QUANTITATIVE ANALYSIS OF LIQUID PHASE TURBULENCE KINETIC ENERGY EQUATION USING DNS DATA OF BUBBLE-TRAIN FLOW

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ABSTRACT

Our research concerns the investigation of bubble-induced turbulence using direct numerical simulation (DNS) of bubbly two-phase flow. DNS computations are performed for the bubble-driven liquid motion induced by a regular train of ellipsoidal bubbles rising through an initially stagnant liquid within a plane channel with two solid walls. DNS data are used to evaluate balance terms in the exact conservation equation for liquid phase turbulence kinetic energy. The evaluation comprises single-phase-like terms (diffusion, dissipation and production) as well as interfacial terms. Special emphasis is placed on the procedure for evaluation of interfacial quantities. Quantitative analysis of the conservation equation of liquid phase turbulence kinetic energy shows the importance of the interfacial terms which are the only source term. The results are further used to validate closure assumptions employed in modelling of the liquid phase turbulence kinetic energy transport in gasliquid bubbly flows. In this context, performance of respective closure relations in the transport equation for liquid turbulence kinetic energy within the twophase k- ε approach is evaluated.

1. INTRODUCTION

The relative motion of bubbles through liquid causes velocity fluctuations in the continuous phase. These fluctuations are induced not only by the nonlinearity of the flow, but also by the discrete buoyancy distribution of the gas phase, the wake motion behind the bubbles and the deformation of bubble interfaces. Such an agitation of the liquid motion gives rise to Reynolds stresses and associated phenomena inherent to turbulence. The phenomenon is called bubble-induced turbulence (BIT). Although BIT shares with ordinary turbulence the fluctuating character, its structure is essentially different from the single phase turbulence.

A large volume of experimental research covering various forms of bubbly flows has been published during last decades. In these investigations turbulence structure is considered as one of the key issues. Different trends have been observed. In most cases the liquid phase turbulence level is increased due to the bubble presence, but an unexpected phenomenon of turbulence suppression by bubbles is, also, reported (Serizawa, Kataoka and Michiyoshi, 1975).

Numerical studies of the phenomenon of BIT have, also, been accumulating quite rapidly last years (a brief overview is given in section 5 of this paper). However, reliable and general models for turbulence in bubbly flows are still missing. In approaches currently used it is common to extend respective transport equations of well-established single-phase turbulence models by closure terms that account for interfacial effects. These interfacial closure terms are modelled more or less empirically with little possibility to include details of basic flow mechanisms.

On the other side, significant progress has been achieved in analytical studies, i.e. in the derivation of basic equations of two-phase flows (Kataoka and Serizawa, 1989). Coupling this matter with recent great improvements in computer performances provided the basis for direct numerical simulations of two-phase flows (DNS). DNS of bubbly flow is based on local instantaneous field equations and auxiliary algorithms for tracking gasliquid interfaces and requires no empirical constitutive equations. Consequently, it offers a significant advantage in studying bubbly flow

dynamics, that is, the full information on the instantaneous three-dimensional flow field around bubbles and the interface topology is available. Although serious limitations concerning the number of bubbles that can be tracked are associated with DNS, this method opens a new promising way to get detailed insight into mechanisms governing BIT and validate existing mathematical models. Namely, important information on BIT can be obtained monitoring the effects of dispersed phase on simple well-investigated single-phase flows. Among these, the simplest case concerns studying liquid phase fluctuations induced by injection of gas bubble(s) into stagnant liquid since the generated fluctuating flow field is a result only of the bubble rise and the influence of the shear-induced turbulence is excluded. A prominent example of such a flow is encountered in bubble columns widely used in chemical and processing industry.

In this context, we performed DNS of bubble driven liquid motion induced by a regular train of ellipsoidal bubbles rising in a rectangular channel. The data obtained are used for statistical analysis of liquid velocity fluctuations. In this paper we present a quantitative analysis of the conservation equation of liquid phase turbulence kinetic energy (k_L) . The presentation is organised as follows. In section 2 an outline of the methodology employed to perform DNS of the bubble-train flow is presented. Further, geometrical and physical input parameters are given. Section 3 deals with theoretical considerations of the exact k_L equation. Methodology used for the evaluation of balance terms in this equation and corresponding results obtained using DNS data on the bubble-train flow are presented in section 4. Comparison of balance terms in the exact k_L equation with closure assumptions employed in the modelled form of this equation is given in section 5. All the results are accompanied by corresponding discussions. The paper is completed by conclusions.

