Numerical simulation of gravity-driven mono- and polydisperse bubbly flows in a three-dimensional column in the framework of the Euler-Euler approach

A S Chernyshev and A A Schmidt
Computational Physics Laboratory, Ioffe Institute, Politekhnicheskaya 26, Saint Petersburg, 194021, Russia
E-mail: alexander.tchernyshev@mail.ioffe.ru

Abstract. The paper presents a comparison of the results of numerical modeling of the three-dimensional flow of mono- and polydisperse media in a rectangular bubble column reactor. The mathematical model used in the paper is based on the Euler – Euler description of a multiphase medium taking into account interphase momentum transfer, turbulence modeling of the carrier phase with bubble induced turbulence and polydispersity in the framework of the inhomogeneous multiple-size group (MUSIG) model. The comparison is carried out of the mono- and polydisperse approaches under the conditions studied for simplified and full formulations. Numerical results are compared with the available experimental data and simulations of other authors.

1. Introduction
The gravity-driven multiphase bubbly flows occurred in a confined space are of a great importance due to their frequent appearance in industrial apparatus. Some cases of such flows are pipeline flows, aerators, sudden valve expansions, chemical reactors (see, for example, [1-3]). Numerical simulations can provide detailed information about such flows which can be used to assess flow regimes for practical implementations or to extend the knowledge about processes under study. In most cases axisymmetrical or two-dimensional simplifications are enough, but they are not always possible because of specific geometrical features or flow regimes which can not be incorporated into the model [4].

The present work is focused on the three-dimensional modeling of the multiphase bubbly flow. The Euler-Euler approach is used as a robust and reliable choice capable of handling of almost arbitrary concentration of dispersed bubbles. In the framework of this approach both carrier and dispersed phases are treated as continuous ones occupying the whole domain. Therefore, the same equation set can be used for all phases which simplifies description of the multiphase medium. The model is extended by incorporation of turbulence effects by k-ω SST turbulence model and the model of polydispersity.

Numerical simulations of gravity-driven three-dimensional mono- and polydisperse bubbly flows inside a rectangular bubble column reactor are carried out. Results obtained on the full geometry are compared with the simplified setup made on a geometry with mirror symmetry as well as with simulations and experimental data of other authors. It is shown that narrow velocity profile of carrier liquid and overestimated peak velocity are obtained in the simplified setup and effect of polydispersity is insignificant for the conditions under study.
2. Mathematical model
The model is based on the Euler-Euler approach to the description of the multiphase medium[5]. In the framework of this approach each phase is treated as a continuum occupied the whole domain and the phase volume fraction $\alpha$ is introduced. Density of each continuum is calculated as a product of the volume fraction per material density $\rho$ of the corresponding phase (sub-index $l$ corresponds to the carrier fluid, $b$ corresponds to the bubbles).

A multi-class model of the bubble size distribution with different velocities per each class of the bubbles (inhomogeneous MUSIG model, [5]) is used to model the effect of polydispersity. A piecewise size distribution with $M$ bubble classes is used with corresponding bubble sizes $R_{ib}$, where $i = 1..M$. The Navier-Stokes set of equations is written with additional terms describing the interphase momentum exchange. Due to the small initial bubble concentration $t_0$ is written with additional terms describing the interphase momentum exchange between bubble classes are omitted in the current work. The initial bubble size distribution is selected on the basis of the experimental data and can be described by the Rosin-Rammler probability distribution function:

$$RR: \frac{k}{2} \left(\frac{R}{\lambda}\right)^{k-1} \cdot \exp\left(-\left(\frac{R}{\lambda}\right)^k\right), R \geq 0.$$  (1)

Here $R$ – bubble radius, $k$ – shape parameter, $\lambda$ – scale parameter.

The Navier-Stokes equations for the polydisperse case per each phase will have the following form:

\begin{align*}
\frac{\partial \alpha_{ib} \rho_{ib} \vec{V}_{ib}}{\partial t} + \text{div}(\alpha_{ib} \rho_{ib} \vec{V}_{ib} \vec{V}_{ib}) &= D_{ib}, \\
\frac{\partial \alpha_{ib} \rho_{ib} \vec{V}_{ib}}{\partial t} + \text{div}(\alpha_{ib} \rho_{ib} \vec{V}_{ib} \vec{V}_{ib} + p \vec{E}) &= S_{ib}, \\
\frac{\partial \alpha_i \rho_i \vec{V}_i}{\partial t} + \text{div}(\alpha_i \rho_i \vec{V}_i \vec{V}_i) &= 0, \\
\frac{\partial \alpha_i \rho_i \vec{V}_i}{\partial t} + \text{div}(\alpha_i \rho_i \vec{V}_i \vec{V}_i + p \vec{E} - \dot{\tau}_i) &= S_i.
\end{align*}  (2)

