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Compressibility induced bubble size variation in bubble column reactors: Simulations by the CFD–PBE

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ABSTRACT

Bubble column reactors can be simulated by the two fluid model (TFM) coupled with the population balance equation (PBE). For the large industrial bubble columns, the compressibility due to the pressure difference may introduce notable bubble size variation. In order to address the compressibility effect, the PBE should be reformulated and coupled with the compressible TFM. In this work, the PBE with a compressibility term was formulated from single bubble dynamics, the mean Sauter diameters predicted by the compressible TFM coupled with the PBE were compared with the analytical solutions obtained by the ideal gas law. It was proven that the mesoscale formulations presented in this work were physically consistent with the macroscale modeling. It can be used to simulate large industrial plants when the compressibility induced bubble size variation is important.

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1. Introduction

Numerous chemical engineering systems involve discrete population of bubbles. One notable example is the bubble column reactors [1]. The information of the flow fields in the bubble column can be predicted by the computational fluid dynamics (CFD) and it is common to employ the two fluid model (TFM) [2] to simulate multiphase flows with high phase fractions [3–11]. However, the hydrodynamic description and the volume averaging approaches employed in the TFM lead to the problem that it is only applicable for monodisperse systems. For the realistic polydisperse system, the evolution of the bubble population in the bubble column can be modeled by means of the population balance equation (PBE) [12], whose unknown is the bubble size distribution (BSD) associated with the bubble population. The BSD can be further distinguished by the length-based BSD or volume-based BSD [13]. By coupling the TFM and the PBE, the knowledge of the BSD in bubble columns can be obtained.

In the past, the TFM–PBE coupling was extensively employed to simulate the bubble columns [9, 10, 14, 15]. In the work of Liang *et al.* [15], the class method was applied to solve the PBE. The TFM–PBE coupling was achieved by the momentum exchange closure term. Three different drag models were employed to investigate the multiphase flow behaviors. The wake acceleration effect of large bubbles was firstly evaluated. In the work of Buffo *et al.* [14], the quadrature-based moment method was employed. The effect of the bubble swarm was investigated by a

correction on the drag model. However, the compressibility induced bubble size variation has never been investigated. For the industrial plants where the operating pressure at the bottom may be much larger than that on the top, the high pressure difference may lead to significant variation of the bubble density and the bubble size.

In such cases the compressibility should be addressed in the TFM and PBE. In this work, the compressible TFM was coupled with the PBE to predict the BSD in conceptual one-dimensional bubble columns with different height. The compressibility induced bubble size variation was novelly introduced by a “growth” term in the PBE which was solved by the method of moments (MOM). The continuous BSD was reconstructed by the log-normal extended quadrature method of moments (EQMOM). Compared with the class method (CM), readers will find that the compressibility induced bubble size variation can be much easily captured in the MOM. Finally, the prediction of the mean Sauter diameter of the bubbles was verified with the analytical solutions.

2. Background Theory

2.1. Compressible TFM

The phase fraction equation of the compressible TFM is reported as the following:

$$\frac{\partial(\alpha_d \rho_d)}{\partial t} + \nabla \cdot (\alpha_d \rho_d U_d) = 0, \quad (1)$$

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where α_d is the volume fraction of the dispersed phase, ρ_d is the density of the dispersed phase, and U_d is the average velocity of the dispersed phase. The volume fraction of the continuous phase (α_c) is generally calculated by knowing that volume fractions sum to unity ($\alpha_d + \alpha_c = 1$). The average velocities of the dispersed phase (U_d) and of the continuous phase (U_c) are calculated by solving the corresponding momentum balance equations:

$$\frac{\partial \alpha_d U_d}{\partial t} + \nabla \cdot (\alpha_d U_d U_d) + \nabla \cdot (\alpha_d \tau_d) + \nabla \cdot (\alpha_d \mathbf{R}_d) = -\alpha_d \nabla p + \alpha_d \mathbf{g} + M_d, \quad (2)$$

$$\frac{\partial \alpha_c U_c}{\partial t} + \nabla \cdot (\alpha_c U_c U_c) + \nabla \cdot (\alpha_c \tau_c) + \nabla \cdot (\alpha_c \mathbf{R}_c) = -\alpha_c \nabla p + \alpha_c \mathbf{g} - M_d, \quad (3)$$

