coefficients for resolved interfaces (see Equation (5)), the proposed system of equations is equivalent the homogeneous model,\(^{16}\) such that the behavior of an algebraic VOF is recovered with the presented method. On the other end, if for dispersed flows closure models of Ishii and Zuber\(^{47}\) and Crowe et al\(^{48}\) are used for drag and virtual mass, respectively, the presented method acts similar to the well-known Euler-Euler model.

### 3.5 Solution procedure

The presented solution procedure utilizes a projection method,\(^{55}\) which consists of the following steps:

1. calculation of predicted phase velocities \( [u^*_{\alpha}] / \) and fluxes \( [\phi^*_{\alpha}] / \) from Equation (16) by omitting pressure contribution \( G \),
2. solution of pressure equation, and
3. obtain correct velocities and fluxes from Equation (16) with pressure contribution.

In the case of incompressible flow, the pressure equation is formulated as

\[ \nabla \cdot ([D_p f] (\nabla p f)) = \nabla \cdot \left( \sum_{\alpha} |r_{\alpha}| f [\phi^*_{\alpha}] f \right) \]

with pressure diffusivity

\[ [D_p f] = \sum_{\alpha} \left[ \frac{|r_{\alpha}| f}{1 + \frac{1}{|\alpha f|} f + \left[ c^D_{\alpha} f \right] f + \left[ c^T_{\alpha} f \right] f + \left[ c^T_{\alpha} f \right] f} \right] f. \]

The entire solution procedure is summarized in Figure 1.
3.6 | Discretization

The presented numerical framework is implemented into OpenFOAM,\textsuperscript{40,54} which is an open-source C++ library based on a finite-volume method formulated for unstructured grids. The solution procedure utilizes a discretization that is second-order accurate in space and provides an implicit time integration scheme of first order. The transport of phase fractions is realized with explicit time integration of phase fraction transport Equation (1). Boundedness is maintained with the multidimensional limiter for explicit solution algorithm (MULES)\textsuperscript{54} together with the flux limiting scheme as proposed by Van Leer\textsuperscript{56} for the discretization of convective transport terms of the phase fractions. Due to the explicit nature of the time integration scheme for phase fractions in OpenFOAM, Courant numbers below unity are required. For the accurate prediction of transient behavior, Jasak\textsuperscript{57} reported that an even smaller maximum Courant number is necessary.

The interface compression mechanism according to Weller\textsuperscript{7} is included in the phase fraction transport algorithm in order to keep resolved interfaces from diffusing with a model constant of $c_a = 1$.

4 | RESULTS AND DISCUSSION

4.1 | Variables

In the cases considering resolved rising bubbles, the initial bubble diameter is referred to as $D_b$, which is used to define any dimensionless length as $\tilde{L} = L/D_b$, where $L$ can be any scalar or vector quantity with a length dimension, for example, a position vector $\tilde{x}$ or diameter of disperse interfacial structures $\tilde{d}$. Furthermore, gravitational velocity and time scales are defined by $U_g = \sqrt{gD_b}$ and $t_g = \sqrt{D_b/g}$, respectively, with gravitational acceleration $g$. Dimensionless time and velocity are defined as $\tilde{t} = t/t_g$ and $\tilde{U} = U/U_g$, respectively.

4.2 | Two-dimensional rising bubble

The first test case setup, which features a two-dimensional gas bubble, rising in a stagnant liquid, has been proposed by Hysing et al.,\textsuperscript{58} who compared the behavior of different codes using level-set methods. Top and bottom walls are modeled with a no-slip condition, whereas both boundaries to the left and right provide a free-slip condition. The gas bubble is
TABLE 1 Overview over gravitational scales and dimensionless numbers in cases of two-dimensional rising gas bubble (G) in liquid (L) according to Hysing et al.\textsuperscript{58}

| Case | $Re_g$ | $Eo$ | $Mo$ | $\rho_L / \rho_G$ | $\mu_L / \mu_G$ | $U_g$ | $t_g$ |
|------|--------|------|------|-----------------|-----------------|-------|-------|
| 1    | 35     | 10   | $6 \times 10^{-4}$ | 10              | 10              | 0.7 m s$^{-1}$ | 0.7143 s |
| 2    | 35     | 125  | 1.3  | 1000            | 100             | 0.7 m s$^{-1}$ | 0.7143 s |

initialized as a circle of diameter $D_b = 0.5$ m in with its center of gravity at position $\mathbf{x}_b(\bar{t} = 0) = (1, 1)$. The computational domain has the dimensions $2D_b \times 4D_b$. According to Hysing et al.\textsuperscript{58} two different bubble regimes are studied considering the corresponding dimensionless numbers, namely gravitational Reynolds number, Eötvös number, and Morton number:

$$Re_g = \frac{\rho_g D_b U_g}{\mu_L}, \quad Eo = \frac{\rho_g D_b^2 \Delta}{\sigma}, \quad Mo = \frac{g \mu_L (\rho_L - \rho_G)}{\rho_G^2 \sigma^3}.$$  \hspace{1cm} (19)

Resulting dimensionless numbers for both cases under investigation are shown in Table 1.

Results are compared in terms of evolution of bubble center of gravity, rising velocity, and circularity over time as well as of interface location at a time $\bar{t} = 4.2$. The center of gravity of the bubble, $\mathbf{x}_b$, is defined as:\textsuperscript{59}

$$\mathbf{x}_b = \frac{\int_G \rho_G \mathbf{x}_G dV}{\int_G \rho_G dV}.$$  \hspace{1cm} (20)

with domain $\Omega \subset \mathbb{R}^2$. The vertical component of $\mathbf{x}_b$ directed opposite to gravitational force is referred to as $y_b$. The rising velocity $U_b$ of the gas bubble is defined accordingly:\textsuperscript{59}

$$U_b = \frac{\int_G \rho_g \mathbf{u}_G dV}{\int_G \rho_G dV}.$$  \hspace{1cm} (21)

Its vertical component is denoted as $U_b$. In two-dimensional space, the circularity is defined as:\textsuperscript{58}

$$c_b = \frac{\pi d_{\text{cir}}}{P_b} \quad \text{with } d_{\text{cir}} = 2 \sqrt{A_b / \pi},$$  \hspace{1cm} (22)

with circle-equivalent diameter $d_{\text{cir}}$, actual bubble area $A_b$, and actual bubble perimeter $P_b$.

