Wissenschaftliche Kurzmitteilung für Chemie Ingenieur Technik

Themenheft „Campus Blasensäulen”

Manuscript number: cite.201200243

Revised version

Toward improved closure relations for the turbulent kinetic energy equation in bubble-driven flows

Zur Entwicklung verbesserter Schließungsbeziehungen für die turbulente kinetische Energiegleichung in Blasen-getriebenen Strömungen

Martin Wörner[1,*], Sercan Erdogan[1]

[1]Karlsruher Institut für Technologie, Institut für Katalyseforschung und -Technologie

Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Deutschland

* Correspondence concerning this article should be address to Dr. M. Wörner

E-mail: martin.woerner@kit.edu, Phone +49 721 608 24477, Fax: +49 721 608 24837

Abstract

There is a considerable interest, within both academia and industry, to develop improved computational fluid dynamic methods for gas-liquid flows in bubble columns in order to support their scale up and optimal design. One main model limitation in current Eulerian two-fluid and multi-fluid models concerns adequate closure relations for turbulence in bubble-driven flows. This article highlights some special features of bubble-induced turbulence, discusses shortcomings of common concepts for closure of the liquid phase turbulence kinetic energy equation and presents the approach for development and validation of improved models within the BMBF project Multi-Phase. Some problematic issues related to the direct numerical simulation of bubble swarms in narrow bubble columns are also discussed.

Keywords: bubble column, bubble induced turbulence, direct numerical simulation, statistical turbulence models

Zusammenfassung

Sowohl im akademischen als auch im industriellen Umfeld besteht ein beträchtliches Interesse daran, verbesserte numerische Methoden für Gas-flüssig Strömungen in Blasensäulen zu entwickeln, und diese für die Skalenübertragung und Entwurfsoptimierung einzusetzen. Eine wichtige Einschränkung in gängigen Euler‘schen Zwei- und Mehr-Fluid-Modellen betrifft das Fehlen adäquater Schließungsbeziehungen für die Turbulenz in Blasen-getriebenen Strömungen. Dieser Artikel erläutert Besonderheiten der Blasen-induzierten Turbulenz, weißt auf Mängel aktueller Konzepte für die Schließung der Erhaltungsgleichung der turbulenten kinetische Energie der Flüssigkeit hin und stellt den Ansatz für die Entwicklung und Validierung verbesserter Modelle im Rahmen des BMBF-Projektes Multi-Phase vor. Problematische Aspekte in Zusammenhang mit der direkten numerischen Simulation von Blasenschwärmen in engen Blasensäulen werden ebenfalls diskutiert.

Schlagwörter: Blasensäule, Blasen-induzierte Turbulenz, Direkte Numerische Simulation, Statistische Turbulenzmodelle

1. Introduction

One main goal of the BMBF project “Multi-Phase” (which started in 11/2011) is the development of reliable multi-scale models which allow the numerical investigation and optimization of industrial scale multiphase reactors. In this context the research at KIT aims on the development and validation of improved statistical models for bubble-induced turbulence (BIT) (also called pseudo-turbulence). Such models are required for computation of chemical multi-phase reactors (such as bubble columns) with engineering computational fluid dynamics (CFD) codes that rely on the Euler-Euler (E-E) approach. The model development is based on direct numerical simulations (DNS) of mono-disperse bubble swarm flows within a sub-region of a flat bubble column, where all details of the interface topologies and the flow field are spatially and temporally resolved. In the development of improved models, particular emphasis is placed on the closure terms in the transport equation for the liquid phase turbulence kinetic energy, k_{L}, which is the cornerstone in many statistical turbulence models. The DNS data shall be used to evaluate existing models, to identify model deficiencies and to develop improved models. These shall be validated by comparing numerical results of the extended E-E model by OpenFOAM with the experimental data of project partners for lab scale, pilot scale and industrial scale bubble columns.

This short communication is organized as follows. In Section 2 we give an overview on various CFD approaches for bubble columns. In Section 3 we discuss the physics of BIT which differs from classical shear-induced turbulence. In Section 4 we present various concepts for closure of the k_{L} equation and related shortcomings. In section 5 we highlight some problems that we face in DNS of bubble swarm flows within narrow flat bubble columns.

2. CFD methods for bubble columns

Bubble columns are widely used as multiphase reactors in chemical, biochemical and petrochemical industries [1, 2]. The ascending gas-phase creates an unsteady buoyancy-driven flow and induces large recirculation loops in the liquid phase (with up-flow in the center and down-flow near the wall). The flow regime can be homogeneous or heterogeneous (with a wide bubble size

distribution). The design of industrial scale bubble columns is mostly done by experience, empirical correlations, one-dimensional convection-dispersion models or compartment models. Such approaches remain somewhat limited when increase of the reactor performance is sought. While multidimensional CFD methods are potentially attractive for this purpose, their use is nowadays often limited to lab scale bubble columns and aqueous liquids.