2. DIRECT NUMERICAL SIMULATION OF BUBBLE-TRAIN FLOW

2.1. Mathematical and numerical background

The direct numerical simulations are performed with our in-house computer code TURBIT-VOF (Sabisch et al., 2001). The code is based on a single set of balance equations for the entire domain which express conservation of mass (equation 1) and momentum (equation 2) for two immiscible incompressible continuous Newtonian fluids:

$$\frac{\partial u_{\alpha}}{\partial x_{\alpha}} = 0 \tag{1}$$

$$\frac{\partial(\rho u_{\alpha})}{\partial t} + \frac{\partial(\rho u_{\alpha} u_{\beta})}{\partial x_{\beta}} = -\frac{\partial p}{\partial x_{\alpha}} + \frac{1}{Re_{ref}} \frac{\partial \tau_{\alpha\beta}}{\partial x_{\beta}} - \frac{(1-f)E\ddot{o}_{ref}}{We_{ref}} \frac{g_{\alpha}^{*}}{g^{*}} + \frac{\kappa n_{\alpha}a_{in}}{We_{ref}}.$$
(2)

The set of equations is completed with the transport equation for the liquid volumetric fraction:

$$\frac{\partial f}{\partial t} + \frac{\partial (u_{\alpha} f)}{\partial x_{\alpha}} = 0.$$
(3)

In the equations above subscripts α and β denote components of Cartesian coordinates. The equations are given in non-dimensional form. The following scaling applies:

$$\vec{x} = \frac{\vec{x}}{L_{ref}^*}; \quad \vec{u} = \frac{\vec{u}}{U_{ref}^*}; \quad t = \frac{t^* U_{ref}^*}{L_{ref}^*};$$

$$\rho = \frac{\rho^*}{\rho_L^*}; \quad \mu = \frac{\mu^*}{\mu_L^*} \text{ and } p = \frac{p^* - \rho_L^* \vec{g} \cdot \vec{x}}{\rho_L^* U_{ref}^{*2}},$$

where L_{ref}^* and U_{ref}^* are reference length and velocity, respectively, and * indicates a dimensional variable. The reference Reynolds (Re_{ref}), Weber (We_{ref}) and Eötvös ($E\ddot{o}_{ref}$) number are defined as:

$$\begin{split} Re_{ref} &= \frac{\rho_{L}^{*} U_{ref}^{*} L_{ref}^{*}}{\mu_{L}^{*}};\\ We_{ref} &= \frac{\rho_{L}^{*} L_{ref}^{*} U_{ref}^{*2}}{\sigma^{*}};\\ E\ddot{o}_{ref} &= \frac{(\rho_{L}^{*} - \rho_{G}^{*}) g^{*} L_{ref}^{*2}}{\sigma^{*}}. \end{split}$$

Using subscripts L and G to indicate quantities of the liquid and gas phase, respectively, the mixture velocity, density and viscosity are expressed as:

$$\vec{u} = \frac{f\rho_L \vec{u}_L + (1-f)\rho_G \vec{u}_G}{\rho}$$
$$\rho = f\rho_L + (1-f)\rho_G$$
$$\mu = f\mu_L + (1-f)\mu_G.$$

Note that \vec{u}_L and \vec{u}_G are not field quantities. However, when they are multiplied with f and (1-f), respectively, the corresponding products are defined for all time and space domains. Therefore, when a mesh cell is fully occupied by the liquid phase the expression for mixture velocity reduces to $\vec{u} = \vec{u}_L$ and in cells occupied only by the gas phase $\vec{u} = \vec{u}_G$. In interfacial cells where 0 < f < 1, the local homogeneous model is employed, i.e. the equality of phase velocities is assumed $\vec{u} = \vec{u}_L = \vec{u}_G$. The same holds for pressure.

The last term in equation (2) expresses the contribution of the surface tension force. There κ is the interface curvature, $\vec{n} = \vec{n}_G = -\vec{n}_L$ is the unit normal vector to the interface pointing from the gas into the liquid and a_{in} is the interfacial area concentration. Details of derivation of equations (1)-(3) are given in Wörner et al. (2001).

To account for the phase-interface evolution the volume fraction of the continuous phase is tracked using Volume of Fluid procedure. The liquid volumetric fraction is advected using equation (3) while the interface within a mesh cell is reconstructed using the PLIC (<u>Piecewise Linear</u> <u>Interface Calculation</u>) method EPIRA (for details see Sabisch et al., 2001).

