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Bubble induced turbulence model improved by direct numerical simulation of bubbly flow

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Highlights

- A single DNS simulation of deformable bubbly flow in a vertical channel is conducted
- Turbulence equations for different turbulent models are evaluated by the DNS data
- The bubble-induced turbulence model is re-evaluated based on DNS simulation

Abstract:

Direct numerical simulations (DNS) provide a description of turbulent flow fields at every point in space and time. Since every statistical quantity can be computed, this data should be useful for the development of closure models. In this paper, models for bubbly turbulent flows, in a two-fluid framework, are investigated using DNS data. A

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front tracking method is employed to simulate turbulent flow with deformable bubbles in a vertical channel. Quantities such as void fraction, average velocities, velocity fluctuations, and turbulence statistics are computed and presented. After processing the DNS data, the turbulence kinetic energy and dissipation equations, based on the k-ε model and explicit algebraic stress model (EASM), are analyzed. The model for bubble-induced turbulence, represented by source terms in the k and ε equations, is re-evaluated using coefficients derived from the DNS results. This work is a first step to show what can be done by using the DNS data to evaluate turbulence closure models. More simulations should be conducted in future works to further improve such models.

Key words:

Direct numerical simulation; Bubbly flow; Turbulence models; Two-fluid model; Explicit algebraic stress model

1 Introduction

Gas-liquid multiphase flows are commonly encountered in bubble columns, stirred tanks and other reactors. The complexity of multiphase turbulent flows causes significant difficulties for the design and scale-up of the reactors. CFD simulation is an effective tool to analyze and predict multiphase flow in reactors, and is widely used to aid design of industrial reactors. The development of suitable models and numerical methods for reliable simulation of multiphase flow characteristic is hence an important task.

Gas-liquid flow can be numerically investigated by various methods. For small-scale simulation of detailed turbulence and bubble movement, direct numerical simulation (DNS) with interface tracking methods such as volume of fluid, level-set or front tracking can be employed [1]. However, these techniques require large computational resources and are not applicable for modeling large industrial systems. For reactor scale simulation, the Euler-Euler two-fluid model is commonly used [2], coupled with the Reynolds-averaged Navier-Stokes (RANS) method. The two-fluid model is preferred for industrial multiphase flow simulation due to its simplicity and the lower computational effort required than for DNS simulations [3]. However, the accuracy of the predictions depends greatly on the closure models employed for the turbulence and the interfacial transfer. The closure model for the momentum transfer is very important for the two-fluid model and will affect the bubble distribution and the flow filed. The drag and lift forces are also of special importance among these interfacial forces for bubbly flow. A number of studies have been done either using experimental methods [4, 5] or CFD simulations [6-8]. Another important issue is the turbulence closure in the two-fluid model. The two-phase k-ε model is widely used to handle the turbulence in the two-fluid method. Though it is easy to carry out and the computational cost is very low in comparison with DNS, the main weakness of the k-ε model is that it fails to predict anisotropic flow, such as the flow in stirred tanks. Recently, Feng et al. [9] employed an explicit algebraic stress model (EASM) to simulate single phase turbulent flow in stirred tanks. The EASM model proposed by Pope [10] is derived from the Reynolds stress model and the Reynolds stress

components are expressed as algebraic correlations of the mean strain rate tensor, the rotation rate tensor and the turbulence quantities. Hence, the anisotropic characteristic is retained and the numerical stability is improved. For multiphase turbulent flow, Feng et al. [11, 12] extended the EASM to a two-phase model based on the two-fluid approach to simulate solid-liquid and liquid-liquid multiphase turbulent flow in stirred tanks. Satisfactory agreement with experimental data was found and the advantage of the EASM among turbulence models was demonstrated. Therefore, it is necessary to improve the accuracy of the closure models for the two-fluid model framework for industrial applications.

Before developing advanced closure relations, it is first necessary to understand the key multiphase turbulence characteristic. Experimental measurements of fluctuating liquid velocities and turbulent quantities become especially difficult in the presence of bubbles. DNS, used as a numerical experiment, is an excellent tool to identify and understand the complex multiphase turbulence mechanisms of interest. DNS simulations resolve all time and length scales of the turbulent flow and provide large amount of accurate data, which can be used to extract information for closing turbulence and interfacial transfer models. For gas-liquid simulation, a comprehensive review of DNS simulation of bubbly flows can be found in Tryggvason et al. [13]. More recently, advanced analysis techniques have also been employed to develop new models for bubbly flow. Ma et al. [14, 15] adopted a machine learning neural network technique to find closure relationships for an average two-fluid model based on DNS simulation of bubbly flows. Such techniques are expected to develop more accurate

models for specific systems.