In this set of equations: $\vec{V}$ – the velocity vector of the carrier or dispersed phases, $p$ – pressure, $\vec{E}$ – the unity tensor, $S$ – source terms responsible for the interphase momentum exchange, $D$ – source terms responsible for the diffusion due to turbulence, $\dot{\tau}$ – the strain rate tensor:

$$\tau_{kl} = \mu_{eff} \left(\frac{\partial v_k}{\partial x_l} + \frac{\partial v_l}{\partial x_k}\right), \mu_{eff} = \mu_{lam} + \mu_{turb}. \quad (3)$$

Here $\mu_{eff}$ is an effective dynamic viscosity coefficient of the carrier phase which is equal to the material viscosity plus turbulent one.

This system should be accomplished by the conservation equations of the number density per each class since the bubble radius can vary with the variation of the bubble gas density:

$$\frac{\partial N_{ib}}{\partial t} + \text{div}(N_{ib} \vec{V}_{ib}) = D_{ln}. \quad (4)$$

Turbulence is taken into account using the k-ω SST Menter model [6], supplemented to the right hand side by the source terms responsible for the generation and dissipation of turbulence due to the relative motion of bubbles and fluid [7]:

$$S_{ibk} = \frac{3}{8} C_{ib} \frac{\alpha_{ib} \rho_i}{R_{ib}} \left|\vec{V}_{irel}\right|^3, S_{ibn} = 0.8 \frac{k}{\mu_{turb}} S_{ibk}, \vec{V}_{irel} = \vec{V}_i - \vec{V}_{ib}. \quad (5)$$

Here $k$ is the kinetic energy of turbulence, $C_{ib}$ – drag coefficient.

Interphase momentum exchange term includes the buoyancy, drag, lift, virtual mass and wall lubrication forces:

$$S_{ib} = \vec{F}_{ib} + \vec{F}_{ibD} + \vec{F}_{ibL} + \vec{F}_{ibWL} + \vec{F}_{ibWM}, S_i = -\sum_{i=1}^{M} (\vec{F}_{ib} + \vec{F}_{ibL} + \vec{F}_{ibWL} + \vec{F}_{ibWM}), \quad (6)$$

$$\vec{F}_{ib} = \alpha_{ib} \cdot (\rho_{ib} - \rho_1) \cdot \vec{g}, \quad (7)$$

$$\vec{F}_{ibD} = \frac{3}{8 R_{ib}} C_{id} \left|\vec{V}_{irel}\right| \vec{V}_{irel}, \vec{V}_{irel} = \vec{V}_i - \vec{V}_{ib}. \quad (8)$$
\[ F_{il} = C_{il} \alpha_{ib} \rho_l \vec{V}_{irel} \times \text{rot} \vec{V}_l, \]  
\[ F_{ivm} = 0.5 \alpha_{ib} \rho_l \left( \frac{D_w V_{iw}}{D t} - \frac{D_l V_{il}}{D t} \right), \]  
\[ F_{iw} = -C_{iw} \alpha_{ib} \rho_l \left( \vec{V}_{irel} - \left( \vec{V}_{irel} \cdot \vec{n}_W \right) \cdot \vec{n}_W \right). \]

Expressions for \( C_{ip}, C_{il}, C_{iw} \) are taken from [8], [9] and [10], respectively and dependent on the variation of the relative velocity \( V_{irel} \) and the bubble shape.

The effect of the bubble dispersion due to the turbulent velocity pulsations of the carried liquid is included by introduction of additional diffusion term into the conservation equations of the volume fraction and the bubble number density [4]:

\[ D_{ia} = \frac{1}{Sc} \nabla \left( \frac{\mu_{eff}}{\rho_l} \nabla \alpha_{ib} \right), \quad D_{IN} = \frac{1}{Sc} \nabla \left( \frac{\mu_{eff}}{\rho_l} \nabla N_{ib} \right). \]

Here \( Sc \) is the Schmidt number.

3. Numerical method

The proposed mathematical model was implemented in the numerical algorithm and the simulation software was developed. The key features of the numerical algorithm are finite volume method and unstructured co-located meshes. To maintain the second-order accuracy and stability the upwind scheme with Minmod limiter is used which satisfies TVD criterion [11]. The modified SIMPLE algorithm with corrections related to multiphase is used for steady-state simulations, while the modified PISO is used for transient simulations to perform non-iterative traversal over time. The model and the code were tested on the available experimental data [5].