2.2. Numerical setup

With the term 'regular bubble train' we indicate a quasi-steady flow pattern where bubbles rise with the same velocity through the channel whose length is much larger than its hydraulic diameter. Bubbles have an identical shape and are uniformly distributed along the channel. In such a situation one can extract a unit cell containing a single bubble that fully characterises bubble-train flow. Taking the dimensions of the computational domain equal to the size of the unit cell (see Figure 1), the bubble-train flow can be successfully simulated keeping the domain fixed and letting bubbles move through it. The presence and influence of the neighbouring unit cells can be taken into account imposing periodic boundary conditions in respective directions. The computational domain used in our DNS of bubble train flow is a cube of (non-dimensional) size $L_x \times L_y \times L_z = 1 \times 1 \times 1$. Boundary conditions are no-slip ones at the lateral rigid walls (z=0 and z=1) and periodic ones in vertical (x) and span-wise (y) direction. The domain is discretized by 64³ uniform mesh cells. The following parameters are specified: reference length L^*_{ref} =4m, reference velocity U^*_{ref} =1m/s, gravity g^* =9.81m/s², density ratio ρ_G^*/ρ_L^* =0.5, viscosity ratio μ_G^*/μ_L^* =1, bubble Eötvös number $E\ddot{o}_B$ =3.065, and Morton number $M=3.06\cdot10^{-6}$. According to these values reference dimensionless numbers are computed: reference Eötvös $E\ddot{o}_{ref}$ =49.05, Weber We_{ref} =2.5, and Reynolds number Reref=100.

Initially, a spherical bubble of the diameter $\frac{1}{4}$ is positioned in the middle of the channel filled with

stagnant liquid. Using the time step width Δt =0.0001 in total 65,000 time steps are computed. Within this time the gas-liquid system has reached the quasisteady state, where the mean velocity of the liquid phase and the bubble rise velocity can be considered as constant. Also, the bubble shape is steady: an axisymmetric ellipsoid with the axis aspect ratio 1.635. Bubble rises along an almost rectilinear path.



Figure 1. Geometry of computational domain.

3. CONSERVATION EQUATION OF LIQUID TURBULENCE KINETIC ENERGY

Under the assumption of incompressibility liquid phase turbulence kinetic energy is defined as:

$$k_L = \overline{u_{L\alpha}^{'2}}/2 \; .$$

For a gas-liquid flow, the production, dissipation and transport of the liquid phase turbulence kinetic energy, k_L , and its interplay with flow parameters such as velocity field, phase distribution, and interfacial structures is mathematically described by the following balance equation (Kataoka and Serizawa, 1989):

$$\frac{D}{Dt} \left(\overline{\Phi_{L}} k_{L} \right) = \frac{\partial \left(\overline{\Phi_{L}} \overline{p_{L}} u_{L\alpha} \right)}{\partial x_{\alpha}} - \frac{\partial \left(\frac{1}{2} \overline{\Phi_{L}} \overline{u_{L\alpha}^{2}} u_{L\beta}^{2} \right)}{\partial x_{\beta}} + \frac{1}{Re_{ref}} \frac{\partial \left(\overline{\Phi_{L}} \frac{\partial k_{L}}{\partial x_{\beta}} \right)}{\partial x_{\beta}} \\ - \overline{\Phi_{L}} \overline{u_{L\alpha}^{2}} u_{L\beta}^{2} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} - \frac{1}{Re_{ref}} \overline{\Phi_{L}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{p_{Lin}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\alpha}^{2}} a_{in} + \frac{1}{Re_{ref}} \overline{u_{Lin\alpha}^{2}} \frac{\partial u_{L\alpha}^{2}}{\partial x_{\beta}} n_{Lin\beta} a_{in} \\ - \overline{p_{Lin\alpha}^{2}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{p_{Lin\alpha}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\alpha}^{2}} a_{in} + \frac{\partial \overline{u_{L\alpha}^{2}}}{Re_{ref}} \overline{u_{Lin\alpha}^{2}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{p_{Lin\beta}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\beta}^{2}} n_{Lin\beta} a_{in} \\ - \overline{p_{Lin\beta}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\beta}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\beta}^{2}} u_{Lin\beta}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{p_{Lin\beta}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\beta}^{2}} u_{Lin\alpha}^{2} \overline{n_{Lin\beta}^{2}} u_{Lin\beta}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{p_{Lin\beta}^{2}} u_{Lin\alpha}^{2} \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \\ - \overline{u_{L\alpha}^{2}} u_{L\alpha}^{2} - \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^{2}}}{\partial x_{\beta}} \frac{\partial \overline{u_{L\alpha}^$$

This equation is obtained using basic conservation equations for the fluctuating components of mass and momentum whose derivation is based on the local instant and averaged formulations of gas-liquid two-phase flow. Therefore, the equation (4) is the exact k_L equation.

The following notation is used. Subscript *in* denotes liquid phase quantities at the gas-liquid interface and Φ_L is the characteristic function of the liquid phase. The single overbar indicates averaging and the double overbar indicates phaseweighted averaging that is for an arbitrary physical quantity, A_L , defined as:

$$\overline{\overline{A_L}} = \overline{A_L \Phi_L} / \overline{\Phi}_L \; .$$

Fluctuating parts of physical quantities (denoted by ' in equation 4) are evaluated as:

$$A_{L}^{'} = A_{L} - \overline{A_{L}}$$
 and
 $A_{Lin}^{'} = A_{Lin} - \overline{A_{L}}$,

where A_L and A_{Lin} are instantaneous values of considered quantity within the cell containing liquid and at the *L* side of the interface, respectively.