For gas-liquid flows, the presence of bubbles will affect the structure and intensity of the local turbulence. In turn, the turbulence also has a strong impact on the bubble behavior, such as bubble dispersion, bubble coalescence and breakup. Therefore, turbulence closures for the two-fluid models need to take the bubble induced turbulence into account. There are two ways to introduce the effect of bubbles into liquid turbulence. Sato et al. [16] adopted an additional viscosity method, in which a viscosity due to the bubble motion is added to the shear induced turbulent viscosity to obtain an effect viscosity. Deen et al. [17] employed this method to simulate the gas-liquid flow in a stirred tank and it has also been used for a vertical pipe [18]. The other way is an additional source term method, in which source terms are added to the turbulence kinetic and energy dissipation equations [19]. This method is widely used for gas-liquid simulations in stirred tanks and other reactors [20, 21]. This model assumes that all energy lost by the bubbles due to drag is converted to turbulent kinetic energy in the wake of the bubbles. Many efforts have been made to improve this additional source method in turbulent transport equations [22, 23]. Rzehak et al. [19] proposed a new bubble-induced model and compared it with other models. Improved predictions for the turbulent kinetic energy were obtained by their new model. Politano et al. [23] also found that modifying the source term coefficients in the k and ε equations resulted in a more realistic profile for the turbulence kinetic energy. However, no general model has been presented in the literatures, due to the empirical and adjustable coefficients.

With the help of DNS simulations, the turbulent interface transfer can be identified and understood. It should, in particular, be possible to derive more general and accurate bubble induced models from the DNS data. Ilic [24] performed DNS to evaluate each term in the turbulent budget equation and determine the relative importance of the various terms under different conditions. Santarelli et al. [25] assessed existing closures for the modeling of the interfacial transfer term and proposed an improved model. Ma et al. [26] employed the SST turbulence model and derived improved coefficients for the source terms based on the DNS data. In most studies, the bubble induced models were derived based on analysis of the turbulent interface transfer term. Since turbulence models are used in the two-fluid method, it is better to derive the bubble induced model direct from an analysis of the turbulent equations for the different models. However, such models are seldom developed directly from the commonly used two-fluid k-ε model and no report has been found for the EASM model. Furthermore, spherical bubbles were used in most of the DNS simulations [25, 26], but the behavior of the deformable bubbles is quite different from the spherical bubbles. Bunner and Tryggvason [27] found that the turbulent kinetic energy induced by the deformable bubbles is larger than for spherical bubbles. Similar findings also show the effect of bubble deformation on turbulence [8, 28]. Feng and Bolotnov [8] evaluated the bubble induced turbulence and found that the magnitude of turbulence enhancement behind a bubble increases with the increase of the bubble deformability. However, only one bubble was simulated and no correlations of the bubble induced turbulence were proposed. Therefore, a bubble

induced model with improved coefficients accounting for the deformability of bubbles is not found in the literature.

In this study, bubble induced turbulence models are investigated by direct numerical simulations, in the context of the two-fluid k-ε model and the EASM model. First, the flow of deformable bubbles in turbulent flow in a periodic vertical channel is computed by a single direct numerical simulation using a front tracking method [1]. The flow field and other quantities of interest, at every temporal and spatial location, are given by the DNS results. The results are then used to find the various averages and statistical quantities in the model equations. Based on the DNS results and statistical analysis, a bubble induced turbulence model with re-evaluated coefficients is developed. This work is a first step in the use of the DNS data to evaluate turbulence closure model, and the development is based on only one DNS run. More studies should be done, considering different conditions, to enlarge the capability of the model for simulating practical gas-liquid flow in industrial reactors in future.

2 Numerical method

DNS simulation is used to follow the evolution of bubbly flow in a vertical channel between two parallel walls. A sketch of the flow configuration is shown in Figure 1. The flow is driven upward by a constant pressure gradient and gravity acts in the negative x direction. x, y and z represent streamwise, wall-normal, and spanwise directions, respectively. No-slip boundary condition is set at the walls. Periodic conditions are imposed in both the streamwise and the spanwise directions.

The parameters used in the calculation are given in Table 1. The computational

domain size is π×2×π/2 in computational units for the streamwise, wall-normal and spanwise directions, respectively. The computational units refer to the (arbitrary) dimensions used for the computations. Here, we define wall units by $l_0^+ = \nu_l / u^+$. ν_l is the viscosity of liquid and u^+ is the friction velocity which is given by $u^+ = \sqrt{\tau_w / \rho_l}$. At steady state, the average wall shear stress τ_w is related to the pressure gradient and the weight of the bubble/liquid mixture by a streamwise momentum balance