where p is the pressure shared by the two phases, τ_d and τ_c are the viscous stress tensors, $\mathbf{R}_d$ and $\mathbf{R}_c$ are the Reynolds-stress tensors, and $\mathbf{g}$ is the gravitational acceleration vector. M_d is the interfacial force term, which describes the momentum exchange between the two phases and requires a certain degree of modeling. It is common to break it down into the axial drag force M_{drag} ; the lateral lift force M_{lift} , which acts perpendicular to the direction of the relative motion of the two phases; the virtual mass force M_{vm} , which is proportional to relative phase accelerations; the wall lubrication force M_{wall} which acts to drive the bubble away from the wall; and the turbulent dispersion force M_{turb} , which is the result of the turbulent fluctuations of the liquid velocity. Specifically, the drag force can be calculated as follows:

$$M_{\text{drag}} = \frac{3}{4} \alpha_d \rho_c C_D \frac{1}{d_d} |U_r| U_r, \quad (4)$$

where C_D is the drag force coefficient, which was calculated by the correlation of Schiller and Naumann [16]; d_d is the diameter of the dispersed phase, or the mean Sauter diameter in each computational cell if the PBE was coupled with the TFM. The lift force can be calculated as follows:

$$M_{\text{lift}} = \alpha_d C_L \rho_c U_r \times (\nabla \times U_r), \quad (5)$$

where C_L is the lift force coefficient. The virtual mass force can be calculated as follows:

$$M_{\text{vm}} = \alpha_d C_{\text{vm}} \rho_b \left(\frac{DU_c}{Dt} - \frac{DU_d}{Dt} \right), \quad (6)$$

where C_{vm} is the virtual mass force coefficient. Readers interested in the theory of the TFM are suggested to other works [17] and the numerical solving procedure was summarized in our previous work [18].

2.2. Compressible PBE

For bubble column simulations, the internal coordinate of the BSD is often characterized by the bubble diameter in order to investigate the size variation intuitively. The one-dimensional length-based BSD transport equation for $n(L, x, t)$ can be written as the following (the dependence on L, x and t is omitted for simplicity):

$$\frac{\partial n}{\partial t} + \frac{\partial u_d n}{\partial x} = 0, \quad (7)$$

where u_d is the advection velocity for the bubbles. At this stage, the possible source terms such as the growth, breakage and coalescence are neglected. To include the compressibility on Eq. (7), one may include the density on each term to address the density variation, and Eq. (7) can be reformulated to

$$\frac{\partial \rho_d n}{\partial t} + \frac{\partial \rho_d u_d n}{\partial x} = 0, \quad (8)$$

where ρ_d is the bubble density which is not spatially homogeneous for the compressible fluids. Unfortunately, it should be stressed here Eq. (8) does not obey the statistic theory from which the PBE is developed and it leads to wrong results.

The bubble size variation due to the compressibility is reported in Fig. 1.

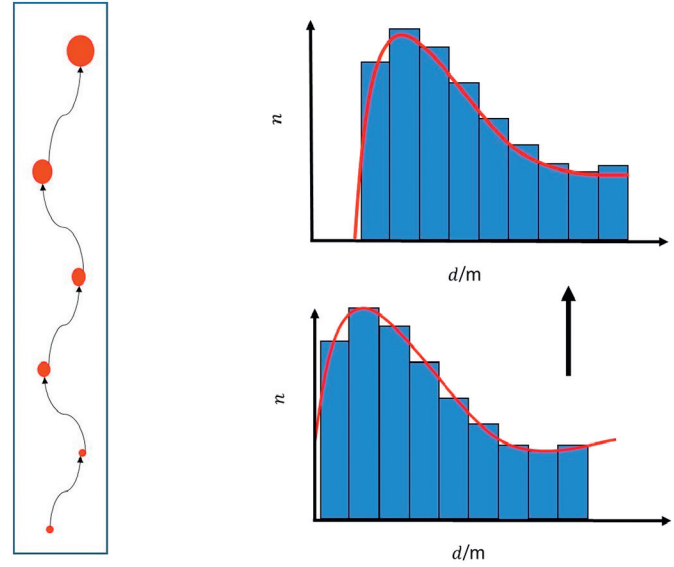


Fig. 1. Left: single bubble growth due to the compressibility from the bottom to the top in a bubble column. Right: the “drift” shape of the BSD due to the compressibility.