The two common approaches for modeling the two-phase flow in bubble columns are the E-E [3] and the Euler-Lagrange (E-L) method [4]. While the E-L method is suitable for bubbly flows with low gas holdup (say below about 5%), the E-E method is much more general and is also suitable for churn-turbulent flows. Within the E-E approach one can distinguish two-fluid models (with a prescribed mean bubble diameter d_{B}) and multi-fluid models which consider bubble-size distributions, e.g. by population balance models [5, 6] or the MUSIG model [7].

In Eulerian multi-fluid simulations of flows in bubble columns, there are model limitations regarding three main aspects [8]: i) closure relations accounting for turbulence effects, ii) closure laws defining interfacial interaction forces between gas and liquid phases, iii) determination of local bubble-size distribution, which affects in return both turbulence phenomena and interfacial forces. Turbulence (which we are interested in here) can be described either by statistical models which are based on the Reynolds-Averaged Navier-Stokes (RANS) equations or by Large Eddy Simulation (LES). The unsteady recirculating flow with coherent structures suggests that LES (or Very-Large Eddy Simulation, V-LES) is more suitable. However, the dimensions of industrial bubble columns (diameters of several meters and height of tens of meters) do not allow a sufficient fine discretization and it is not possible to simulate sufficient long times necessary for a reliable statistical evaluation. Hence, the only viable approach seems to be RANS. Here, one can distinguish eddy-viscosity models (such as the $k-\varepsilon$ and $k-\omega$ models) and Reynolds stress models (RSM) which can better account for the inherent an-isotropy of the buoyancy-driven flow in bubble columns.

Several papers in literature investigated the suitability and limitations of different modeling concepts for bubble columns by comparing computed mean profiles for gas-holdup, gas and liquid velocity, and turbulent kinetic energy (TKE) with experimental data from dedicated lab-scale bubble

column experiments. Though the conclusions are not definite, several authors report that predictions of the mean flow (mean velocities, mean gas-hold-up) and the turbulent kinetic energy obtained by using the $k-\varepsilon$ models are comparable to those obtained by using RSM or LES (at least away from the sparger, where the performance of LES is clearly superior) [9-12]. Therefore, in our research we focus on $k-\varepsilon$ type models and discuss in Section 4 the status of respective closure assumptions.

3. Physics of pseudo-turbulence

For reliable mathematical modeling of pseudo-turbulence in bubble swarms it is essential to understand the underlying physics. Experiments show that statistical features of pseudo-turbulence considerably differ from those in conventional shear turbulence.

3.1 *Liquid velocity fluctuations*

Velocity fluctuations in BIT are often characterized by the probability distribution function (PDF) and the energy spectrum. In BIT, the PDFs are non-Gaussian and exhibit a self-similar behavior when scaled with $\alpha_{\mathrm{G}}^{0.4}$ [13-15]. The spectrum differs from that in shear-driven turbulence and follows in a certain range a power law with a slope close to -3 of the wave number [13, 16, 17] (in contrast to the Kolmogorov -5/3 law for homogeneous single-phase turbulence). The difference in scaling is attributed to the immediate dissipation of eddies in the bubble wake in pseudo-turbulence [16, 18]. The slope -3 and its origin have been recently confirmed by DNS [19] while E-L simulations based on the point-particles approach do not give the correct scaling observed in experiments [20]. This indicates that resolving the finite size of the bubble in the DNS is essential.

We remark that the evaluation of liquid spectra in bubbly flows from experimental or numerical data is not trivial since signals arise as segments of different length. In general, spectra are computed from signals which are interpolated during the intervals when bubbles are present at the measuring point; therefore the kind of interpolation has an impact on the spectra themselves [21]. To circumvent this problem, spectra are sometimes measured behind the rising bubble swarm [13].

3.2 *Bubble clustering*

The clustering of bubbles modifies the rise behavior of the swarm as compared to an isolated bubble (hindering or cooperative rise) and changes the local volume fraction and is thus important for consideration of swarm effects in the bubble forces. At the same time the interaction of the bubble wakes modifies the liquid velocity fluctuations as compared to single bubbles. Bubble clustering is often characterized by the pair correlation function [17, 22] or radial probability distribution functions [23]. Experiments show that PDFs of all components of the bubble velocity have non-Gaussian form [17]. DNS investigations [22, 24] suggest that the bubble deformability and the associated inversion of the lift force play a crucial role in determining the orientation of the clustering; close to spherical bubbles have a higher probability of aligning horizontally [23] while non-spherical preferentially align in the vertical direction.