$$\tau_w = -\left(dP_0 / dz + \rho_{av} g\right) h = -\beta h, \tag{1}$$

which is found by taking a simple force balance for the whole domain. Here h is the half-width of the channel and β is a computational parameter which represents the driving force of the bubbly flow. Since the liquid and the bubbles are taken to be incompressible, ρ_{av} is constant, and the value of β is therefore constant. The direction of the flow depends on the sign of β, and $\beta<0$ leads to the upflow condition. In order to set β, we first have to give the friction Reynolds number, $Re^+ = u^+ h / \nu_l$. Here, we assume that the imposed pressure gradient does not change and set the β to insist that the friction Reynolds number is equal to 150. Then we get $u^+ = 0.0375$, $\tau_w = 0.0014$ and $\beta = -0.0014$. After this, the wall unit is calculated as $l_0^+ = 1/150 = 0.0067$. Therefore, the size of the channel is 471×300×235.5 for the present set up. The friction Reynolds number is 150, which is a little lager than the values used in Lu and Tryggvason [29, 30].

The mesh used for the simulation has 384, 256 and 192 grid points in the three directions, or about 19 million computational cells in total. The grid points are uniformly spaced in the spanwise and streamwise direction, but stretched in the

wall-normal direction to increase the resolutions at the walls. The grid spacing in wall unit is $\Delta x^+ = \Delta z^+ = 1.227$ and $0.675 \le \Delta y^+ \le 1.513$. 21 bubbles with diameter of 0.3 or 45 wall units are simulated. There are on average 36 grid points per diameter of the bubble. Thomas et al. [31] concluded that when the bubble was resolved with at least 20 nodes across bubble diameter, the interfacial forces between bubble and liquid could provide appropriate resolution.

A grid resolution study, is typically not done for DNS simulations because of the high computational cost for an individual run [8]. Here, we check the grid resolution in two ways. First, we can calculate the Kolmogorov length scale by using $\eta = \left(\nu_l^3 / \varepsilon\right)^{0.25}$. The turbulent energy dissipation rate can be estimated by $\varepsilon = \left(u^+\right)^3 / k y_b$. Here k=0.42 is the von Kármán constant and y_b is the bubble average distance from the wall, and is assumed to be 0.5 [30]. The energy dissipation rate is 2.511×10^{-4}, and the Kolmogorov length scale is 0.0158 or 2.370 wall units. The largest grid spacing in this work is 1.537 in wall units, which is smaller than the Kolmogorov scale. Besides, 36 grid points per diameter of the bubble are used in the simulation. In some recent works, about 25 grid points were used for DNS simulation of bubble flow [8, 30]. Therefore, we believe that the mesh used in this work is adequate for DNS simulation of the bubbly flow.

To make the simulations as easy as possible, the density of the bubbles is taken to be one-tenth of the liquid density. The dynamic viscosities of the bubbles and of the liquid are taken to be equal, so the kinematic viscosity of the bubbles is ten times that of the liquid, which is comparable to what it is for air and water. Although the

numerical values have been chosen for computational convenience, the system could be realized at least approximately by an aqueous solution of sugar in water [29]. The average void fraction is 0.03, since higher void fraction is likely to lead to bubble coalescence in real systems. The *Eo* and *Mo* number are commonly used to characterize the shape of bubbles or drops moving in a surrounding fluid, and are defined by

$$Eo = \frac{\rho_l g d^2}{\sigma} \quad ; \quad Mo = \frac{g \mu_l^4}{\rho_l \sigma^3}. \tag{2}$$

It can be expected that the bubbles will deform under these parameters.

A front-tracking method [1] is used to simulate the bubbly flow in a vertical channel, fully resolving the turbulent flow and the bubbles. The one-fluid formulation of the governing equation is the key to this method, by which the flow in the whole domain, including both the bubbles and the carrying liquid, is solved. The one-fluid Navier-Stokes equation can be written as

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot \mathbf{u}\mathbf{u} = -\nabla p + \rho \mathbf{g} + \nabla \cdot \left(\mu \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) + \int_F \sigma \kappa_f \mathbf{n}_f \delta(\mathbf{x} - \mathbf{x}_f) dA_f \tag{3}$$

The last term represents the interface force and only exists at the interface. The surface tension σ is taken to be constant and δ is a three-dimensional delta function constructed by repeated multiplication of one-dimensional delta functions; κ_f is twice the mean curvature, $\mathbf{n}_f$ is a unit vector normal to the front, $\mathbf{x}$ is the point at which the equation is evaluated, and $\mathbf{x}_f$ is the position of the front. This equation fully resolves the fluid flow around each bubble and accurately captures the movement and

deformation of the bubbles. The governing equation is solved by an explicit projection method on a fixed, staggered grid. The time term is discretized by second order scheme and a QUICK scheme is employed for the advection term.