It can be seen that the bubble size variation is continuous, which implies that it is not physically reasonable to address the compressibility effect as first-order or higher-order point processes [13]. It is therefore reasonable to qualify the bubble size variation due to the compressibility by adding a zero-order point process (e.g., a “growth” term) in Eq. (7). Under such assumption, the BSD transport equation with the growth term can be written as

$$\frac{\partial n}{\partial t} + \frac{\partial u_d n}{\partial x} + \frac{\partial G n}{\partial L} = 0, \quad (9)$$

where G is the diameter-based growth coefficient, which can be calculated by

$$G = \frac{dL}{dt}. \quad (10)$$

It represents the continuous rate of change of bubble length L . The unknown growth coefficient introduced by the compressibility should be derived from the single bubble dynamics. The relationship between the pressure and the volume can be represented by the ideal gas law as follows:

$$V = \frac{NRT}{p}, \quad (11)$$

where V is the volume, p is the pressure, N is the mole number, R is the universal gas constant, and T is the temperature. Using this assumption, we obtain

$$\frac{DV}{Dt} = \frac{DV}{Dp} \frac{Dp}{Dt} = -\frac{NRT}{p^2} \frac{Dp}{Dt} = -\frac{V}{p} \frac{Dp}{Dt}, \quad (12)$$

where $\frac{D}{Dt}()$ is the material derivative. The bubble volume can be calculated by $V = k_v L^3$, where k_v is the shape coefficient which equals $\pi/6$

for sphere bubbles. Meanwhile, the substantial derivative of the bubble volume can be calculated from the substantial derivative of the bubble diameter by

$$\frac{DV}{Dt} = 3L^2 k_v \frac{DL}{Dt}. \quad (13)$$

Combining Eqs. (12) and (13) yields

$$\frac{DL}{Dt} = -\frac{L}{3p} \frac{Dp}{Dt}. \quad (14)$$

Substituting Eq. (14) into Eq. (9) leads to the BSD transport equation with effect of the compressibility due to the pressure difference:

$$\frac{\partial n}{\partial t} + \frac{\partial u_d n}{\partial x} - \frac{1}{3p} \frac{Dp}{Dt} \frac{\partial Ln}{\partial L} = 0. \quad (15)$$

In this work, Eq. (15) was numerically solved by the method of moments (MOM) and the continuous BSD was reconstructed by the extended quadrature method of moments (EQMOM) [19]. The corresponding moment transport equations are defined by

$$\frac{\partial m_k}{\partial t} + \frac{\partial u_d m_k}{\partial x} = -\frac{k}{3} \frac{1}{p} \frac{Dp}{Dt} m_k. \quad (16)$$

The details of the MOM and EQMOM are neglected here. Reader interested in this subject is suggested to other latest works [13]. It should be stressed here that Eq. (8) can be also transformed to the moment transport equations as follows:

$$\frac{\partial m_k}{\partial t} + \frac{\partial u_d m_k}{\partial x} = -\frac{1}{p} \frac{Dp}{Dt} m_k. \quad (17)$$

It can be seen that the R.H.S. of Eqs. (16) and (17) is different when $k \neq 3$. For example, the R.H.S. of Eqs. (16) and (17) for m_2 is $-\frac{2}{3} \frac{1}{p} \frac{Dp}{Dt} m_2$ and $-\frac{1}{p} \frac{Dp}{Dt} m_2$, respectively. If Eq. (17) was employed to predict the

mean Sauter diameter (m_3/m_2), it overpredicts the value compared with the analytical solution due to the larger sink source term. In the following test case, the correctness of Eq. (16) was proved by comparisons between numerical predictions with analytical solutions.

3. Numerical Test Case

3.1. 1-meter-high bubble column

A one-dimensional conceptual bubble column was employed in this work to investigate the effect of the compressibility on the bubble size variation. The grids include 75 cells in height (1 m), as this results in grid-independent predictions. Further refinement of the mesh (e.g., 150 cells) did not improve the predicted results. The computational domain was initially fed by mixture of water and gas. The inlet boundary of the gas phase fraction was 9.549%. The inlet gas velocity was $0.1 \text{ m} \cdot \text{s}^{-1}$ as the Dirichlet boundary condition, and the flow fields were assumed to be laminar. The operating pressure at the top of the column was set to 101325 Pa. The boundary conditions are reported in Table 1. The information of the flow fields was calculated by the compressible TFM solver in OpenFOAM-5.x.