In order to assess the influence of spatial resolution, a mesh study is carried out with the domain being spatially discretized with $20 \times 40, 40 \times 80, 80 \times 160$, and $160 \times 320$ grid points, which results in $\Delta_x = 1/10, \Delta_x = 1/20, \Delta_x = 1/40$, and $\Delta_x = 1/80$, respectively. Time step sizes are set to $\Delta t = 1.4 \times 10^{-2}, \Delta t = 7 \times 10^{-3}, \Delta t = 3.5 \times 10^{-3}$, and $\Delta t = 1.75 \times 10^{-3}$, respectively, such that the Courant number stays $C_o < 0.12$ for each individual mesh level. The solver is set up, such that the number of inner loops is fixed to three, whereas outer loops are done until the initial pressure residual at the beginning of an outer loops is lower than $1 \times 10^{-4}$. Subsequently, one final outer iteration is done before proceeding with the next time step. Vertical bubble position $y_b$, rising velocity $U_b$, and bubble circularity $c_b$ over time as well as the interface location ($r_G = 0.5$) at $\bar{t} = 4.2$ are presented in Figure 2.

For the vertical bubble position, no major differences can be observed, while the rising velocity noticeably differs between mesh levels $\Delta_x = \{1/10, 1/20\}$ and $\Delta_x = 1/80$ at time $\bar{t} \approx 1$. For $\bar{t} = 4.2$, the rising velocity on the coarsest mesh is significantly larger than on the finer ones. Almost no differences in rising velocity can be observed between meshes $\Delta_x = \{1/20, 1/40, 1/80\}$ at $\bar{t} = 4.2$. On coarse meshes, circularity values of $c_b \approx 1$ can be observed in the beginning of the simulation. Mathematically, the circularity of an object cannot be larger than unity, as the circle, which has $c_b = 1$ by definition, is the shape with the lowest possible ratio of perimeter to surface area. The simulation results can be explained with the error of the procedure for estimating the perimeter of the bubble, which is quite large on coarse grids. Nevertheless, the qualitative behavior of the bubble is recovered with all meshes used. While the resulting differences between the coarsest and the finest meshes are large, minor deviations between the results of the meshes $\Delta_x = \{1/40, 1/80\}$ can be observed for $\bar{t} > 3$. The interface position at $\bar{t} = 4.2$ converges nicely with refinement of the computational grid and meshes $\Delta_x = \{1/40, 1/80\}$ deliver nearly identical results. Hence, mesh level $\Delta_x = 1/40$ is chosen for further investigations of
this case. Although the presented results suggest that total bubble volume changes between meshes of different spatial resolution, gas volume is conserved. This is evident by integrating $r_G$ over the domain, giving a relative volume error of $1.02 \times 10^{-8}$ for $0 < \tilde{t} < 4.2$ for the coarsest mesh. The reason, why bubbles appear smaller on a coarse mesh with the interface definition of $r_G = 0.5$ is that the interface smears over several grid cells, which is typical for algebraic VOF methods.

Figure 3 shows the results of case 1, namely vertical bubble rising velocity $\tilde{U}_b$ and circularity $c_b$ over time, as well as the interface position ($r_G = 0.5$) at $\tilde{t} = 4.2$ and the relative pressure residuals for each inner and outer loop for the latest time step at $\tilde{t} = 4.2$. The present solver’s performance is compared with the results, which Hysing et al.\textsuperscript{58} obtained with the level-set solver TP2D, and with the results of Klostermann et al.\textsuperscript{60} who use the VOF solver interFoam without interface reconstruction, similarly to the presented method but considering a homogeneous model. For both groups, the mesh resolution taken for comparison is $\Delta x = 1/160$ (originally denoted as $1/h = 320$) for this case.

Extreme values of rising velocity $\tilde{U}_b$ and circularity $c_b$, as well as values of $\tilde{U}_b$, $c_b$ and vertical bubble position $\tilde{y}_b$ at time $\tilde{t} = 4.2$ are listed in Table 2. For the maximum rising velocity $\tilde{U}_{b,\text{max}}$, the present solver predicts a value, which is in between both reference values, being slightly closer to the data of Klostermann et al.\textsuperscript{60} than to the ones of Hysing et al.\textsuperscript{58} The same accounts for the period of time, which is needed until maximum rising velocity is reached. Subsequently, the bubble slows down, which is most pronounced in the results of the present solver. Finally, at $\tilde{t} = 4.2$, the rising velocity as predicted by the presented model is slightly higher than the one of Klostermann et al.\textsuperscript{60} but at the same time lower than the value predicted by Hysing et al.\textsuperscript{58} For the circularity, the present solver predicts a minimum value of $c_{b,\text{min}}$, which is below the values of the reference data from both sources. At $\tilde{t} = 4.2$, the circularity value obtained with the presented model is between the reference values. The bubble shape at this point of time slightly differs from the results of Hysing et al.\textsuperscript{58} but is very close to the ones of Klostermann et al.\textsuperscript{60} At $\tilde{t} = 4.2$, the present solver predicts a value for the vertical bubble position that again lies between the results of both references. Regarding the relative pressure residuals over inner and outer loops of the recent time step at $\tilde{t} = 4.2$, a good convergence behavior is observed inside each individual outer loop as well as over the progress of all outer loops. The four outer loops express in the four peaks and the final relative residual for the whole time step is quite low with a value below $10^{-8}$.
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FIGURE 3  Bubble rising velocity and bubble circularity over time as well as interface position \( r_G = 0.5 \) at \( \bar{t} = 4.2 \) and relative pressure residuals over inner and outer loops over a single time step at \( \bar{t} = 4.2 \) for two-dimensional rising bubble, case 1 [Colour figure can be viewed at wileyonlinelibrary.com]