On the right-hand-side of equation (4) two distinguishing groups of terms appear. The first one is the group of terms associated with the mean liquid volumetric fraction, $\overline{\Phi}_L$. Except for being multiplied with $\overline{\Phi}_L$, these terms are basically of the same form as the ones involved in the single-phase turbulence kinetic energy equation. Therefore, one can recognize diffusion, production and dissipation term. For this reason these are called single-phase-like terms. The last two terms associated with the interfacial area concentration, a_{in} , represent interfacial turbulence transport due to bubbles and are called interfacial terms.

4. EVALUATION OF BALANCE TERMS IN EXACT k_L EQUATION

4.1. Averaging procedure

In the problem considered the bubble rises in vertical (x) direction. Since all the analyses performed concern developed flow regime, the mean velocity of the liquid phase in x direction is constant, i.e., averaged quantities show no gradients in this direction. Besides this, when periodic boundary conditions at the inlet/outlet of the channel are taken into account, one may claim that the turbulence structure along a certain x line (y=const, z=const) is

homogeneous. In such a situation averaging along x lines can be applied. In the context of the equation 4 this line averaging corresponds to the single overbar). The procedure is here demonstrated on the example of evaluation of the mean liquid volumetric fraction:

$$\overline{\Phi}_L = \overline{\Phi}_L^i(j,k) = \sum_{i=1}^{IM} f(i,j,k) / IM ,$$

where: f is the local liquid volumetric fraction, IM is the number of cells in x direction and i, j, k are mesh cell indices in x, y and z direction, respectively.

4.2. <u>Evaluation of liquid phase interfacial</u> <u>quantities</u>

Using the DNS data provided by TURBIT-VOF in procedures described in the text above one can evaluate all the single-phase-like terms in equation (4). On the other side, for the evaluation of interfacial terms some additional information is necessary. Namely, TURBIT-VOF simulations provide the data on the pressure and velocity in interfacial cells. However, since these cells are occupied with two-phase mixture, and locally homogeneous two-phase flow model is used, these data can not be used as representative quantities of the liquid phase at the interface.

The problem of determining the liquid interfacial pressure, p_{Lin} , is solved assuming that it is equal to the pressure in a neighbouring cell fully occupied with liquid phase.

The procedure used for evaluation of the liquid phase interfacial velocity, \vec{u}_{Lin} , is more complicated and is here shortly outlined. Since no phase change is considered, the phase interfacial velocities are equal and the following notation is used hereafter:

$$\vec{u}_{Lin} = \vec{u}_{Gin} = \vec{u}_{in} .$$
 (5)

The velocity u_{in} can be split into its tangential, u_{int} , and normal, \vec{u}_{inn} , component:

$$\vec{u}_{in} = \vec{u}_{int} + \vec{u}_{inn} \,. \tag{6}$$

Tangential component is defined to be equal to the tangential velocity of a fluid particle lying at the interface (Ishii, 1975). As in our case interfacial cells contain two-phase mixture, \vec{u}_{int} is set to be equal to the tangential component of the mixture velocity \vec{u}_t :

$$\vec{u}_{int} = \vec{u}_t = \vec{u} - \left(\vec{u} \cdot \vec{n}_L\right) \cdot \vec{n}_L \,. \tag{7}$$

The normal component of interfacial velocity can be presented in the following way:

$$\vec{u}_{inn} = \left(\vec{u}_{in} \cdot \vec{n}_L\right) \cdot \vec{n}_L \,. \tag{8}$$

The projection of interfacial velocity on the normal vector is given as (Kataoka, 1986):

$$\vec{u}_{in} \cdot \vec{n}_L = \frac{\partial F/\partial t}{\sqrt{\left(\partial F/\partial x\right)^2 + \left(\partial F/\partial y\right)^2 + \left(\partial F/\partial z\right)^2}}$$
(9)

where: F(x, y, z, t) = 0 is the equation of the gasliquid interfacial surface. In TURBIT-VOF at any time step, the interface is defined via the unit normal vector, $\vec{n}_L(n_{Lx}, n_{Ly}, n_{Lz})$, and a point lying on the interface, $M(b_x, b_y, b_z)$ (Sabisch et al., 2001):

$$F(x, y, z, t) = (b_x - x) \cdot n_{Lx} + (b_y - y) \cdot n_{Ly} + (b_z - z) \cdot n_{Lz} = 0.$$
 (10)

Therefore, the problem of determining $\partial F/\partial t$ arises. The procedure applied for solving this problem is as follows. Consider two subsequent time steps t_0 and $t_1=t_0+\Delta t$ in which the interfacial surface passes through the point $M_0(b_{x0},b_{y0},b_{z0})$ and through the point $M_1(b_{x0}+\partial x,b_{y0}+\partial y,b_{z0}+\partial z)$, respectively, i.e. the surface equation satisfies:

$$F(b_{x0}, b_{y0}, b_{z0}, t_0) = 0$$
(11)
$$F(b_{x0} + \delta x, b_{y0} + \delta y, b_{z0} + \delta z, t_0 + \Delta t) = 0.$$
(12)