It can be seen in Fig. 2 that the plots of the predicted phase fraction by Eq. (1) and the $\frac{p}{6} m_3$ calculated from Eq. (16) overlap. It is because that when $k = 3$, Eq. (16) can be written as

$$\frac{\partial m_3}{\partial t} + \frac{\partial u_d m_3}{\partial x} = -\frac{m_3}{p} \frac{Dp}{Dt}, \quad (18)$$

which is mathematically equivalent to the compressible phase fraction equation [18]:

$$\frac{\partial \alpha_d}{\partial t} + \frac{\partial u_d \alpha_d}{\partial x} = -\frac{\alpha_d}{p} \frac{Dp}{Dt}. \quad (19)$$

The overlapped plots verify the correctness of Eq. (16), whereas Eq. (17) is incorrect. Moreover, it can be seen that the gas phase fraction inside the bubble column (around 2.5%) is much smaller than that at the inlet (9.549%) due to the upward buoyant force.

Let us now analyze the bubble size variation due to the compressibility. For the test case investigated in this work, the pressure can be calculated analytically by $p = p_0 + \rho_g g h$. From Eq. (11), the analytical solution for the bubble size can be written as

$$\left(\frac{L}{L_0}\right)^3 = \frac{p^0}{p}, \quad (20)$$

where L_0 and p^0 are the reference diameter and pressure, respectively. The reference pressure can be calculated from the hydrodynamics, and it equals 111115 Pa at the bottom of the one-meter-high column. The corresponding mean Sauter diameter is 3.136 mm. The comparison

Table 1
Numerical schemes and boundary conditions used in the test cases

Variable	Scheme	Boundary conditions at walls
Bubble vol. frac.	Second-order TVD scheme with vanLeer flux limiter	Zero grad.
Bubble velocity	Second-order TVD scheme with vanLeer flux limiter	No-slip
Cont. liquid velocity	Limited second-order central scheme	No-slip
Pressure	Limited second-order central scheme	Zero grad.

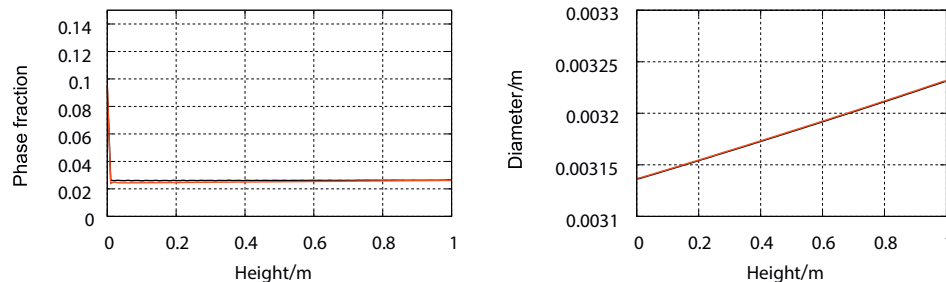


Fig. 2. Left: plots of the predicted phase fraction α_d by Eq. (1) (black line) and $\frac{p}{6} m_3$ by Eq. (16) (red line). Right: plots of the mean Sauter diameter predicted by Eq. (16) (black line) and the analytical solution (red line).

of the predicted mean Sauter diameter ($d_{32} = m_3/m_2$) with the analytical solution calculated by Eq. (20) was reported in Fig. 2. It can be seen that the predicted mean Sauter diameter predicted by Eq. (16) agrees well with the analytical solution.

The reconstructed BSD predicted by the log-normal EQMOM was reported in Fig. 3 in order to verify the drift phenomenon as reported in Fig. 1. It can be seen that the shape of the BSD shifts horizontally from left to the right, which implies the bubble literally grows due to the compressibility. Such drift phenomenon of the reconstructed BSD predicted by the EQMOM is consistent with Fig. 1.

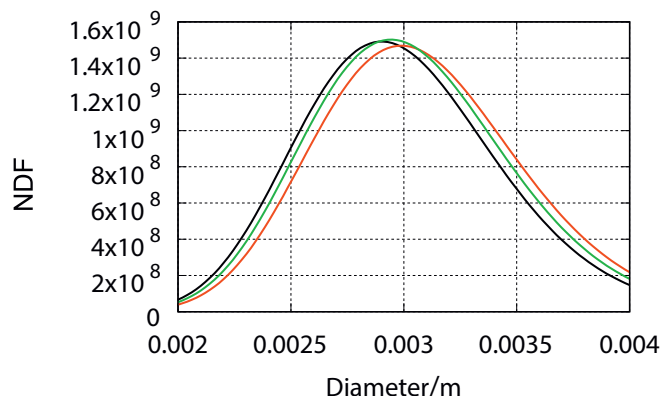


Fig. 3. Plots of the reconstructed BSD predicted by the log-normal EQMOM for $x = 0$ m (black line), $x = 0.5$ m (green line) and $x = 1$ m (red line).