4. Turbulence closures in $k-\varepsilon$ type models

Kataoka & Serizawa [25] derived the exact equations for k and ε for a gas-liquid flow consisting of two incompressible phases. In non-dimensional form, the transport equation for the liquid phase turbulent kinetic energy $k_{\mathrm{L}} = \overline{\overline{\mathbf{u}_{\mathrm{L}}^{'2}}}/2$ can be written as [26]

$$\frac{\partial}{\partial t}\left(\alpha_{\mathrm{L}} k_{\mathrm{L}}\right) + \nabla\cdot\left(\alpha_{\mathrm{L}} k_{\mathrm{L}} \overline{\overline{\mathbf{u}_{L}}}\right) = \underbrace{\frac{1}{Re_{\mathrm{ref}}}\nabla\cdot\left(\alpha_{\mathrm{L}}\,\overline{\overline{\tau_{\mathrm{L}}^{'}\cdot\mathbf{u}_{\mathrm{L}}^{'}}}\right) - \nabla\cdot\left[\alpha_{\mathrm{L}}\left(\overline{\overline{p_{\mathrm{L}}^{'}\mathbf{u}_{\mathrm{L}}^{'}}} + \frac{1}{2}\overline{\overline{\mathbf{u}_{\mathrm{L}}^{'2}\mathbf{u}_{\mathrm{L}}^{'}}}\right)\right]}_{DIFFUSION} \underbrace{-\alpha_{\mathrm{L}}\,\overline{\overline{\mathbf{u}_{\mathrm{L}}^{'}\mathbf{u}_{\mathrm{L}}^{'}}} : \nabla\overline{\overline{\mathbf{u}_{\mathrm{L}}}}}_{PRODUCTION\ BY\ SHEAR}$$
$$\underbrace{-\frac{1}{Re_{\mathrm{ref}}}\alpha_{\mathrm{L}}\,\overline{\overline{\tau_{\mathrm{L}}^{'}:\nabla\mathbf{u}_{\mathrm{L}}^{'}}}}_{DISSIPATION} + \underbrace{\overline{\left[\frac{1}{Re_{\mathrm{ref}}}\tau_{\mathrm{L,i}}^{'} - p_{\mathrm{L,i}}^{'}\mathbb{I}\right]\cdot\mathbf{u}_{\mathrm{L,i}}^{'}\cdot\hat{\mathbf{n}}_{\mathrm{L,i}}a_{\mathrm{i}}}}_{PRODUCTION\ BY\ INTERFACIAL\ TERM} \tag{1}$$

Here, subscript “i” denotes liquid phase quantities at the gas-liquid interface and $\alpha_{\mathrm{L}} = \overline{X_{\mathrm{L}}}$ is the mean liquid volumetric fraction defined via the characteristic function of the liquid phase, X_{L}. The single overbar indicates averaging while the double overbar denotes phase-weighted (conditional) averaging. For an arbitrary physical quantity φ_{L}, the respective definitions are $\overline{\overline{\varphi_{\mathrm{L}}}} = \overline{\varphi_{\mathrm{L}} X_{\mathrm{L}}}/\overline{X_{\mathrm{L}}}$ and $\varphi_{\mathrm{L}}' = \varphi_{\mathrm{L}} - \overline{\overline{\varphi_{\mathrm{L}}}}$. A similar equation is obtained for k_{G}.

In Eq. (1), all terms on the right-hand side must be modeled to close the system of equations. The terms involving α_L have essentially the same form and meaning as in the single-phase k equation. The last term in Eq. (1) contains the specific interfacial area a_i and is specific for two-phase flows as it represents a source/sink of turbulence due to the presence of interfaces.

Detailed literature reviews on turbulence models for CFD simulations of flows in bubble columns with various closures for the k equation can be found in [11, 27, 28]. Here, we mentioned only the most important concepts. In general, one can distinguish (seldom adopted) models that account for the turbulence in both phases and (more common) models that neglect the turbulence in the disperse phase (as it is considered as laminar) and model the turbulence in the continuous phase only. In the former case, usually no separate transport equation for k_G is solved. In [29] a mixture $k-\varepsilon$ model is proposed where the disperse phase turbulence is algebraically related to that of the continuous phase through a turbulence response coefficient.

For closure of the k_L equation it is common practice to adopt for the single-phase like terms closure relations and model coefficients from the standard single-phase $k-\varepsilon$ model. For considering the pseudo-turbulence two approaches exist. In the more general one, the interfacial term in Eq. (1) is explicitly modeled and several closure relations have been proposed in literature (see e.g. [9, 30]). In the second approach, the interfacial term is neglected (i.e. set to zero) so that the single-phase $k-\varepsilon$ equation is solved for the continuous phase. The BIT is taken into account by a two-phase multiplier for the shear-induced turbulent kinetic energy [31] or by an extra (linearly superposed) contribution to the eddy viscosity, e.g. by the model of Sato [32, 33]. The latter approach has two main drawbacks. First, it can only increase the turbulent viscosity in bubbly flow and is thus unable to reproduce the attenuation of turbulence observed in several bubbly flow experiments. Second, the influence of the bubbles on the turbulent kinetic energy and its dissipation rate are neglected.