If the distance between
$$M_0$$
 and M_1 is small, function F given by equation (12) can be expanded into a Taylor series. Assuming that terms of second and higher order in this expansion can be neglected, after some simple mathematical rearrangements, one obtains the expression for the time derivative of function F needed in equation (9):

$$\frac{\partial F}{\partial t} = -\frac{1}{\Delta t} \left(n_{Lx0} \delta x + n_{Ly0} \delta y + n_{Lz0} \delta z \right).$$
(13)

In practice, the evaluation of equation (13) from our DNS data is not straightforward. The problem appears because the data in restart files are available only for certain time instances (here for every 500th). The data required in equation (13), i.e. coordinates of the point M_1 are determined as follows. Firstly, the advection algorithm implemented in TURBIT-VOF is employed. After this, the data on liquid volumetric fraction at time

 $t_0+\Delta t$ are known and the TURBIT-VOF reconstruction step can be performed providing the information on position of the point M_1 .

4.3. Balance of k_L equation for bubble-train flow

Before presenting results for the balance terms in the k_L equation we give profiles of turbulence kinetic energy itself. Thus, in Figure 2 wall-normal profiles of k_L evaluated using the DNS data on the bubble-train flow are presented.



Figure 2. Wall-normal profiles of turbulence kinetic energy (displayed with dimension $[m^2/s^2]$) for the following span-wise positions, $y: \bullet 0.492 \bullet 0.523$ $\bullet 0.555 \lor 0.586 \diamondsuit 0.617 \blacktriangleleft 0.648$.

In Figure 3 wall-normal profiles of the terms on the right-hand-side of the exact k_L equation for different span-wise positions are presented. The following can be observed. Profiles of all the terms are symmetric with respect to the channel axis. Nonzero values of all the terms are noticed only in the central part of the channel, i.e. in the domain where bubbles are rising. Strong gradients of the liquid phase quantities in the region between the part of the channel through which bubbles rise and the one that is always occupied with liquid phase cause sharp peaks of all the terms at these locations. These peaks are especially remarkable for the diffusion term. In Figure 3 one can see that both, the profiles of the mean gas volumetric fraction, $\overline{\Phi_{G}} = 1 - \overline{\Phi_{L}}$, and the balance terms, are continuous, but not continuously differentiable. Consequently, the peaks are expected to be reduced in a bubbly flow with smoother profiles of $\overline{\Phi_{a}}$, i.e. when instead of the bubble-train a bubble swarm flow is considered.

The term that is called production, and in shear flows is always positive, is negative here.



Figure 3. Wall-normal profiles of balance terms in equation (4) calculated for different span-wise positions. Legend: \blacksquare diffusion, \bullet production, \blacktriangle dissipation, \checkmark interfacial terms calculated from equation (4) \blacklozenge interfacial terms estimated from equation (14). Balance terms from k_L equation are displayed with dimension $[m^2/s^3]$. Mean value of gas phase volumetric fraction is represented by solid red line.

Although this result can seem surprising and bring into discussion the name of this term, physics lying behind it is easy to understand taking into account that the movement of the liquid phase is caused by rising bubbles, i.e. that the energy in the liquid flow is transferred from the fluctuating velocity field caused by moving bubbles to the mean flow.

Taking into account that the diffusion term does not have any net contribution, but represents the redistribution of turbulence kinetic energy over the flow domain, the following can be stated. In the case of the bubble driven liquid motion considered here the turbulence kinetic energy of liquid phase is gained only by interfacial terms, while it is lost not only through the dissipative, but also through the production term (magnitude of production is lower than that of dissipation). This conclusion confirms the importance of studying the interfacial terms.

For a fully developed flow the magnitude of the terms on the left-hand-side of equation (4) is approximately zero. Consequently, the magnitude of interfacial terms can be estimated via the sum of the single-phase-like terms, i.e.:

$$IF_{balance} = -(D + P + \varepsilon), \qquad (14)$$

where D is diffusion, P is production and ε is dissipation term. Comparison of results obtained applying equation (14) with the interfacial terms evaluated according to equation (4) shows good agreement in the central part of the channel. Discrepancies appear at the bubble hips due to already mentioned strong gradients of liquid phase quantities in these regions. This situation becomes evident in Figure 3 in the graph for span-wise position y=0.648.