In the front tracking method, the interface is tracked by connected marker points that are moved with the fluid velocity, interpolated from the fixed fluid grid. Once the marker points have been advected, an index function is constructed from the new interface location. The front is used to construct the density and viscosity fields and also to compute the surface tension, which is then smoothed onto the fluid grid and added to the discrete Navier–Stokes equations. As the interface deforms, the front is dynamically updated by adding and deleting points in order to fully resolve the interface. The method has been applied to several multiphase problems and validated in a number of ways. The original method has been described in detail by Tryggvason et al. [32] and implemented for fully three-dimensional flows, as well as for two-dimensional and axisymmetric ones. Applications and extensions of the method to homogeneous bubbly flows, atomization, flows with variable surface tension, solidification, and boiling were presented. The method was also compared to the Lattice Boltzmann method (LBM) and the comparison of the results showed excellent agreement [33]. Other numerical test and validations include the comparisons with analytical solution for simple problems [34], validation tests described by Esmaeeli and Tryggvason [35, 36] and comparisons with experiments [1, 37].

3 Results and discussion

3.1 DNS results for bubbly flow

3.1.1 Detailed DNS results

The DNS results give a detailed description of the flow at each time step and space location. At the initial time, the bubbles are spherical and distributed randomly in the computational domain. Then the simulation is run for a sufficiently long time (580 computational time units) so that the flow has reached a statistically steady state. The computations were continued so that various averages could be computed at the statistically steady state. The averaging was done for the time interval of 581-643, in computational units. Figure 2 shows the instantaneous bubble distribution and the flow field in the x-y plane at z=0.7854, at time t=581. A snapshot of the bubble distribution is shown in Figure 2(a). Iso-contours of the vertical velocity in the plane are also plotted. It can be seen that the deformable bubbles are distributed in the middle part of the channel. It should be noted that in the simulations presented here, we do not allow the bubbles to coalesce and breakup, which is reasonable when the average volume fraction is low. The flow with deformable bubbles is quite different from the situation with clean spherical bubbles, in which most of the bubbles move towards the wall due to lift force [6, 27]. The velocity changes most rapidly near the walls, but is relatively uniform in the middle. Figure 2(b) shows the instantaneous flow field. It is also clear that the flow is upward in the whole domain, driven by the pressure gradient. As the bubbles rise, the local structure of the flow field is changed due to the movement and deformation, as can be seen in detail in Figure 2(c).

Figure 3 shows the vortical structures in the channel by the λ-2 method [38] at three different times. The color of the vortices represents the vertical velocity. The

toroidal vortices around and behind the bubbles and a few vortex loops on the wall are clearly visible. This shows that some of the vortices are generated at the wall, and some by the bubbles. Feng and Bolotnov [8] also found that turbulent eddies were periodically generated on the surface of deformable bubbles. The turbulent eddies plotted by the Q-criterion are similar to our results. There are more vortex loops at the wall than in the middle, suggesting that more turbulence are generated at the wall. The bubble distributions at three times are similar, but the movement and deformation of each individual bubble are quite different, showing the instantaneous flow characteristic.

Before processing the DNS data, we have to ensure that the flow has reached the steady state. Two parameters, the flow rate and the wall shear stress, can be used to check whether the flow is steady. The flow rate Q and the average wall shear stress τ_w are calculated by

$$Q = \int_0^H \langle u \rangle \, dy \; ; \quad \tau_w = \mu_l \left. \frac{\partial \langle u \rangle}{\partial y} \right|_{y=0} \tag{4}$$

where A is the area of the walls. < > means an average over planes parallel to the wall. The flow rate is the integration of the plane-averaged velocity over the width of the channel. The wall shear stress is calculated using the shear rate at the wall. In Figure 4, the flow rate and the wall shear stress are showed for the time interval 581 to 643. At steady state, the wall shear should balance the pressure gradient and the weight of the mixture, as shown by Eq. 1. According to the equation, the theoretical value of the wall shear stress should be equal to $-\beta h$. In this work β is set to -0.0014 and h is the half-width of the channel which is 1. Therefore, the theoretical value of the wall shear

is 0.0014. It is shown that the flow rate is essentially constant and while the wall shear stress fluctuates slightly as the flow accelerates and decelerates, it is close to its theoretical value. The flow has been at steady state from time 581 to 643, which we use to collect data for averaging.