The performance of the above concepts and variants of the $k-\varepsilon$ model (standard, realizable, RNG, SST) in the E-E approach is investigated in several papers [8, 34-39]. In such numerical studies it is important to use higher order schemes since low order schemes (like upwind) have a large amount of numerical diffusion which masks the eddy viscosity of the turbulence model [8, 34]. Despite

their apparent similarities, the Standard, RNG and Realizable versions perform different when applied to flows in bubble columns (with the RNG model being the best) [8]. The impact of the BIT term, despite being negligible on the computation of velocity fields and gas holdup, is significant on the estimation of turbulent quantities [8]. While the above comparative studies are useful to identify which model performs best for a certain experiment, their value for development of improved closure relations is limited.

It is well known that the constants in the $k-\varepsilon$ equation are not universal, even in the case of single-phase flow. Furthermore, statistical features of BIT differ from that of shear turbulence (cf. Section 3). It is therefore obvious that for two-phase flows specific models and coefficients should be developed for closure of Eq. (1). Experimentally, it is difficult to obtain detailed information on the individual terms in the k_{L} equation especially under non-dilute conditions. By applying molecular tagging velocimetry to a turbulent bubbly flow in a vertical square duct, Hosokawa et al. [40] studied the effect of the bubbles on the TKE budget and carried out a priori tests of closure assumptions of the standard and low Reynolds number $k-\varepsilon$ model. They found that the $k-\varepsilon$ can reasonably predict the production rate of TKE but fails in evaluating the diffusion rate in the near wall region.

More detailed and complete information about the TKE budget can be obtained by DNS, where the governing equations are solved numerically on sufficiently fine grids so that all continuum length and time scales are fully resolved. In order to ensure that DNS results are of relevance for bubble columns, it is - for two reasons - essential to consider a computational domain with walls. First, in triple periodic computational domains the possibility of occurrence of large scale recirculating flow structures that are typical for bubble columns is reduced [19]. Second, statistical quantities (i.e. all terms in the k_{L} equation) depend on the wall distance. DNS investigations of turbulent bubbly flow in a vertical channel were performed by Lu & Tryggvason, both for up-flow [41] and down-flow [42].

Ilić [30] performed DNS studies of laminar bubbly flow in a narrow vertical channel in rather viscous liquids (Morton number $M = g(\rho_{\mathrm{L}} - \rho_{\mathrm{G}})\mu_{\mathrm{L}}^4 / \rho_{\mathrm{L}}^2\sigma^3 > 3\cdot 10^{-6}$) and evaluated all terms in Eq. (1) for a single bubble [26] and a swarm consisting of eight bubbles [43]. For this purpose, the local instantaneous data for phase distribution, velocity field and pressure field are averaged over wall-

normal planes and are additionally averaged in time. By this averaging procedure, the wall-normal profile of the budget of k_L is obtained; it indicates the relative importance of the various terms in Eq. (1). For the parameters investigated in [43] it is found, that a gain of k_L is mainly due to the interfacial term while the production by shear stresses is almost negligible. The interfacial term and the dissipation are not in local equilibrium. Therefore the redistribution of k_L by diffusive transport is very important. Besides giving inside in the TKE budget, the DNS data are used for a-priori-testing of closure assumptions. For this purpose, the wall-normal profile of any closure term in Eq. (1) as evaluated from the DNS data is compared with the profile predicted by a model for this closure term, where all flow quantities entering into the model are taken by the respective profiles evaluated from the DNS data. In [43] it was found that all models for the production by shear stresses yield a strong overestimation, while the turbulent diffusion is strongly underestimated by all models used in engineering codes. For the interfacial term a large number of models are analyzed and one promising model could be identified. However, all the other closure terms in the turbulent kinetic energy equation need further improvement for bubble driven flows.

The concept of a-priori testing of model assumptions for closure terms is certainly useful for the development of improved models. However, it does not consider that in practical CFD computations the quantities entering into the model (e.g. the mean void fraction and velocity profiles) are influenced by the model itself as it is part of the governing equations and therefore affects the solution for the mean quantities. Since this feedback is non-linear, the a-posteriori testing of any potential model refinement in full E-E simulations is necessary and validation by experiments is mandatory.