5. EXACT VERSUS MODELLED k_L EQUATION

In engineering applications turbulence models with a modelled form of liquid phase turbulence kinetic energy equation are employed. Among these the most popular approach employs the two-phase k- ε model that is derived by an extension of the well known single-phase k- ε model. Turbulence kinetic energy equation in the two-phase k- ε model contains closure assumptions for diffusion and production terms (dissipation is modelled by separate transport equation) and a model term that accounts for the existence of gas-liquid interfaces. A short overview of corresponding approximations follows.

5.1. <u>Overview of closure assumptions in modelled</u> <u>*k_L* equation</u>

Closure assumptions used for modelling the production term are given in Table 1 and the ones for the diffusion term in Table 2. The following notation is used: *I* is the unit tensor, $\overline{S}_{L\alpha\beta}$ is the mean strain rate imposed to the liquid phase and v_L^t is the eddy viscosity expressed in the same way as in the single-phase $k - \varepsilon$ model: $v_L^t = 0.09k_L^2/\varepsilon_L$. It is noted that, due to the normalisation, reference Reynolds number appears instead of the molecular viscosity.

Several authors dealt with modelling interfacial terms. All of them use the approach that the interfacial terms in k_L equation can be expressed as the work of interfacial forces. In these models the contribution of the work of drag force, W^D , is considered to be dominant one.

Table 1. Closure assumptions for production term used in k_L equation of two-phase k- ε model.

	Reference	Production term [-]	
P1	Troshko and Hassan, 2001; Morel, 1997; Hill et al.,1995;	$\alpha_{L}\left[2v_{L}^{t}\overline{S}_{L\alpha\beta}k_{L}-\frac{2}{3}\left(k_{L}+v_{L}^{t}\frac{\partial\overline{u}_{L\alpha}}{\partial x_{\beta}}\right)I\right]\frac{\partial\overline{u}_{L\alpha}}{\partial x_{\beta}}$	
P2	de Bertodano et al., 1994; Boisson and Malin, 1996; Lain et al., 2001 ;	$\alpha_{L} \Big[2\nu_{L}^{t} \overline{S}_{L\alpha\beta} \Big] \frac{\partial \overline{u}_{L\alpha}}{\partial x_{\beta}}$	
Р3	Pfleger and Becker, 2001; Grienberger and Hofmann, 1992; Svendsen et al.,1992;	$\alpha_{L}\left[2\left(\frac{1}{Re_{ref}}+v_{L}^{t}\right)\overline{S}_{L\alpha\beta}\right]\frac{\partial\overline{u}_{L\alpha}}{\partial x_{\beta}}$	

Table 2. Closure assumptions for diffusion term used in k_L equation of two-phase $k - \varepsilon$ model.

	Reference	Diffusion term [-]	
D1	Lain et al.,2001; Pfleger and Becker,2001; Svedsen et al. 1992; Grienberger and Hofmann, 1992; Hill et al. 1995;	$\frac{\partial}{\partial x_{\beta}} \left[\alpha_{L} \cdot \left(\frac{1}{Re_{ref}} + \frac{v_{L}^{t}}{\sigma_{k}} \right) \cdot \frac{\partial k_{L}}{\partial x_{\beta}} \right]$	
D2	Lopez de Bertodano et al.,1994; Morel, 1987; Troshko and Hassan, 2001; Boisson and Malin, 1996;	$rac{\partial}{\partial x_eta} igg(lpha_{_L} \cdot rac{oldsymbol{v}_{_L}^{\iota}}{oldsymbol{\sigma}_{_k}} \cdot rac{\partial k_{_L}}{\partial x_eta} igg)$	

Reference		$M_{L\alpha}^{D}$ [-]	$C_{D}[-]$
Morel, 1997	$M^{D}_{Llpha}\overline{u}_{Rlpha}$	$\frac{3}{1}\alpha_{G}\frac{C_{D}}{2}\overline{U}_{R}\overline{u}_{R\alpha}$	$\frac{2}{3}\sqrt{E\ddot{o}_{\scriptscriptstyle B}}\cdot f(\alpha_{\scriptscriptstyle L})$
de Bertodano et al.,1994		$4 \circ D_b$	not given
Pfleger and Becker, 2001	$1.44 \alpha_L M_{L\alpha}^D \overline{u}_{R\alpha}$		0.44
Svendsen et al., 1992	$0.75 M_{L\alpha}^{D} \overline{u}_{R\alpha}$	not given	
Hill et al., 1995	$\frac{3}{4} \frac{\alpha_G C_D}{D_b} \overline{U}_R \left(\frac{\overline{u}_{R\alpha} \partial \alpha_G / \partial x_\alpha}{0.3 R e_{ref} \alpha_L \alpha_G} + 2k_L (C_t - 1) \right)$	not contained explicitly in expression for W^D	$\frac{2}{3}\sqrt{E\ddot{o}_{\scriptscriptstyle B}}\cdot f(\alpha_{\scriptscriptstyle L})$