TABLE 2  Results of bubble rising velocity \( \bar{U}_b \), circularity \( \bar{c}_b \), and vertical position \( \bar{y}_b \) obtained with present solver and reference data from Hysing et al\(^{58}\) and Klostermann et al\(^{60}\) as well as relative deviation with respect to the reference data for two-dimensional rising bubble case 1

|                  | Present solver | Hysing et al\(^{58}\) | Klostermann et al\(^{60}\) |
|------------------|----------------|-----------------------|---------------------------|
| \( \bar{U}_{b,\text{max}} \) | 0.3413          | 0.3453                | −1.158% 0.3354 1.759%     |
| \( \bar{h} \bar{U}_{b,\text{max}} \) | 1.3090          | 1.2898                | 1.3322                     |
| \( \bar{c}_{b,\text{min}} \) | 0.8964          | 0.9013                | −0.544% 0.9044 −0.885%    |
| \( \bar{h} \bar{c}_{b,\text{min}} \) | 2.6985          | 2.6657                | 2.7475                     |
| \( \bar{y}_{b,\bar{t}=4.2} \) | 2.1418          | 2.1626                | −0.962% 2.1392 0.122%     |
| \( \bar{U}_{b,\bar{t}=4.2} \) | 0.2676          | 0.2767                | −3.289% 0.2649 1.019%     |
| \( \bar{c}_{b,\bar{t}=4.2} \) | 0.9160          | 0.9206                | −0.500% 0.9130 0.329%     |

For case 2, the geometrical setup is identical to the one in the first test case. Gravitational acceleration and material properties are chosen, such that they result in the dimensionless numbers of this case, as defined by Hysing et al\(^{58}\) and listed in Table 1. As for case 1, a convergence study regarding spatial resolution is carried out as well. Additionally to the meshes investigated for case 1, another mesh refinement level with a grid spacing of \( \Delta \bar{x} = 1/160 \) is used together with a time step size of \( \bar{t} = 8.75 \times 10^{-4} \). The time step sizes for all other mesh refinements levels are set according to the refinement study in case 1. The results of this mesh study regarding the bubble’s position, vertical rising velocity and circularity over time as well as the interface position \( r_G = 0.5 \) at \( \bar{t} = 4.2 \) are shown in Figure 4.

It turns out that a higher bubble rising velocity is predicted on finer meshes, which results in the highest bubble position for the finest mesh refinement level. In the beginning of the simulation for \( \bar{t} < 2 \), except for the coarsest mesh, the results show only minor differences in terms of rising velocity. Subsequently, a second local velocity maximum appears, which is most pronounced on fine meshes. This results in a persistent velocity difference between the results of the different mesh levels. With the coarsest mesh, the second local velocity maximum is not captured at all. In terms of circularity value \( \bar{c}_b \), a convergent behavior can be observed with increasing spatial resolution with the largest differences
FIGURE 4  Bubble vertical position, rising velocity, circularity, and interface position \((r_G = 0.5)\) at \(\bar{t} = 4.2\) for different spatial resolutions in two-dimensional rising bubble case 2 [Colour figure can be viewed at wileyonlinelibrary.com]

just between the coarsest mesh \(\Delta_x = 1/10\) and the next finer mesh level \(\Delta_x = 1/20\). Comparing the interface position \((r_G = 0.5)\) at \(\bar{t} = 4.2\), large differences are present between the results of different spatial resolution levels. On the coarsest mesh, the skirt in the lower part of the bubble cannot be captured. Mesh level \(\Delta_x = 1/20\) results in a bubble skirt, which is of nearly uniform thickness. With increasing mesh resolution, the skirt becomes more and more slim in the center, while the lower part nearly retains its thickness. Finally, with the finest mesh \(\Delta_x = 1/160\), two gas portions are already detached from the skirt at \(\bar{t} = 4.2\). For further investigations, mesh resolution \(\Delta_x = 1/160\) is chosen for this case.

As for case 1, the results obtained with the present solver are again compared with the data of Hysing et al.\textsuperscript{58} who used the TP2D solver and a mesh resolution of \(\Delta_x = 1/320\) (originally denoted as \(1/h = 640\)), as well as with the data obtained by Klostermann et al.\textsuperscript{60} with interFoam and a mesh resolution of \(\Delta_x = 1/160\) (\(1/h = 320\)). In Figure 5, vertical bubble rising velocity and circularity over time as well as interface position \((r_G = 0.5)\) and relative pressure residuals for time \(\bar{t} = 4.2\) are shown.

Numerical values of local extrema, as well as vertical bubble position \(\bar{y}_b\), rising velocity \(\bar{U}_b\), and circularity \(c_b\) at time \(\bar{t} = 4.2\) are reported in Table 3. For the first local maximum of the rising velocity \(\bar{U}_{b,\text{max}}\), the value obtained with the present solver again lies between the results of Hysing et al.\textsuperscript{58} and Klostermann et al.\textsuperscript{60} with a tendency of being closer to the latter reference. When approaching the second local velocity maximum \(\bar{U}_{b,\text{max}}\), the value predicted with the present solver is slightly lower than both references but still close to the value of Klostermann et al.\textsuperscript{60} (about 1% deviation), while Hysing et al.\textsuperscript{58} report a value, which is significantly higher. Subsequently, the rising velocity drops significantly faster in the results obtained with the present solver and of Klostermann et al.\textsuperscript{60} compared with the ones of Hysing et al.\textsuperscript{58} The circularity values of all simulations are quite close to each other in the beginning of the simulation until \(\bar{t} \approx 3.4\). At this time, Hysing et al.\textsuperscript{58} predict a breakup of the skirt region, which leads to a strong increase of the circularity, which is an integral quantity.
FIGURE 5 Bubble rising velocity and bubble circularity over time as well as interface position \((r_G = 0.5)\) at \(\bar{t} = 4.2\) and relative pressure residuals over inner and outer loops over a single time step at \(\bar{t} = 4.2\) for two-dimensional rising bubble, case 2 [Colour figure can be viewed at wileyonlinelibrary.com]