Most of the above references consider mono-disperse flows. For poly-disperse flows, literature indicates that bubble population balances cannot be applied in a satisfactory manner because of the inability of $k-\varepsilon$ models to predict correctly the turbulent dissipation rate, thus causing a large underestimation of bubble break-up rates [3, 5, 6]. To solve this issue, further developments of coalescence [44] and break-up kernels [45] seem to be required on the one hand, while on the other hand improved closure relations for k and ε are necessary for bubble-driven flows. We note that for closure of the two-phase source/sink term in the ε equation, it is common practice to relate it to the

two-phase source/sink term in the k_L equation by means of a time scale (for which essentially four options exist, see [46]). Simulations with the MUSIG model clearly show that the kind of turbulence modeling affects sensitively the bubble coalescence and break-up so that different bubble size distributions are obtained for different turbulence models [47].

5. Issues in DNS of bubble swarms in narrow bubble columns

In this project we extend the DNS study of Ilić [30, 43] on BIT in mono-disperse bubble swarms to lower values of the Morton number ($M = 10^{-7} - 10^{-10}$) and larger numbers of bubbles. The simulations are performed by an in-house code which uses a volume-of-fluid (VOF) method with piecewise linear interface reconstruction for describing the interface evolution [48, 49]. The computational domain is cubic and represents a sub-region of a flat bubble column, see Fig. 1. The wall distance is about 4 to 6 bubble diameters (which is of the order of millimeters).

For achieving convergence of statistical data it is necessary to consider large enough domains and simulation time. In order to identify parameters which allow efficient simulations without compromising the physics, a number of test runs were performed for single bubbles. These showed that a grid resolution of 20 cells per bubble diameter and a liquid-to-gas density ratio of 25 are sufficient to obtain results that are independent on both, the mesh size and ρ_G.

In multi-bubble simulations we encounter two problems. The first once concerns the approach of bubbles toward the wall. When a part of the bubble enters the mesh cell layer that is closest to the wall, the liquid film between the bubble and the wall is not resolved. This may lead to artificial wall contact of the bubble. To circumvent this problem we intend to use a grid which is non-equidistant in z direction with refinement near the side walls. The second and more severe problem concerns bubble coalescence. To limit the physical complexity, only mono-disperse flows shall be considered in the project Multi-Phase, both in experiments and simulations. Coalescence is an unresolved problem in DNS of interfacial flows as some methods (e.g. front-tracking) suppress it while others like VOF lead to artificial coalescence [50]. In Fig. 2 we show close-up visualizations of a bubble swarm simulation ($M = 2.8 \cdot 10^{-8}$, Eötvös number $Eo = g(\rho_L - \rho_G)d_B^2 / \sigma = 1.265$) at four slightly different instants in

time. When the distance between the two approaching bubbles (Fig. 2 a) becomes less than one mesh cell, both interfaces connect (Fig. 2 b) and form a gas bridge (Fig. 2 c) which grows in time (Fig. 2 d) and finally leads to coalescence. Since the spatial resolution of the gas bridge is only a few mesh cells, the estimation of interface normal vector and curvature is rather inaccurate and leads to large erroneous velocity vectors (Fig. 2 c and d). It is obvious that the initialization of the coalescence process in these simulations depends on the mesh size. While numerical coalescence can be prevented by using for each bubble a separate VOF function [51], the associate computational effort strongly increases with the number of bubbles.

6. Conclusions

Numerical methods for computation of bubble-driven gas-liquid flows require adequate closure relations for turbulence. In bubble columns, the large scale liquid recirculation generates shear-induced turbulence (especially near the walls) which is superposed to the BIT. Statistical features of bubble-induced turbulence considerably differ from conventional shear-induced turbulence. Eulerian computations of flows in bubble columns with statistical turbulence models often ignore the complex physics of the turbulence and adopt standard single-phase closure laws and coefficients. The development of improved turbulence closure relations for bubble-driven flows is hindered by the lack of detailed experimental data on the various closure terms in the turbulence kinetic energy equation. Direct numerical simulations of bubble swarms can provide such data but suffer from imprecise treatment of coalescence, which is – depending on the numerical method – either completely suppressed or artificially enhanced.

The development and validation of improved statistical turbulence models for gas-liquid flows in bubble columns is a long-term task which requires an integrated approach involving various computational methods (DNS, E-E) and experiments on various scales (single bubbles, bubble swarms, lab-scale, pilot-scale and production scale bubble columns). The BMBF project Multi-Phase presents one step toward this goal.

Acknowledgement

We gratefully acknowledge the support of the Federal Ministry of Research for funding this project (BMBF FKZ 01RC1102).