4. Results

Numerical simulations are carried out for the rectangular bubble column reactor which has a square cross-section in a plane parallel to the bottom of the column and dimensions of the column are 0.15x0.15x0.45 m (WxDxH) (see Figure 1). Initially the column is filled with water. An aerator is flash mounted in the center of the bottom of the column and has a square shape with side edge of 35.5 mm. Air is supplied through the aerator into the domain with superficial velocity of 4.9 mm/s. Top boundary is assumed as a free surface which lets bubbles leave the column. The buoyancy force causes bubbles to move towards the top boundary which in turn accelerates fluid in the column. Two types of bubble distributions are used at the aerator inlet: uniform with constant bubble size of 2 mm, non-uniform with 7 classes and bubble radius \( R_{ib} \) varies from 0.5 mm to 3.45 mm and the most probable bubble radius is equal to 2 mm. Conditions of the experiment are the same used in [13]. Simulations are carried out at normal conditions with pressure is equal to 101350 Pa and temperature is equal to 297 K.

![Figure 1. Schematic of the computational domain. Geometry is clipped along the vertical (H) direction for simplicity.](image)

Placement of the aerator, free surface boundary and a quarter of the geometry for steady state simulations (dashed gray lines) are presented.

Because of mirror symmetry, one set of simulations is carried out on a one quarter of the domain, which stands for the simplified setup. A steady state flow pattern is obtained on this configuration which is used to assess an applicability of this approach.

3
A full-scale domain is constructed to perform transient simulations. An instability of a bubble plume produced by the aerator can cause formation of a non-symmetrical transient flow structure which could be captured by modeling the entire domain with time resolution.

Figure 2. Comparison of vertical velocity profiles for experimental data and LES simulation (Deen, 2011), steady-state mono- and polydisperse and transient monodisperse cases (current work) in 0.35 m cross-section.

Figure 3. Comparison of vertical velocity profiles for experimental data and LES simulation (Deen, 2011), steady-state mono- and polydisperse and transient monodisperse cases (current work) in 0.25 m cross-section.

Figure 4. Comparison of vertical velocity profiles for experimental data and LES simulation (Deen, 2011), steady-state mono- and polydisperse and transient monodisperse cases (current work) in 0.15 m cross-section.

Vertical velocity component of the carried liquid is presented (Figures 2-4). The data is sampled in the middle vertical plane in 3 horizontal cross-sections at different heights: 0.15 m, 0.25 m and 0.35 m from the bottom surface. Transient data is averaged over 200 seconds of computational time, first 50 seconds are skipped to get to the fully developed transient regime.
Comparing mono- and polydisperse steady-state cases, it can be seen that the only slight difference is at the initial stage of the developing bubble plume, at 0.15 m location in the middle of the column. At the other locations both distributions are similar. That can be addressed to the small variation of the drag coefficient for big bubbles which provides similar values of relative velocity for different bubble classes and same behavior in the bubble cloud.

Steady state formulation for the simplified geometry cannot provide adequate description of the flow pattern inside the column, leading to the overestimated velocity value in the middle with fast velocity decrease towards the side walls. In contrast, transient simulation predicts well the velocity profile shape close to the outlet (0.25 and 0.35 m), but significantly underestimates peak velocity value which can be addressed to the overestimation of the bubble path dispersion. LES simulation, as expected, behaves better than unsteady RANS, but also unable to predict correctly the velocity profile close to the inlet which can be addressed to the insufficient mesh resolution.

5. Conclusion
Numerical simulations of the gravity-driven three-dimensional mono- and polydisperse bubbly flows inside the rectangular bubble column reactor were carried out. Obtained results were compared with available experimental and numerical results, feasibility of the proposed approach was verified.

It can be seen that under conditions provided the polydisperse treatment of the bubbly medium doesn't provide any advantages over monodisperse approach. Still, additional investigations should be made involving simulations for smaller bubbles or possibility of bubble’s interaction at higher concentrations.

Simulations on the simplified geometry which resulted in steady-state solution doesn't provide adequate prediction of the multiphase flow structure inside the whole domain. Transient approach provides better resolution of the flow inside the bubble column but overpredicts bubble dispersion and, as a result, underestimates velocity of the carried liquid. LES approach seems more promising, but requires detailed mesh to provide reasonable quality of the solution.

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