for the whole domain. The separated gas structures can be observed in the interface position at \(\bar{t} = 4.2\), where the results of Hysing et al\(^{58}\) show two small gas structures, which are located in a large distance to the large gas bubble. At that point of time, Klostermann et al\(^{60}\) and the present solver predict that the skirt region is still more pronounced and two slightly larger gas structures just separate from there. Those results show only minor differences, which can also be observed in the evolution of the circularity value with a final deviation of about 1.5%. The initial relative pressure residual over inner and outer loops shows a convergent behavior, even though the final level of convergence is, with a value of about \(10^{-6}\), not as deep as in case 1. At the final time step, five outer loops are necessary to reach the criterion of \(10^{-4}\), which expresses in the five peaks in the residuals.

In summary, the present solver is able to recover the dynamics considering a single two-dimensional rising gas bubble. Moderate deviations are observed in comparison with the results obtained with a level-set method by Hysing et al\(^{58}\) while very small differences occur in comparison with results of the VOF method without interface reconstruction by Klostermann et al\(^{60}\).

4.3 Three-dimensional rising bubble

The three-dimensional case setup was proposed by Balcázar et al\(^{61}\) who investigated the performance of a level-set method and compared results with experimental data. The gas bubble is initialized as sphere with diameter \(D_b\), with the center position \(2D_b\) above the bottom. The computational domain is described as a cylindrical vessel with diameter \(8D_b\) and height \(12D_b\). As in the two-dimensional cases, a free-slip condition is applied to the side wall of the cylindrical
TABLE 3 Results of bubble rising velocity $\bar{U}_b$, circularity $c_b$, and vertical position $\bar{y}_b$ obtained with present solver and reference data from Hysing et al.\textsuperscript{58} and Klostermann et al.\textsuperscript{60} as well as relative deviation with respect to the references for two-dimensional rising bubble case.

|                | Present solver | Hysing et al.\textsuperscript{58} | Klostermann et al.\textsuperscript{60} |
|----------------|----------------|----------------------------------|----------------------------------|
| $\bar{U}_b^{\max}$ | $0.356$        | $0.3606$                         | $0.3534$                         |
| $\bar{t} | \bar{U}_b - c_b^{\max}$ | $1.029$                    | $1.0265$                         | $1.0018$                        |
| $\bar{U}_b^{\max}$ | $0.3346$        | $0.3477$                         | $0.3361$                         | $-0.346\%$                     |
| $\bar{t} | \bar{U}_b - c_b^{\max}$ | $2.8298$                    | $2.8987$                         | $2.8066$                        |
| $c_b | \bar{t} = 2.8$ | $0.6829$                    | $0.6918$                         | $0.6862$                         | $-0.481\%$                     |
| $\bar{y}_b | \bar{t} = 4.2$ | $2.2423$                    | $2.2795$                         | $2.2436$                         | $-0.058\%$                     |
| $\bar{U}_b | \bar{t} = 4.2$ | $0.2833$                    | $0.3095$                         | $0.2853$                         | $-0.701\%$                     |
| $c_b | \bar{t} = 4.2$ | $0.4912$                    | $0.7157$                         | $0.4984$                         | $-1.445\%$                     |

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Two cases have been selected from the ones investigated by Balcázar et al.\textsuperscript{61} whose corresponding dimensionless numbers are shown in Table 4. Additionally to the dimensionless numbers, which are introduced in the previous section, flow regimes are categorized by the bubble Reynolds number

$$Re_{b}^{Bal} = \frac{\rho_{L} U_{b}^{Bal} D_{b}}{\mu_{L}} \quad (23)$$

with rising velocity $U_{b}^{Bal}$, which is the numerical result for the bubble rising velocity of Balcázar et al.\textsuperscript{61} In the same fashion, a bubble Reynolds number $Re_{b}^{Bha}$ is defined, based on the bubble rising velocity $U_{b}^{Bha}$, which Bhaga and Weber\textsuperscript{62} obtained experimentally. The gas bubble relaxes for $-3.132 < \bar{t} < 0$, before gravitational acceleration is finally switched on at time $\bar{t} = 0$. In three-dimensional space, bubble position $x_b$ and rising velocity $U_b$ are evaluated by means of Equations (20)
Table 4 Overview over gravitational scales and dimensionless numbers of cases of rising gas bubble (G) in liquid (L) of Balcázar et al.\textsuperscript{61}

| Case | \(Re_b\) | \(Re_{BL}^{Bal}\) | \(Re_{BL}^{Bha}\) | \(Eo\) | \(Mo\) |
|------|--------|----------------|----------------|-----|-----|
| 1    | 11     | 6.94          | 7.16          | 116 | 41.1|
| 2    | 31     | 17.46         | 18.3          | 339 | 43.1|

Case | \(\rho_L/\rho_G\) | \(\mu_L/\mu_G\) | \(U_g\) | \(t_g\) |
|------|----------------|----------------|--------|--------|
| 1    | 100            | 100            | 3.132 ms\(^{-1}\) | 0.319 s |
| 2    | 100            | 100            | 3.132 ms\(^{-1}\) | 0.319 s |

**FIGURE 7** Bubble vertical position, rising velocity, and sphericity over time as well as interface position (\(r_G = 0.5\)) at \(\bar{t} = 12.53\) for different spatial resolutions in three-dimensional rising bubble case 1 [Colour figure can be viewed at wileyonlinelibrary.com]

\[s_b = \frac{\pi d_{Sph}^2}{S_b} \quad \text{with} \quad d_{Sph} = \sqrt[6]{\frac{6V_b}{\pi}}.\] (24)

The computational domain is discretized, such that in the center of the domain, where the bubble is located, computational cells are orthogonal and of constant grid sizing. Outside the core region, cells are getting larger the further their distance to the core is in order to save computational cost.