Symbols used

a_i	[m^{-1}]	specific interfacial area
d_B	[m]	bubble diameter
Eo	[-]	Eötvös number
k	[$m^2 s^{-2}$]	turbulent kinetic energy
M	[-]	Morton number
$\hat{n}$	[-]	unit normal vector to interface
p	[Pa]	pressure
Re	[-]	Reynolds number
t	[s]	time
$\mathbf{u}$	[$m\,s^{-1}$]	velocity field
x, y, z	[m]	Cartesian co-ordinates
X	[-]	phase indicator function

Greek symbols

α	[-]	volume fraction
ε	[$m^2 s^{-3}$]	dissipation rate of k
ρ	[$kg\,m^{-3}$]	density
τ	[Pa]	shear tress tensor
φ		arbitrary quantity

Subscripts

G	gas phase
i	interface
L	liquid phase

References

[1] W.-D. Deckwer, R. W. Field, *Bubble column reactors*. John Wiley and Sons, **1992**.
[2] N. Kantarci, F. Borak, K. O. Ulgen, *Process Biochem* **2005,** *40 (7)*, 2263-2283.
[3] H. A. Jakobsen, H. Lindborg, C. A. Dorao, *Ind Eng Chem Res* **2005,** *44 (14)*, 5107-5151.
[4] S. Lain, D. Bröder, M. Sommerfeld, M. F. Göz, *Int J Multiph Flow* **2002,** *28 (8)*, 1381-1407.
[5] P. Chen, J. Sanyal, M. P. Dudukovic, *Chem Eng Sci* **2004,** *59 (22-23)*, 5201-5207.
[6] K. Ekambara, K. Nandakumar, J. B. Joshi, *Ind Eng Chem Res* **2008,** *47 (21)*, 8505-8516.
[7] Y. X. Liao, D. Lucas, E. Krepper, M. Schmidtke, *Nucl Eng Des* **2011,** *241 (4)*, 1024-1033.
[8] C. Laborde-Boutet et al., *Chem Eng Sci* **2009,** *64 (21)*, 4399-4413.
[9] D. Zhang, N. G. Deen, J. A. M. Kuipers, *Chem Eng Sci* **2006,** *61 (23)*, 7593-7608.
[10] M. T. Dhotre, B. Niceno, B. L. Smith, *Chem Eng J* **2008,** *136 (2-3)*, 337-348.
[11] M. V. Tabib, S. A. Roy, J. B. Joshi, *Chem Eng J* **2008,** *139 (3)*, 589-614.
[12] M. K. Silva, M. A. d'Avila, M. Mori, *Comput Chem Eng* **2012,** *44*, 34-44.
[13] G. Riboux, F. Risso, D. Legendre, *J Fluid Mech* **2010,** *643*, 509-539.
[14] J. Martinez-Mercado, C. A. Palacios-Morales, R. Zenit, *Phys Fluids* **2007,** *19 (10)*, 103302-1 - 103302-13.
[15] F. Risso, K. Ellingsen, *J Fluid Mech* **2002,** *453*, 395-410.
[16] M. Lance, J. Bataille, *J Fluid Mech* **1991,** *222*, 95-118.
[17] J. M. Mercado et al., *J Fluid Mech* **2010,** *650*, 287-306.
[18] F. Risso et al., *Philos T R Soc A* **2008,** *366 (1873)*, 2177-2190.
[19] I. Roghair et al., *Int J Multiph Flow* **2011,** *37 (9)*, 1093-1098.
[20] I. M. Mazzitelli, D. Lohse, *Phys Rev E* **2009,** *79 (6)*, 066317-1 - 066317-9.
[21] M. Ilic, M. Wörner , D. G. Cacuci, in *6th International Conference on Multiphase Flow*,Leipzig, Germany **2007**.
[22] B. Bunner, G. Tryggvason, *J Fluid Mech* **2002,** *466*, 17-52.
[23] B. Figueroa- Espinoza, R. Zenit, *Phys Fluids* **2005,** *17 (9)*, 091701-1 - 091701-4.
[24] B. Bunner, G. Tryggvason, *J Fluid Mech* **2002,** *466*, 53-84.
[25] I. Kataoka, A. Serizawa, *Int J Multiph Flow* **1989,** *15 (5)*, 843-855.
[26] M. Ilic, M. Wörner, D. G. Cacuci, *J Nucl Sci Technol* **2004,** *41 (3)*, 331-338.
[27] J. B. Joshi, *Chem Eng Sci* **2001,** *56 (21-22)*, 5893-5933.
[28] A. Sokolichin, G. Eigenberger, A. Lapin, *AIChE J* **2004,** *50 (1)*, 24-45.
[29] A. Behzadi, R. I. Issa, H. Rusche, *Chem Eng Sci* **2004,** *59 (4)*, 759-770.
[30] M. Ilic, Wissenschaftliche Berichte Forschungszentrum Karlsruhe FZKA 7199,**2006**.
[31] S. Hosokawa, A. Tomiyama, *Int J Heat Fluid Flow* **2004,** *25 (3)*, 489-498.
[32] Y. Sato, K. Sekoguchi, *Int J Multiph Flow* **1975,** *2*, 79-95.
[33] Y. Sato, M. Sadatomi, K. Sekoguchi, *Int J Multiph Flow* **1981,** *7 (2)*, 167-177.
[34] A. Sokolichin, G. Eigenberger, *Chem Eng Sci* **1999,** *54 (13-14)*, 2273-2284.
[35] D. Bothe, H. Shirzadi, H. J. Warnecke, *Chem Eng Res Des* **2007,** *85 (A11)*, 1491-1496.
[36] J. Gimbun, *Journal of the Institution of Engineers, Malaysia* **2009,** *70 (4)*, 57-64.
[37] K. Ekambara, M. T. Dhotre, J. B. Joshi, *Chem Eng Sci* **2005,** *60 (23)*, 6733-6746.
[38] K. Ekambara, M. T. Dhotre, *Nucl Eng Des* **2010,** *240 (5)*, 963-969.
[39] H. Marschall et al., *Chem Eng Technol* **2011,** *34 (8)*, 1321-1327.
[40] S. Hosokawa, T. Suzuki, A. Tomiyama, *Exp Fluids* **2012,** *52 (3)*, 719-728.
[41] J. C. Lu, G. Tryggvason, *Phys Fluids* **2008,** *20 (4)*, 040701-1 - 040701-6.
[42] J. C. Lu, G. Tryggvason, *Phys Fluids* **2006,** *18 (10)*, 103302-1 - 103302-10.
[43] M. Wörner, B. E. Ghidersa, M. Ilic, D. G. Cacuci, *Houille Blanche* **2005,** *(6)*, 91-104.
[44] Y. X. Liao, D. Lucas, *Chem Eng Sci* **2010,** *65 (10)*, 2851-2864.
[45] Y. X. Liao, D. Lucas, *Chem Eng Sci* **2009,** *64 (15)*, 3389-3406.
[46] R. Rzehak, E. Krepper, *Nucl Eng Des* **2013,** *258*, 57-65.