Table 3. Contribution of the work of drag force in interfacial terms

Different approaches used to express W^D are listed in Table 3. The following notation is used: $\overline{U}_R = \sqrt{\overline{u}_{R\beta}\overline{u}_{R\beta}}$ is the intensity and $\overline{u}_{R\alpha} = \overline{u}_{G\alpha} - \overline{u}_{L\alpha}$ is α component of the mean relative velocity, $\alpha_L = \overline{\Phi}_L$ and $\alpha_G = 1 - \overline{\Phi}_L$ are volumetric fraction of the liquid and gas phase, respectively; C_D is the drag coefficient and D_b denotes the equivalent bubble diameter. Function $f(\alpha_L)$ is defined as:

$$f(\alpha_L) = \left\{ (1 + 17.67\alpha_L^{1.3}) / (18.67\alpha_L^{1.5}) \right\}^2.$$

For the definition of C_t in model of Hill et al. (1995) see the corresponding reference.

The contribution of the work of other interfacial forces is neglected by most of the authors. Only Morel (1997) took into account work of the added-mass force:

$$W^{AM} = \frac{1}{2} \left(\overline{u}_{G\alpha} - \overline{u}_{L\alpha} \right) \frac{1 + 2\alpha_G}{\alpha_L} \alpha_G \left(\frac{D_G \overline{u}_{G\alpha}}{Dt} - \frac{D_L \overline{u}_{L\alpha}}{Dt} \right).$$

5.2. <u>Validation of closure assumptions employed</u> in modelled k_L equation

Using DNS data on bubble-train flow both the single-phase-like (production and diffusion) and interfacial terms are evaluated employing the closure assumptions presented in Tables 1-3. When results are compared with terms evaluated via the exact k_L equation the following can be seen.

According to all the closure assumptions listed in Table 1 positive values of production term are evaluated, that is opposite to the exact one which is always negative (see Figure 4). The exact production term is almost zero in the central part of the channel. On the other side non-zero values within this domain are evaluated by models, especially when the molecular viscosity is taken into account (model P3 in Table 1). In Figure 5 the comparison between the wallnormal profiles of the exact and modelled diffusive term is given. A strong underestimation of this term is obtained when closure relations given in Table 2 are employed. Analysing the profiles of sub-terms contained in the exact diffusive term, we observed that the pressure correlation dominates the triple correlation and molecular diffusion. In k- ε model the pressure diffusion term is, however, grouped with the triple correlation and the sum assumed to behave as a gradient-transport process:

$$\frac{1}{2}\overline{\overline{u_{L\alpha}^{'2}u_{L\beta}^{'}}} + \overline{\overline{p_{L}^{'}u_{L\beta}^{'}}} \propto -v_{L}^{\prime}\frac{\partial k_{L}}{\partial x_{\beta}}$$

From the results presented here the following can be stated: the closure relation for pressure correlation used in the k- ε model is not appropriate for bubble driven liquid flows. A similar observation was reported by Wörner and Grötzbach (1998) who analysed DNS data on the single-phase natural convection in horizontal fluid layers.

Finally, some encouraging results concerning modelling interfacial terms are presented in Figure 6. Namely, when the profiles of these terms evaluated from the model of Morel (1997) are compared to the ones obtained according to the exact expression, great discrepancies are not observed. Taking into account the high lateral inhomogenity of the flow field considered here (only one bubble within computational domain), one can expect that the model of Morel (1997) will give even better results for the case of the liquid motion driven by bubble swarms.

It is noted that the contribution of the work of added-mass force is an order of magnitude lower than that of drag force. This result seems reasonable since the evaluation is performed only for the steady flow regime.

Both the model of Hill (1995) and the model of Pfleger and Becker (2001) underestimated the magnitude of interfacial terms.



Figure 4. Wall-normal profiles of production term (dimension $[m^2/s^3]$) at y=0.586. Exact term is denoted by \blacksquare and models from Table 1 by: $\blacktriangle P1 \bullet P2 \lor P3$.



Figure 5. Wall-normal profiles of diffusion term (dimension $[m^2/s^3]$) at y=0.586. Exact term is denoted by \blacksquare and models from Table 2 by: \bigcirc D1 \blacktriangle D2.



Figure 6. Wall-normal profiles of interfacial terms (dimension $[m^2/s^3]$) at different span-wise positions, y. • indicates exact term. Model assumptions listed in Table 3 are denoted as: • Morel (1997) A Pfleger and Becker (2001) • Hill et al. (1995). The black solid line represents mean gas volumetric fraction.