Influence of spatial resolution is assessed via comparison of results obtained with computational grids of spacings \(\Delta_x = 1/8\), \(\Delta_x = 1/16\), and \(\Delta_x = 1/32\). Time step sizes are set to \(\Delta t = 1.25 \times 10^{-1}\), \(\Delta t = 6.25 \times 10^{-2}\), and \(\Delta t = 3.13 \times 10^{-2}\), respectively, and the Courant number is \(Co < 0.12\) for all simulations. As in the two-dimensional cases, the number of inner loops is set to a fixed number of three. Outer loops are run until the initial pressure residual is lower than a value of \(1 \times 10^{-3}\), before the final outer iteration is carried out. Figure 7 shows evolutions of vertical position, rising velocity, and sphericity of the bubble over time as well as bubble interface position (\(r_G = 0.5\)) at \(\bar{t} = 12.53\) for the different mesh levels in case 1.

On the coarsest mesh with \(\Delta_x = 1/8\), the predicted bubble rising velocity decreases over time after it reaches its maximum value at \(\bar{t} \approx 2\), while the value of rising velocity is maintained on the finer meshes. Therefore, for the coarse mesh, vertical bubble position increases slower over time compared with finer spatial resolutions, which leads to a significant vertical distance at \(\bar{t} = 12.53\) between the bubble on the coarse and on both finer meshes. Between \(\Delta_x = 1/16\)
and \( \Delta_\xi = 1/32 \), slight differences in bubble rising velocity can be observed for \( 1 < \bar{t} < 6 \) with a lower value with the finer mesh, before they approach each other again. In terms of bubble sphericity \( s_b \), unphysical values larger than unity can be observed for both the coarser meshes, which has the same reason as explained for bubble circularity \( c_b \) in the two-dimensional cases. Furthermore, the graph of the sphericity for \( \Delta_\xi = 1/8 \) appears to be very jagged for the same reason that the precision of the interface reconstruction for postprocessing is very poor for coarse spatial resolutions. For the finer meshes, the graphs are smooth and moderately differ from each other for \( \bar{t} < 10 \), before they take very similar values. In terms of final interface position at \( \bar{t} = 12.53 \), the bubble shape obtained with the coarsest mesh is too wide and flat compared with the results on the other meshes. A direct comparison of bubble shapes from \( \Delta_\xi = 1/16 \) and \( \Delta_\xi = 1/32 \) shows that the shape is very similar in the upper region, while the dent between the skirt structures is less pronounced on the finest mesh. The overall differences between the results obtained with both finer meshes are moderate and, hence, mesh \( \Delta_\xi = 1/32 \) is chosen for further investigations.

The performance of the present solver is compared with the experimental results of Bhaga and Weber\(^{62}\) as well as to the numerical results of Balcázar et al,\(^{61}\) who used a mesh of spatial resolution of \( \Delta_\xi = 1/30 \). Additionally, the three-dimensional bubble is simulated with a solver based on the homogeneous model \((\text{interFoam}, ^{54})\) with mesh spacing \( \Delta_\xi = 1/32 \). Bubble rising velocity \( \bar{U}_b \) and sphericity \( s_b \) over time as well as interface location \((r_G = 0.5)\) at time \( \bar{t} = 12.53 \) for case 1 are shown in Figure 8. It is worth noting that the data for interface position from both Bhaga and Weber\(^{62}\) and Balcázar et al\(^{61}\) have neither been provided with a scale nor with positional information for a specified time and, therefore, both parameters are adjusted to match the present results.

Values of velocity extrema and their point of time as well as of vertical position \( \bar{y}_b \), rising velocity \( \bar{U}_b \), and sphericity \( s_b \) at \( \bar{t} = 12.53 \) are shown in Table 5. For \( \bar{t} < 4 \), the rising velocity predicted with the present solver is noticeably smaller than the one obtained with \text{interFoam}. In the second half of the simulation, both values approach each other. Throughout the whole simulation, the values for rising velocity reported by Balcázar et al\(^{61}\) are even higher compared with \text{interFoam} with moderate deviations in the first and minor ones in the second half of the simulation. The present results for \( \bar{U}_b \) at \( \bar{t} = 12.53 \) deviate from aforementioned ones by \(-0.28\%\). The values for bubble rising velocity obtained with the present solver are approximately \( 3\% \) lower, compared with the experimental results of Bhaga and Weber\(^{62}\). In terms of bubble...
TABLE 5 Results of rising velocity $\tilde{U}_b$, sphericity $s_b$, and vertical position $\tilde{z}_b$ of the bubble and relative deviation of results between the present solver, interFoam, and Balcázar et al.\textsuperscript{61} as well as Bhaga and Weber\textsuperscript{62} in three-dimensional rising bubble case 1

| Present solver | interFoam | Balcázar et al.\textsuperscript{61} |
|----------------|-----------|-----------------------------------|
| $\tilde{U}_{b,max}$ | 0.4871 | 0.4905 | −0.69% | 0.4944 | −1.48% |
| $\tilde{t}_{D_b=0.5}$ | 1.2528 | 1.1159 | 1.2455 |
| $\tilde{U}_{b,min}$ | 0.4848 | 0.4860 | −0.25% | 0.4876 | −0.57% |
| $\tilde{t}_{D_b=0.5}$ | 2.3804 | 2.8502 | 3.6011 |
| $\tilde{z}_b$ | 7.9845 | 8.0174 | −0.41% |
| $s_b$ | 0.7680 | 0.7773 | −1.20% |
| $U_b$ | 0.4907 | 0.4909 | −0.04% | 0.4921 | −0.28% |
| $U_b$ | 0.5103 | 3.84% |