[47] F. Z. Kendil et al., *Nucl Eng Des* **2011,** *241 (10)*, 4111-4121.
[48] W. Sabisch, M. Wörner, G. Grötzbach, D. G. Cacuci, *Chem-Ing-Tech* **2001,** *73 (4)*, 368-373.
[49] M. C. Öztaskin, M. Wörner, H. S. Soyhan, *Phys Fluids* **2009,** *21 (4)*, 042108-1 - 042108-17.
[50] M. Wörner, *Microfluid Nanofluid* **2012,** *12 (6)*, 841-886.
[51] E. Coyajee, B. J. Boersma, *J Comput Phys* **2009,** *228 (12)*, 4444-4467.

Figure captions

Fig. 1: Sketch of a flat bubble column and a sub-region representing the computational domain (with no-slip conditions at the two lateral side walls and periodic boundary conditions in vertical (x) and span-wise (y) direction).

Fig. 2: Coalescence process of two bubbles at four different instants in time. The small boxes indicate individual mesh cells.

Figures

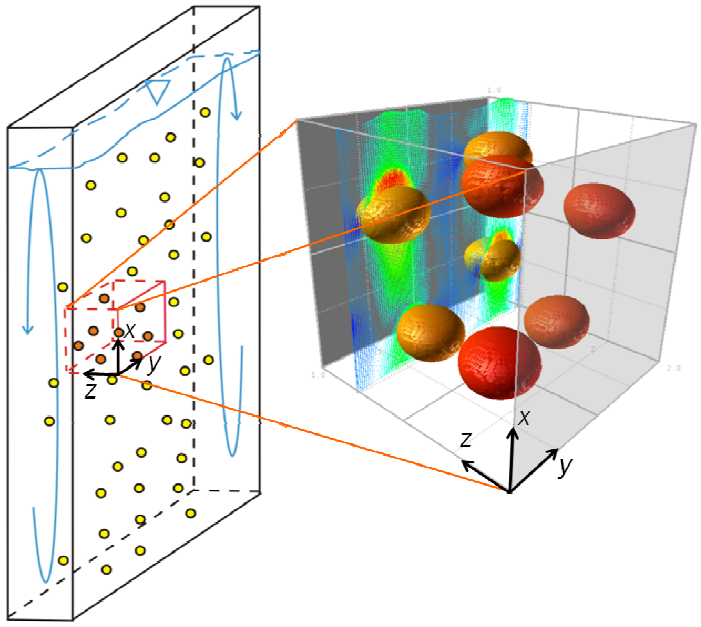
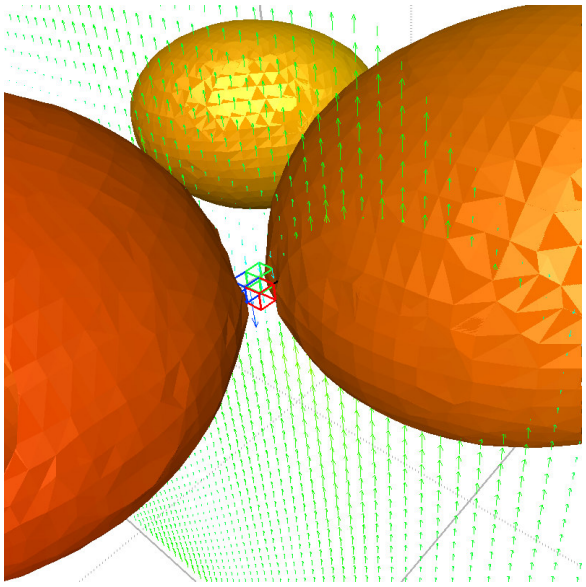
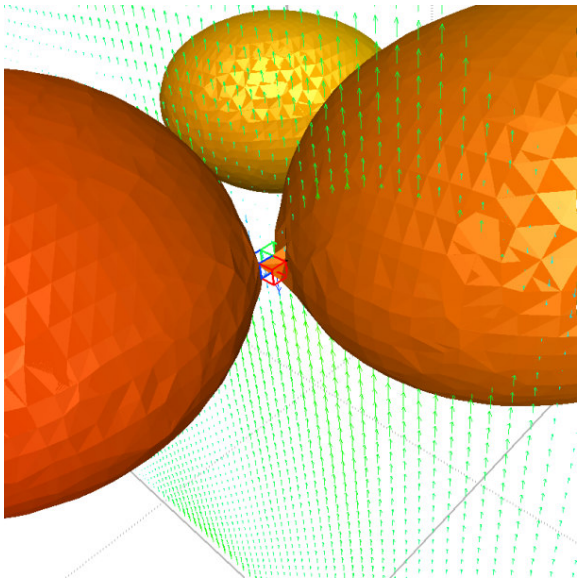