3.1.2 Averaged DNS results

The two-fluid model is derived by averaging the microscopic governing equations. In order to make the DNS data and the two-fluid model comparable, the DNS results are therefore processed by averaging operations. A commonly used average procedure for a quantity A over time or space is defined as

$$\overline{A} = \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} A dt, \quad \langle A \rangle = \frac{1}{|\Lambda|}\int_{\Lambda} A d\Lambda \tag{5}$$

where $\overline{\ }$ represents time average and < > means space average. Λ may be a line, a plane or a volume. Phase-weighted average is also employed to get the values for the liquid phase or the gas phase, and is given by

$$\overline{A_q} = \frac{\overline{A\phi_q}}{\overline{\phi_q}}, \tag{6}$$

where q represents a different phase: l for liquid and g for gas. ϕ is an indicator function such that ϕ_l=1 in the liquid phase and ϕ_l=0 in the gas phase. The turbulence quantities are based on the velocity fluctuations, which are given by

$$u' = u - \overline{u}. \tag{7}$$

After the averaging, the velocity, the void fraction, the fluctuations and any other quantity of interest can be calculated. The channel flow is almost homogeneous in the streamwise and the spanwise directions. Therefore, a plane average parallel to the

wall is often used. In this work, the quantities are processed by time and plane average for all the grid points in the streamwise and spanwise directions to obtain profiles along the wall-normal direction. Figure 5 shows the averaged void fraction, velocities and turbulence quantities across the channel.

Figure 5(a) shows that almost all the deformable bubbles are located in the middle of the channel, and there are almost no bubbles close to the walls. The mean streamwise velocities for both phases are shown in Figure 5(b), and are calculated by the phase-weighted average of the velocities from the DNS simulations. The velocity profile changes most rapidly near the walls, which is similar to a single phase channel flow and characteristic of typical turbulent flow. The slip velocity, obtained by taking the difference of the liquid and bubble velocities, is almost constant in the center of the channel, but is reduced at the walls. Figure 5(c) shows the root mean square velocities in three directions. The streamwise component is larger than the other two components. In the middle of the channel, it is about 1.47 times larger and the other components are almost identical. The profiles of the RMS velocity agree well with the DNS results from Kawamura and Kodama [39], in which the streamwise component is about 1.21 times larger than the other two. The results show that the flow is typically anisotropic, although the flow is homogeneous [8]. The turbulence are strong near the wall and reduces in the middle of the channel, indicating that the wall turbulence are still dominant, even when bubbles are present, which can also be found from the vortex distribution in Figure 3. The turbulence kinetic energy shown in Figure 5(d) gives the same profile as that in Figure 5(c), since it is calculated from the

normal Reynolds stresses. The energy dissipation rate obviously shows the highest value at the walls, and reduces in the middle of the channel.

3.2 Bubble induced turbulence model

3.2.1 Two phase *k*-*ε* model and EASM model

The bubble induced turbulence model is based on the Eulerian-Eulerian two-fluid method. First, we focus on the two phase *k*-*ε* model, which has been widely used in various multiphase flow simulations. The two phase model is an extension of the single phase model, in which the Reynolds stress is defined by the relationship

$$\overline{u'_{qi}u'_{qj}} = \frac{2}{3}k\delta_{ij} - \nu_t\left(\frac{\partial \overline{u_{qi}}}{\partial x_j} + \frac{\partial \overline{u_{qj}}}{\partial x_i}\right), \tag{8}$$

where k is the turbulence kinetic energy, ν_t is the turbulent viscosity, and subscript q represents different phases. We assume that the turbulent viscosity is given in the standard way by

$$\nu_t = C_\mu k^2 / \varepsilon, \tag{9}$$

where C_μ=0.09, and the turbulent kinetic energy and the energy dissipation rate in liquid phase are calculated by

$$k = \frac{1}{2}\overline{u'_{li}u'_{li}}; \qquad \varepsilon = -\nu_l\overline{\left(\frac{\partial u'_{li}}{\partial x_j} + \frac{\partial u'_{lj}}{\partial x_i}\right)\frac{\partial u'_{li}}{\partial x_j}}. \tag{10}$$

In the two-phase *k*-*ε* model, the k and ε in the liquid phase are assumed to be governed by evolution equations which at steady state are [40]:

$$\begin{aligned}
\nabla\cdot\left(\overline{\alpha_l}\rho_l\overline{\mathbf{u}_l}k\right) &= \nabla\cdot\left(\overline{\alpha_l}\frac{\mu_t}{\sigma_k}k\right) + \overline{\alpha_l}\left(\Pi - \rho_l\varepsilon\right) + S_k, \\
\nabla\cdot\left(\overline{\alpha_l}\rho_l\overline{\mathbf{u}_l}\varepsilon\right) &= \nabla\cdot\left(\overline{\alpha_l}\frac{\mu_t}{\sigma_\varepsilon}\varepsilon\right) + \overline{\alpha_l}\frac{\varepsilon}{k}\left(C_{\varepsilon 1}\Pi - C_{\varepsilon 2}\rho_l\varepsilon\right) + S_\varepsilon.
\end{aligned} \tag{11}$$