sphericity, the present solver and interFoam perform very similar regarding the first time period $\tilde{t} < 4$. Subsequently, the value predicted with the presented model drops slightly lower compared with the homogeneous model with a relative deviation of $−0.41\%$ at the final time $\tilde{t} = 12.53$. No data regarding bubble sphericity have been reported by Balcázar et al.\textsuperscript{61} or Bhaga and Weber.\textsuperscript{62} Concerning the interface position at final time, the numerically obtained bubble shape reported in the literature shows blunt tips for both skirt regions, which is in contrast to the results obtained with interFoam, which show a steeper rise of the interface in the inward direction of both skirt regions. With the present solver a bubble shape is predicted, which has even more pronounced ligaments of the skirt with the tip region being more sharp than the one obtained with interFoam. That is completely in line with the numerical values for bubble sphericity at final time. Apart from the skirt regions, nearly no differences in bubble shape can be observed between the results of both solvers and of Balcázar et al.\textsuperscript{61} The comparison with the experimentally obtained bubble shape shows a good agreement.

For assessment of influence of spatial resolution in case 2, the same computational grids as for the investigation in case 1 are used together with the according time step sizes. Additionally to that, another level of mesh refinement is added with $\Delta x = 1/64$ with a time step size of $\Delta t = 1.56 \times 10^{-3}$. With this setup, Courant numbers of $Co < 0.18$ are achieved on all mesh levels. Results in terms of bubble vertical position $\tilde{y}_b$, rising velocity $\tilde{U}_b$, and sphericity $s_b$ over time as well as interface location at time $\tilde{t} = 12.53$ for case 2 are shown in Figure 9. As before, the definition of the interface location for meshes $\Delta x = 1/16$ and finer is $r_G = 0.5$ but for $\Delta x = 1/8$ the interface smears out strongly and the distribution of the phase fraction of the gas is so dilute that the criterion mentioned before is met nowhere. Therefore, an interface definition of $r_G = 0.1$ is used for that coarsest mesh level.

As it turns out, the coarsest mesh cannot capture the flow dynamics at all and the bubble breaks up into multiple small, quite dilute gas structures. Connected to that are very low values of rise velocity and vertical position compared with results obtained on finer meshes. Accordingly, the evolution of sphericity over time becomes very jagged and rapidly rising in the second half of the simulation. In terms of vertical position, rising velocity sphericity, and final interface position, all other meshes show a convergent behavior with increasing mesh resolution and only minor deviations are observed between the values obtained with meshes $\Delta x = 1/32$ and $\Delta x = 1/64$. Hence, mesh $\Delta x = 1/32$ is chosen for further investigations.

For case 2, Figure 10 shows results in terms of bubble rising velocity $\tilde{U}_b$ and sphericity $s_b$ over time as well as the location of the gas-liquid interface ($r_G = 0.5$) at time $\tilde{t} = 12.53$, which are obtained with the present solver, the homogeneous model solver, experimentally obtained by Bhaga and Weber\textsuperscript{62} and numerically by Balcázar et al.\textsuperscript{61} For the reference data from literature, rising velocity information is provided in terms of a single value for the bubble Reynolds number $Re_b^{Bal} = 17.46$ and $Re_b^{Bha} = 18.3$ (cf Table 4). Furthermore, literature reference data for interface position are scaled and shifted, analogously to case 1.

In contrast to case 1, the rising velocity shows two pronounced and one flat local maximum value, $\tilde{U}_{b,max}$, $\tilde{U}''_{b,max}$, and $\tilde{U}'''_{b,max}$ in the early phase of the simulation ($\tilde{t} < 6$). Numerical values of those velocity extrema and their time of occurrence as well as values of vertical bubble position, rise velocity, and sphericity at time $\tilde{t} = 12.53$ are presented in Table 6. Considering rise velocity and sphericity, both the present model and the homogeneous model perform very similar
FIGURE 9  Bubble vertical position, rising velocity, and sphericity over time as well as interface position ($r_G = 0.5$) at $\tilde{t} = 12.53$ for different spatial resolutions in three-dimensional rising bubble case 2 [Colour figure can be viewed at wileyonlinelibrary.com]

with relative deviations below 1%. While the homogeneous model predicts $\tilde{U}_b$ to be slightly higher in the beginning of the simulation than the presented model does, the situation is vice versa for $\tilde{t} > 2$. Both solvers predict that the bubble slowly decelerates in the second half of the simulation, making it more than 3% slower than reported by Balcázar et al.\textsuperscript{61} The deviation of the present result from the experimental value of Bhaga and Weber\textsuperscript{62} in terms of final rising velocity is approximately −8%. In terms of bubble shape, the results of Balcázar et al\textsuperscript{61} show that the bubble is nearly flat in the lower region between the ligaments of the skirt region. In contrast to that, the other solvers predict a bulge of the interface in the region of the symmetry axis. Moreover, the ligaments are predicted to be longer and more slender compared with the results of Balcázar et al\textsuperscript{61}. The bubble shape as obtained with the presented solver has ligaments, which are slightly more blunt at the tips compared to the homogeneous model solver. In contrast to the numerical results, the experimentally obtained bubble shape shows that ligaments at the lower end of the gas structure are pinched toward the center line, while deviations regarding interface position at the upper part of the bubble are rather small.

Overall, the presented model framework performs very similar to the solver, which is based on the homogeneous model, while deviations from the results of Balcázar et al\textsuperscript{61} are moderate.