Fig. 1: Sketch of a flat bubble column and a sub-region representing the computational domain (with no-slip conditions at the two lateral side walls and periodic boundary conditions in vertical (x) and span-wise (y) direction).

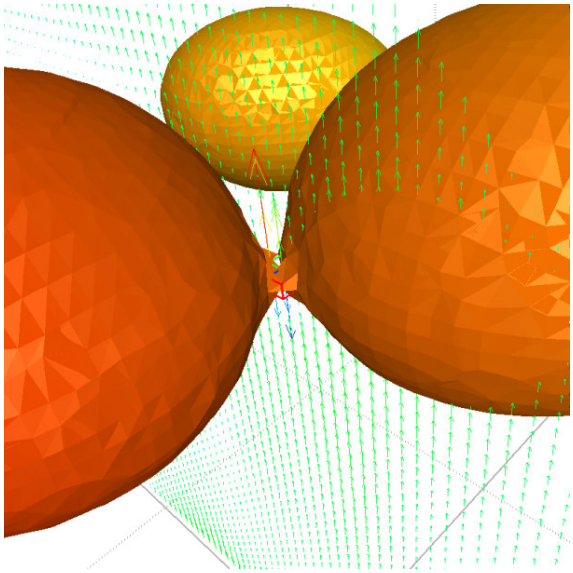
a) t = 0.0593 s



b) t = 0.0595 s



c) t = 0.0597 s



d) t = 0.0598 s

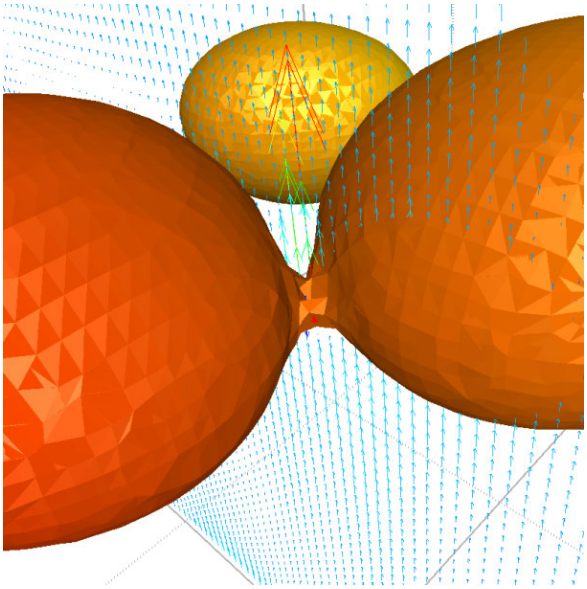


Fig. 2: Coalescence process of two bubbles at four different instants in time. The small boxes indicate individual mesh cells.

Text for table of contents section

Numerical methods for computation of gas-liquid flows in bubble columns require adequate closure relations for turbulence. This article discusses shortcomings of common concepts for closure of the liquid phase turbulence kinetic energy equation and presents the approach for development and validation of improved closures within the BMBF project Multi-Phase.