Here, α_l is the volume fraction of liquid, ρ_l is the density of liquid, $\mathbf{u}_l$ is the average liquid velocity, and $\mu_t=\nu_t\rho$. The standard values of the parameters are σ_k=1.0, σ_ε=1.3, $C_{\varepsilon 1}$=1.44, and $C_{\varepsilon 2}$=1.92. The turbulence production term is given by

$$\Pi = -\overline{u'_{li}u'_{lj}}\frac{\partial \overline{u_{li}}}{\partial x_j}. \tag{12}$$

The EASM is derived from RSM by tensor polynomial expansion theory. There is no turbulent viscosity when calculating the Reynolds stress. Instead, the Reynolds stress tensor is first expressed as an anisotropy tensor

$$\overline{u'_{qi}u'_{qj}} = \frac{2}{3}k\delta_{ij} + kb_{qij}. \tag{13}$$

The anisotropy tensor is given by

$$\begin{aligned} b_{qij} &= \beta_1 S_{ij} + \beta_3(\omega_{il}\omega_{lj} - \tfrac{1}{3}\eta_2\delta_{ij}) + \beta_4(S_{il}\omega_{lj} - \omega_{il}S_{lj}) \\ &+ \beta_6(S_{il}\omega_{lm}\omega_{mj} + \omega_{il}\omega_{lm}S_{mj} - \tfrac{2}{3}\eta_4\delta_{ij}) + \beta_9(\omega_{il}S_{lm}\omega_{mn}\omega_{nj} - \omega_{il}\omega_{lm}S_{mn}\omega_{nj}), \end{aligned} \tag{14}$$

where β_i are expansion coefficients and η_i are independent invariants, which can be found in Feng et al. [11, 12], along with further details. S_{ij} and ω_{ij} are the normalized mean strain rate tensor and the mean rotation rate tensor, respectively, which are defined in a two-phase formation as

$$S_{ij} = \frac{1}{2}\frac{k}{\varepsilon}\left(\frac{\partial \overline{u_{qi}}}{\partial x_j} + \frac{\partial \overline{u_{qj}}}{\partial x_i}\right), \quad \omega_{ij} = \frac{1}{2}\frac{k}{\varepsilon}\left(\frac{\partial \overline{u_{qi}}}{\partial x_j} - \frac{\partial \overline{u_{qj}}}{\partial x_i}\right). \tag{15}$$

The EASM also needs to solve the k and ε equations, but those are a little different from the k-ε model for the diffusion term, which are written as:

$$\begin{aligned} \nabla\cdot\left(\overline{\alpha_l}\rho_l\overline{\mathbf{u}_l}k\right) &= \nabla\cdot\left(\overline{\alpha_l}\rho_l c_k\frac{k^2}{\varepsilon}\nabla k\right) + \overline{\alpha_l}\left(\Pi - \rho_l\varepsilon\right) + S_k, \\ \nabla\cdot\left(\overline{\alpha_l}\rho_l\overline{\mathbf{u}_l}\varepsilon\right) &= \nabla\cdot\left(\overline{\alpha_l}\rho_l c_\varepsilon\frac{k^2}{\varepsilon}\nabla\varepsilon\right) + \overline{\alpha_l}\frac{\varepsilon}{k}\left(C_{\varepsilon 1}\Pi - C_{\varepsilon 2}\rho_l\varepsilon\right) + S_\varepsilon, \end{aligned} \tag{16}$$

where c_k=0.25 and c_ε=0.15, as suggested by Launder et al. [41]. The source terms are

the same as in the k-ε model.

Here, we use the additional source method to describe the influence of bubble on the turbulence, and add the source terms S_k and S_ε to the governing equations. These terms originate from the interfacial term in the turbulence budget equation, which represent the interfacial transport of turbulent kinetic energy, and account for the energy transfer into the liquid at the phase boundary due to the presence of bubbles [16]. It is expressed by a term related to the pressure fluctuations and a term related to the fluctuation of the viscous forces at the interface. Some researchers have used either DNS simulations [25, 26, 42] or experiment [43] to evaluate this term and also developed new models.

The starting point for the k-ε model or the EASM is averaging of the full Navier-Stokes equations and the averaging unavoidably results in loss of information. The various closure terms are intended to compensate for the missing information, in part and in an average sense, in such a way that the model predictions come as close as possible to the results of averaging the DNS results. While the advection, diffusion, production and dissipation terms in the model equations all follow directly from the structure of the original equations, some terms have to be modeled, based on dimensional analysis and intuition. The modeling of the interfacial transfer as additional source terms is, in particular, more speculative, but it seems reasonable to assume that it depends on the slip velocity between the phases and the void fraction or the area concentration. However, the availability of DNS data allows us to evaluate each term in the model equations and once the advection, diffusion, production and

dissipation terms have been computed, what remains are the interfacial source terms.