4.4  Two-dimensional bubble rising in liquid with micro gas bubbles

In order to demonstrate the present solver’s capability to describe the interplay between large and finely dispersed interfacial structures, the two-dimensional case setup 1 from Section 4.2 is modified such that a large gas bubble rises trough liquid with a layer of micro bubbles, which consist of the same gas. In contrast to the original setup in Section 4.2, the computational domain is extended in vertical direction, resulting in dimensions of $2D_h \times 20D_h$. The spatial resolution is kept constant, such that $80 \times 800$ grid points are used for discretization. Micro bubbles are modeled as disperse Eulerian
FIGURE 10  Bubble rising velocity and sphericity over time as well as interface position \((r_G = 0.5)\) at \(\tilde{t} = 12.53\) for three-dimensional rising bubble case 2, data for interface position of Balcázar et al\(^{61}\) and Bhaga and Weber\(^{62}\) are adjusted in terms of scale and position [Colour figure can be viewed at wileyonlinelibrary.com]

![Graphs showing bubble rising velocity and sphericity over time.](image)

TABLE 6  Results of rising velocity \(\bar{U}_b\), sphericity \(s_b\), and vertical position \(\bar{z}_b\) of the bubble and relative deviation of results between the present solver, interFoam, and results of Balcázar et al\(^{61}\) as well as Bhaga and Weber\(^{62}\) in three-dimensional rising bubble case 2

|                  | Present solver | interFoam | Balcázar et al\(^{61}\) |
|------------------|----------------|-----------|------------------------|
| \(\bar{U}_b\)_{\text{max}} \ | 0.6119         | 0.6158    | −0.63%                 |
| \(i|\bar{U}_b-C_{\text{max}}\) \ | 0.7517         | 0.7517    | 0.34%                  |
| \(\bar{U}_b\)_{\text{max}} \ | 0.5889         | 0.5869    | 0.22%                  |
| \(i|\bar{U}_b-C_{\text{max}}\) \ | 2.5996         | 2.6310    |                        |
| \(\bar{U}_b\)_{\text{max}} \ | 0.5581         | 0.5569    | 0.22%                  |
| \(i|\bar{U}_b-C_{\text{max}}\) \ | 5.5125         | 5.6378    |                        |
| \(\bar{z}_b|\tilde{t}=12.53\) \ | 8.8599         | 8.9061    | −0.52%                 |
| \(s_b|\tilde{t}=12.53\) \ | 0.3273         | 0.3259    | 0.43%                  |
| \(\bar{U}_b|\tilde{t}=12.53\) \ | 0.5429         | 0.5415    | 0.26%                  |
| \(\bar{U}_b|\tilde{t}=63\) \ | 0.5905         | 0.5634    | −3.64%                 |

phase (d) with fixed bubble diameter for interfacial models of \(d_G = 2 \times 10^{-3} D_b\). The disperse phase is initialized with a void fraction of \(r_G = 0.1\) in the region of \(3 < \bar{y}_b < 4\). Disperse drag and virtual mass formulations as described in Section 2 are applied to model momentum exchange between disperse and continuous phases. All walls are modeled with free-slip conditions for the disperse phase. As in case 1 of Section 4.2, time step size is fixed to \(\Delta \tilde{t} = 3.5 \times 10^{-3}\), which results in \(Co < 0.133\). The large gas bubble is rising and deforming just as described in Section 4.2 and after it passes the region, where the micro bubbles are present, a portion of dispersed phase gets entrapped into the wake region of the large gas structure. The velocity fields of the large bubble and the distribution of entrapped micro bubbles at time \(\tilde{t} = 63\) are shown in Figure 11.

At this time, the bubble’s vertical position is \(\bar{y}_b|\tilde{t}=63\) = 17.27. It turns out that the micro bubbles distribute in close relation to the streamlines of the liquid-phase velocity outside the large gas structure and, therefore, the majority of
Large rising gas bubble with wake region and entrapped micro bubbles at time \( t = 63 \) with the large bubble's vertical position \( \tilde{y}_b = 17.27 \); A, magnitude and streamlines of velocity of continuous phases \( \tilde{\mathbf{u}}_c \) in moving frame of large gas bubble's center of gravity \( \tilde{\mathbf{u}}_b \mid_{t=63} = (0.26) \) and, B, contours of volume fraction of disperse gas phase (micro bubbles) \( r_d \) together with streamlines of velocity of continuous phases \( \mathbf{u}_c - \mathbf{u}_b \); the gas-liquid interface \( (r_G = 0.5) \) of the large gas bubble is shown as white and black solid lines for figures A and B, respectively. [Colour figure can be viewed at wileyonlinelibrary.com]

them stays in the recirculating liquid flow for a long time. Inside the resolved gas bubble, the continuous gas phase also develops quasisteady vortex structures and, as dispersed and continuous gas phases have identical material properties, mixes with the disperse gas phase, which concentrates at the lower part of the gas bubble. From there, small disperse gas portions get sucked upward to the bubble cap by the internal coherent vortex structures. In the frame of the Euler-Euler method is not a drawback, as the phase fraction represents a probability due to the implicated averaging procedure. This demonstrates that the present solver is able to handle both subgrid and supergrid interfacial structures at the same time. Further modeling is required to handle interactions of small bubbles with a resolved interface properly.