Comparison of forms of models proposed by Morel (1997) and Pfleger and Becker (2001) and their performances for the case of the bubble-train flow revealed the following. In both approaches the same definition of the drag force is used. Pfleger and Becker (2001) try to incorporate the characteristics of the flow introducing liquid volume fraction, α_l , in the expression for the work of the drag force, W^{D} . On the other side, they use the constant value of the drag coefficient, $C_D=0.44$. Morel (1997) applies 'standard' definition of the work of the drag force. However, through the correlation for C_D not only the global flow characteristics are taken into account (through α_L and α_G), but also some of the local details concerning bubbles (through $E\ddot{o}_B$). Since this approach gave better results a conclusion can be drawn: in the development of improved model assumptions for evaluation of interfacial terms in modelled turbulence kinetic energy equation details of local flow features should be incorporated as much as possible.

6. CONCLUSION

The present paper deals with the quantitative analysis of the conservation equation for the turbulence kinetic energy of the liquid phase (k_L equation). According to this equation there are two governing mechanisms which determine the turbulence characteristics. The first group of terms is associated with liquid phase volumetric fraction and includes turbulence energy diffusion, dissipation and production terms. The other group of terms is associated with the interfacial area concentration and is thus peculiar to two-phase flow systems.

To provide the data for the analysis, direct numerical simulations of a regular train of ellipsoidal bubbles rising through an initially stagnant liquid are performed using the computer code TURBIT-VOF.

The analysis of the budget of the liquid phase turbulence kinetic energy reveals the importance of interfacial terms. Namely, these terms are the only source of turbulence kinetic energy. Surprisingly, the production term is negative. In the diffusive term the contribution of the pressure correlation is dominant.

The present analysis is further used for scrutiny and validation of closure assumptions employed in k_L equation of two-phase k- ε model. As concerns the case of the bubble-train flow studied here, the conventional modelling of production and diffusion terms totally fails: the production term predicted by models is positive while it should be negative and the diffusive term is strongly underestimated. When modelled interfacial terms are tested against the exact ones the importance of taking into account local flow details is recognised. The model of Morel (1997) includes some of these information through the correlation for coefficient of the drag force. The interfacial terms evaluated using

this model showed rather good agreement with the exact ones. Closure assumptions used by other authors did not perform well.

Finally, one can argue that the case of regular bubble train considered in this paper is somewhat academic and this can be the reason why certain models do not perform well. However, this flow configuration is convenient for developing the computational tool to perform the quantitative analysis of the exact k_L equation and the validation of closure relationships employed in its modelled form. In future work we intend to apply the presented methodology to the case of liquid motion induced by a rising bubble swarm.

REFERENCES

Boisson, N. and Malin, M.R., 1996, Int. J. Numer. Methods Fluids, Vol. 23, pp. 1289-1310

- Lopez de Bertodano, M., Lahey, R.T., Jr. and Jones, O.C., 1994, J. Fluids. Eng. Trans. ASME, Vol. 116, pp. 128-134
- Grienberger, J. and Hofmann, H., 1992, Chem. Eng. Sci., Vol. 47, pp. 2215-2220

Hill, D.P., Wang, D.M., Gosman, A.D. and Issa, R.I., 1995, Proc. of 2nd Int. Conf. Multiphase Flow, Kyoto, Japan

Ishii, M., 1975, *Thermo-fluid Dynamic of Two-phase Flow*, Eyrolles, Paris

Jakobsen, H.A., Sannaes, B.H., Grevskott, S. and Svedsen, H.F., 1997, Ind. Eng. Chem. Res., Vol. 36, pp. 4052-4074

Kataoka, I., 1986, Int. J. Multiphase Flow, Vol. 5, pp. 745-758

Kataoka, I. and Serizawa, A., 1989, Int. J. Multiphase Flow, Vol. 15, pp. 843-855

Lain, S., Bröder, D., Sommerfeld, M. and Göz, M.F., 2002, Int. J. Multiphase Flow, Vol. 28, pp. 1381-1407

Morel, C., 1997, 11th Symposium on Turbulent Shear Flows, Grenoble, France, pp. P3.10-16

Pfleger, D. and Becker, S., 2001, Chem. Eng. Sci., Vol. 56, pp. 1737-1747

Sabisch, W., Wörner, M., Grötzbach, G. and Cacuci, D.G., 2001, Proc. of 4th Int. Conf. Multiphase Flow, New Orleans, USA.

Serizawa, A., Kataoka, I. and Michiyoshi, I., 1975, Int. J. Multiphase Flow, Vol.2, pp. 235-246

Svedsen, H.F., Jakobsen, H.A. and Torvik, R., 1992, Chem. Eng. Sci., Vol. 47, pp. 3297-3304

Troshko, A.A. and Hassan, Y.A., 2001, Int. J. Multiphase Flow, Vol. 27, pp. 1965-2000

Wörner, M. and Grötzbach, G., 1998, Int. J. Heat Fluid Flow, Vol. 19, pp. 150-158

Wörner, M., Sabisch, W., Grötzbach, G. and Cacuci, D.G., 2001, Proc. of 4th Int. Conf. Multiphase Flow, New Orleans, USA.