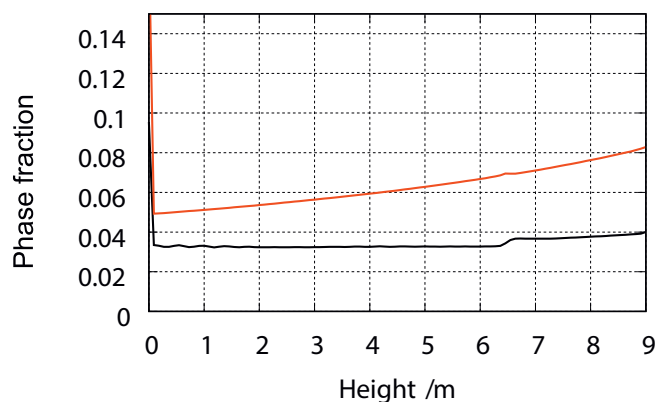


Fig. 4. Plots of the predicted phase fraction ($\frac{m_3}{6}$) by PBE with (red line) and without (black line) the compressibility induced term.

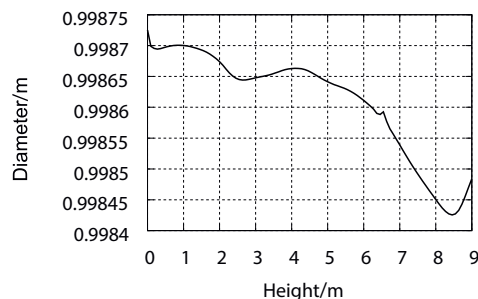
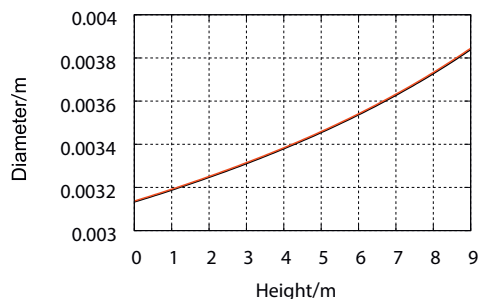


Fig. 5. Left: plots of the mean Sauter diameter predicted by Eq. (16) (black line) and the analytical solution (red line). Right: plot of the relative value of the predicted mean Sauter diameter with analytical solution.

3.2. 9-meter-high bubble column

In this test case, the bubble column was heightened to 9 m, which is a common operating height for industrial gas–liquid flows [20]. The plots of the predicted phase fraction are reported in Fig. 4. It can be seen that the predicted phase fraction ($\frac{m_3}{6}$) by the PBE with the compressibility induced term captures the bubble volume growth due to the pressure difference in the bubble column. However, the predicted bubble volume by PBE without the compressibility induced term keeps constant due to the absence of the source term in Eq. (18), which is not physically meaningful. The plots of the predicted mean Sauter diameters are reported in Fig. 5. It can be seen that the predicted mean Sauter diameter predicted by Eq. (16) agrees well with the analytical solution. It was further proven by that the relative value of the predicted mean Sauter diameter with analytical solution is approximately 1.

At last, it is interesting to discuss the relative importance of the compressibility induced bubble size variation compared with the breakage/coalescence induced bubble size variation. From the 9-meter-high bubble column test case, the bubble diameter increases from 3.14 mm to 3.83 mm due to the compressibility effect. The variation is approximately 20% which should not be overlooked. Moreover, when the PBE was coupled with the TFM, the predicted $\frac{m_3}{6}$ and α_d should be identical. If the compressibility term was neglected or not correct (e.g., Eq. (17)), the predicted $\frac{m_3}{6}$ by the PBE deviates with the predicted α_d by the compressible TFM. Last but not least, the compressibility term should be included together with the breakage/coalescence source term in the PBE, since it scales up/down the bubble size on the basis of the bubble size variation due to the breakage/coalescence.

4. Conclusions

In this work, the bubble size variation due to the compressibility was investigated by the compressible TFM coupled with the PBE. The predicted mean Sauter diameters were compared with the analytical solutions by virtue to the ideal gas law. The drift phenomenon of the BSD was successfully predicted by the log-normal EQMOM. It was proven that the PBE with the compressibility effect derived from single bubble dynamics is physically reasonable compared with Eq. (8). For the 9-meter high bubble column test case, the compressibility induced bubble size variation is approximately 20% which cannot be overlooked. We suggest employing Eq. (15) in the CFD–PBE simulations for industrial bubble column reactors.

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