### 4.5 Two-dimensional stagnant stratification of water and oil with air bubbles

In order to further demonstrate the solvers capability to handle interactions between disperse phases and interfaces between continuous phases at the same time, dispersed air bubbles of diameter \( d_{air} \) are introduced into a stagnant stratification of oil and water. The two-dimensional computational domain of dimensions \( 0.15 \text{ m} \times 0.5 \text{ m} \) is discretized with \( 30 \times 100 \) grid points, and at time \( t = 0 \text{ s} \), the lower half of the domain is filled with continuous water phase, whereas the upper part is filled with continuous oil phase. The top boundary is setup to provide a fixed-pressure condition. For lateral and bottom boundaries no-slip conditions are imposed for the continuous water and oil phases. For the disperse air phase, these boundaries act as free-slip walls. At the bottom region between \( 0.05 \text{ m} < x < 0.1 \text{ m} \), disperse air is introduced into the domain with a volume fraction of \( r_d = 0.26 \) and a wall-normal velocity of \( U_d = 0.197 \text{ m s}^{-1} \), where both \( r_d \) and \( U_d \) are linearly ramped up from zero values for time \( 0 \text{ s} < t < 0.3 \text{ s} \), kept constant until \( t = 0.6 \text{ s} \) and again ramped down linearly to zero values for \( 0.6 \text{ s} < t < 0.7 \text{ s} \). Again, drag and virtual mass closure formulations from Section 2 are applied to model interactions between disperse air phase and both continuous water and oil phases. Time step size is fixed to a value of \( \Delta_t = 0.03 \text{ s} \), resulting in a Courant number \( Co < 0.296 \). It is expected that the dispersed air bubbles rise due to gravity \( g = 9.81 \text{ m s}^{-2} \) and pass the water-oil interface smoothly. The bubble rise velocity should slightly change after passing the interface. Physical properties for the present case are reported in Table 7. The initial residuals for the solution of pressure Equation (17) over one single time step at \( t = 1.7 \text{ s} \) are shown in Figure 12. A total number of \( i = 10 \) outer and \( j = 2 \) inner loops is used.

It turns out that initial residuals stay nearly constant over the outer loops for \( i \geq 5 \) with relative residuals smaller than \( 2 \times 10^{-7} \) for each second iteration \( (j = 2) \). Figure 13 shows the temporal evolution of spatial distribution of disperse air volume fraction \( r_d \).
TABLE 7  Material properties of water, oil, and air in case of a two-dimensional stagnant water-oil stratification with air bubbles

| Unit       | Water  | Oil    | Air      |
|------------|--------|--------|----------|
| $\rho_\alpha$ | kg m$^{-3}$ | 997    | 900      | 1.185    |
| $\mu_\alpha$ | Pa s   | $1 \times 10^{-2}$ | $1 \times 10^{-2}$ | $1.84 \times 10^{-4}$ |
| $d_{\text{air}}$ | m      | —      | —        | $3 \times 10^{-3}$ |
| $\sigma_{\text{water-oil}}$ | N m$^{-1}$ | 0.0244 |          |          |

FIGURE 12  Initial relative residuals for the solution of the pressure equation over all outer and inner loops of a single time step at $t = 1.7$ s [Colour figure can be viewed at wileyonlinelibrary.com]

After starting to rise in the water from the bottom, the swarm of air bubbles forms a mushroom-like shaped cloud, which then hits the water-oil interface at $t \approx 1.6$ s, penetrates it and continues rising to the top boundary, where it exits the computational domain. The water-oil interface becomes temporary deformed by the bubble swarm and keeps sloshing for some time without being completely disrupted. After the air has left the domain through the outlet, the resolved interface almost perfectly recaptures its initial vertical position of $y|_{t=0} = 0.25$ m, which means that the total amount of water is conserved in the domain over the course of the simulation within an accuracy of 0.398% after $t = 10$ s. From the contours of the vertical component of the air velocity $U_{a,y}$ (Figure 13H-N) it becomes clear that the dispersed air phase passes the sharp water-oil interface smoothly without any oscillatory behavior in the phase velocity field. Furthermore, in the air velocity field a region can be identified ahead of the bubble swarm, where air bubbles have a nearly constant rising velocity, which results from the force balance between buoyancy and drag between small bubbles and the continuous liquid around. Figure 14 shows vertical profiles of phase volume fraction $r_\alpha$ as well of vertical phase velocity components $U_{a,y}$.

It is visible that the interface between water and oil phases maintains its relatively small thickness, even when dispersed air phase is present at the same location. Phase velocities $U_{a,y}$ of water and oil are close to be perfectly identical everywhere in the domain, which is the desired behavior and results of the choice of the interfacial drag formulation by Štrubelj and Tiselj$^{42}$ together with the small value for relaxation time $\tau_r$. The vertical air velocity is also nearly identical to the ones of continuous phases, wherever air volume fraction is close to zero. In regions, where air is present, its vertical velocity component is approximately $0.15$ m s$^{-1}$ higher than vertical velocity components of the continuous phases, which results from the buoyancy force acting on the gas bubbles and accelerating them in vertical direction. Again, all velocity profiles turn out to be very smooth, especially in the interface region, where three phases are present in this case.

5 SUMMARY AND CONCLUSIONS

The compact momentum interpolation method was applied to the multifield two-fluid model. Special care was taken to properly define phase coupling in regions of large, resolved interfacial structures by applying the interfacial drag formulation of Štrubelj and Tiselj.$^{42}$ The resulting stiffness of the system of multiple momentum conservation equations for the individual phases was resolved in an approximate fashion by extending the idea of partial elimination$^{43}$ to an arbitrary number of phases by maintaining a sum formulation, wherever more than two phases are present. This method worked out to resolve phase coupling in the investigated test cases with a maximum of three phases while preventing the solution procedure from heavy underrelaxation effects. Furthermore, this method was extended to consistently treat the virtual
mass force, which is a momentum exchange model for description of dispersed flows in the used multifield two-fluid model. For the first time it has been shown that dispersed as well as resolved interfacial structures can be simultaneously solved with the same set of equations considering interactions between flow and interfacial structures of different length and time scales in a computationally efficient way.

The next steps are to include further interfacial closure models, namely lift, wall lubrication, and turbulent dispersion forces, so that the typical set of momentum exchange closure models for dispersed flows can be applied. Furthermore, mass transfer between phases describing different morphologies of the same physical phase, such as dispersed air bubbles.
and continuous air, will be added, for example, in order to model the bursting of small air bubbles at a large water-air interface. Further extensions are the consideration of drag modeling regarding resolved interfaces in an underresolved manner by allowing for interfacial slip, subgrid scale modeling in the fashion of large-eddy simulations as well as modeling of further multiphase morphologies such as froth.

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