There are several approaches to model the interfacial transport and give the source terms, as reviewed by Ilic [24]. The most commonly encountered model for bubbly flow was proposed by Troshko and Hassan [22], based on the k-ε model. In this method, the interfacial term is modeled as the work of the interfacial force per unit of time, and only the drag force is taken into account. For the turbulence kinetic energy equation, the source term is given by

$$S_k = C_k S_{term}, \quad S_{term} = \left|\overline{\mathbf{F}}\right|\left|\left(\overline{\mathbf{u}_g} - \overline{\mathbf{u}_l}\right)\right|, \tag{17}$$

where C_k is an empirical parameter, and in the work of Troshko and Hassan [22], C_k is 1.0. Other researchers give different values for C_k. Pfleger and Becker [44] used C_k =1.44 and the bubble void fraction was multiplied by S_k term in the model. Olmos el al. [45] took C_k =0.75 and modified the expression for C_D by accounting for the effect of the mean void distribution. Recently, Santarelli et al. [25] proposed a C_k related to the turbulence kinetic energy. Ma et al. [26] modified the parameter assuming that it depends on the bubble Reynolds number.

The source term in the dissipation equation is given by

$$S_\varepsilon = C_\varepsilon \frac{\varepsilon}{k} S_k. \tag{18}$$

Several values have also been used for the parameter C_ε. C_ε=0.45 from Troshko and Hassan [22], C_ε=1.92 from Politano et al. [23], C_ε=2.0 from Rzehak and Krepper [19], and C_ε=0.3C_D from Ma et al. [26]. The coefficients in the previous models are either from experiments or from an analysis of the turbulent interface transfer term. In this work, the bubble induced model is derived from an analysis of the turbulent equation

of the two-fluid *k-ε* model and the EASM model using the DNS data. Besides, most of the studies above and the coefficients used in the model are based on spherical bubbles. Here, the bubbles can deform.

3.2.2 Turbulence models and DNS results

In order to develop improved two phase turbulence models, the results from the *k-ε* model and the EASM model are first calculated and compared with the DNS results. Figure 6 shows the Reynolds normal stress, the shear stress and the turbulence production computed by the two methods. For the normal stress simulation, it shows that the *k-ε* model cannot differentiate between the three directions due to its use of an isotropic turbulence viscosity. The DNS results show clearly the difference and the EASM captures this well, but the streamwise component is a little underestimated by the EASM, although still better than the *k-ε* model. The Reynolds shear stress and the production calculated by the *k-ε* model agree with the DNS results in the middle region of the channel, but have a large discrepancy at walls. Hosokawa et al. [43] analyzed the turbulence kinetic energy budget in bubbly flows in a vertical duct using experimental measurements. They compared the measured turbulence production with different turbulence models and also found that the *k-ε* model overestimated production significantly near walls but agreed well with the measurements in the middle. In contrast, the EASM predictions of the Reynolds shear stress and production agree well with the DNS data both in the middle of the channel and at walls. Therefore, the results show the superiority of the EASM when simulating the anisotropic flow in comparison with the *k-ε* model.

3.2.3 Coefficient of bubble induced model

All the terms in the k and ε equations of both k-ε model and EASM model, such as the advection term, the diffusion term, the production term and the dissipation term, can be computed from the DNS data. Then the source term is calculated from the balance equation (Eq. 11, 16), which is shown as "res" term. Figure 7 shows each term versus the wall-normal coordinate for both two models. Due to the large error in the calculation of the production term by the k-ε model, the "res" terms also vary significantly at the walls. The terms calculated by the EASM are more reasonable, and the differences between the terms are also shown clearly. Since the bubbles are distributed in the middle of the channel, and are rarely near the walls, the results near the walls are not considered in the following calculations.

After we get the "res" terms, we can also calculate the source terms in terms of the bubble induced model, shown as Eq. 17. The source term in the turbulent energy equation is considered first. Eq. 17 shows that the drag force and the slip velocity are needed. There are many ways to find the drag force, such as by empirical equations or from the DNS data by integration of pressure and viscous stress over the bubble surface. In this work, the drag force is calculated using an even simpler way directly from the DNS data. For a steady state bubbly flow, it can be assumed that the drag force is balanced by the buoyancy. The volume of the deformable bubble is known so the drag force can be calculated by the force balance. Then the drag force is distributed to each location according to the local volume fraction. Figure 8(a) shows the results for the "res" terms from the budget equations of the k-ε model and the

EASM, as well as the source term from the model, calculated by multiplying the drag force and the slip velocity without the coefficient. The coefficient can then be calculated simply by division of the two terms. The production term calculated by the DNS data is also plotted. It can be seen the production term is lower than the production by the bubbles in the middle of the channel. But the production term increases with the location closer to the wall, because of the rapid velocity changes near the wall. It is surprising to find that the bubbles seem to reduce the turbulence near the walls, but something similar is seen for drag reduction by deformable bubbles in turbulent flows, although we note that the slip velocity is very small for those situations. It is shown in Figure 8(a) that the source term and the "res" terms are almost flat and an average C_k can be obtained, which is given in Table 2. Figure 8(b) shows the source terms and the "res" terms in the energy dissipation equation for both models. We can also get an average C_ε from the results. It can be seen that the coefficients for the k-ε model is close to the values used in other works. However, the C_ε for the EASM model is quite different. It should be noted that when the EASM model is used, a matched coefficients of bubble induced model should also be adopted.

Most researchers have used a uniform value of the coefficient for the bubble induced model. Some works showed that the coefficients varied with other parameters such as bubble Reynolds number or local turbulent kinetic energy. Here, we show how the coefficient C_k varies with bubble Reynolds number $\mathrm{Re}_b = \left|\left(\overline{\mathbf{u}_g} - \overline{\mathbf{u}_l}\right)\right| d / \nu_l$. Since the DNS simulation can yield all the local values, the local C_k at each grid point with bubbles is calculated. Figure 9 shows how the C_k varies with Re_b. The trend

clearly shows that C_k decreases when the Re_b increases, which is different from what is seen for spherical bubbles [26]. If we use a simple power fitting, $y=ax^b$, for the variation of C_k with Re_b, we can get the values of a and b and also the R^2, shown in Table 2. Unfortunately, the R^2 for the fitting of k-ε model and EASM are only 0.3146 and 0.2556, respectively. The fittings are not good for both of the models. If we look close to the data shown in Figure 9, we see a significant scatter in the data and a deviation from the fitting line. There are two possible reasons. One is due to the averaging method used in this work. We do a time and phase average of the DNS data to get averaged variables at each grid point. The averaged data is analyzed in a two-fluid framework, but there are lots of locations with very low gas volume fraction, such as near the wall. Though most points are neglected when conducting the fitting, there are still lots of bad points. This may be improved if an unsteady analysis is made without time averaging. The other problem may result from the wrong choose of the variables for the fitting. The effect of bubble Reynolds number, turbulent kinetic energy or other variables on the coefficient is still unknown. More simulations with different conditions should be done to get more data in order to find reasonable correlations. When C_k has been established, C_ε can also be calculated from the source term in the turbulent dissipation equation. We find that the values of the coefficient calculated are also scattered and no correlations are made for the C_ε. The averaged values of the coefficients are listed in Table 2. For a bubble Reynolds number that varies from 100-400, the C_k calculated from the fitting equations varies from 0.2-6.3 for the k-ε model and 0.3-3.5 for the EASM. It can be seen that the averaged values calculated from each grid point is larger than the previous values. This is also attributed to the average method discussed above.

4 Conclusions

A single DNS simulation of bubbly flow in a vertical channel between two parallel walls is conducted. Based on the DNS data, the turbulence equations in the two-fluid model are examined and a bubble induced turbulence model with re-evaluated coefficients is presented for both the k-ε model and the EASM model. The present study is a very preliminary step, and the application of the model is limited to a gas-liquid system of specific *Eo* and *Mo* number with bubble Reynolds number from 100-400.The use of DNS to provide quantitative data to improve closure terms in model equations for the average flow is a topic of growing interest and the detailed information available should allow a thorough revaluation of existing model, adjustment of the various model parameters, and improvements of their structures. In addition, model predictions and experimental results can disagree for many reasons, including because of missing physical effects. DNS results are based on solving fully known equations, so there is no ambiguity in what physics is included. However, the number of DNS runs is limited by the huge computational cost, particularly if large range of parameters is considered. On one hand, DNS simulations depend on the development of fast supercomputer, but on the other hand, advanced data mining such as deep learning technology is also needed for future deep analysis of DNS data.

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Table 1. Calculation parameters

Domain Size(x_L,y_L,z_L)	π×2×π/2
Mesh (x,y,z)	384×256×192
Re^+(u^+)	150 (0.0375)
Re (U_b)	4200 (0.525)
Number of bubble	21
Bubble diameter	0.3
Density(fluid/bubble)	1/0.1
Viscosity(fluid/bubble)	2.5×10^{-4}/2.5×10^{-4}
Gravity	0.1
Surface tension	0.00225
Average void fraction	3%
Eo	4.0
Mo	4.4×10^{-8}

Table 2. Coefficients of model and fitting parameters

	C_k	C_ε	a	b	R^2	$C_{k,ave}$	$C_{\varepsilon,ave}$
k-ε model	0.693	2.0	252323.5	-2.291	0.3146	1.63	5.05
EASM	0.314	7.78	7382.2	-1.654	0.2556	0.99	18.74

List of tables and figures