

# STATUS AND CHALLENGES OF CFD-MODELLING FOR POLY-DISPERSE BUBBLY FLOWS

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## ABSTRACT

A clear progress was achieved during the last 20 years in the qualification of CFD-codes for problems of the nuclear safety research. Especially two-phase flows are important, e.g. for LOCA scenarios, but up to now the predictive capabilities of CFD-methods for such flows are limited. Two-phase flows are determined by complex interactions between the phases. Some of them are not yet well understood at the local scale and, therefore, CFD models are limited. This paper discusses such local phenomena and their reflection in presently available CFD-models. It turns out that most of the assumptions in the formulation of closure models for the multi-fluid approach reflect the real phenomena only in a coarse way. Possible uncertainties are listed. Nevertheless, the simulation results obtained by the HZDR baseline model for poly-disperse flows in which all models including model parameter are fixed show in general a rather good agreement with experimental data. One sensitive issue seems to be how to handle the bubble size. In case of poly-disperse flows the sub-division of the gas phase with respect to the bubble size is important and the exact choice of the limits for this division sensitively influences the simulation results.

## KEYWORDS

bubbly flow, CFD, multi-fluid model, closure models

## 1. INTRODUCTION

Computational Fluid Dynamics (CFD) becomes more and more important for issues of Nuclear Reactor Safety (NRS) research. Single phase CFD is widely used for industrial applications, e.g. in automotive and aviation industries. Also for applications in NRS single phase CFD-simulations show promising results as e.g. demonstrated in several OECD benchmark simulations. However, CFD is not yet mature for two-phase flows which are often of interest in NRS in relation to Loss Of Coolant Accident (LOCA) scenarios. Due to decreasing pressure boiling occurs, i.e. steam bubbles are generated and may grow up to large gas structures. To simulate such processes reliable models for poly-disperse bubbly flows with phase transfer are required. However, the predictive capabilities of CFD-simulations are even limited for adiabatic bubbly flows up to now.

The main reason for the existing shortcomings is the complex structure of the gas-liquid interface. On the one hand, this interface determines the interaction between the phases; on the other hand, it is also formed by such interactions. In a flow simulation in medium or large sized domains as in nuclear reactors not all details of such interfaces can be resolved. Instead in most simulations the Euler-Euler two- or multi-fluid model is applied. It bases on the assumption of interpenetrating phases and simulates probabilities for the local and instantaneous occurrence of the phases. All information on the interface gets lost and has to be brought into the model by closure laws.

The closure models have to reflect all relevant flow phenomena which are not resolved in a simulation, i.e. which occur at a scale in the order of the size of the numerical mesh cells or below. A lot of proposals for such models can be found in literature, but there is no general agreement on the question which closure models should be used for a specific flow situation. In the result, depending on suggestions from code suppliers, personal or research group preferences in most publications different sets of closures are used. This clearly limits the possibilities to draw well-based conclusions from comparisons of the results obtained with different model setups. The published CFD-simulations are in almost all cases post-test simulations on one or only few experimental configurations. Often the selection of closures is done aiming on a good agreement with experimental data. Such investigations demonstrate the general capabilities of CFD codes to simulate two-phase flow problems and can provide valuable insights into flow characteristics, but the predictive capabilities are rather limited.

Basing on the long-term experiences on CFD model development and validation, recently so-called baseline models were developed for poly-dispersed bubbly flows (Rzehak et al., 2015) and stratified flows (Höhne and Mehlhoop, 2014). These HZDR baseline models are characterized by an exact definition of all closure models to be used including the definition of all model constants. Such fixed setups have to be applied to many different flows situations without any tuning and modification. For cases with deviations from experimental data the reasons for these problems have to be identified. Basing on these identified shortcomings model improvements can be proposed and tested. However, an update of the baseline model should only be done in the case of an overall improvement of the simulation results, i.e. only if the cases with previously good agreement will not become worse. The baseline model strategy seems to be the only way to obtain predictive multiphase CFD tools in future. This strategy is presented and discussed in detail by Lucas (2014). Beside closure models also issues of numerical solution procedures, discretization, consideration of best practice guidelines (Bestion, 2012) and some others have to be considered. This paper discusses some of these issues to identify possible reasons for uncertainties in the Euler-Euler approach on poly-disperse flows.

## **2. PHENOMENA IN POLY-DISPERSE BUBBLY FLOWS IN VIEW OF THE TWO-OR MULTI-FLUID MODEL**

One important reason for the open issues is the lack of knowledge on the phenomena which take place at local scale. This applies especially in dense gas-liquid flows. There are many detailed measurements on single bubbles and for diluted bubbly flows with gas volume fraction up to several percent. Open questions result from the interpretation of these data and the formulation of closure models reflecting these observations in frame of an Euler-Euler-simulation.

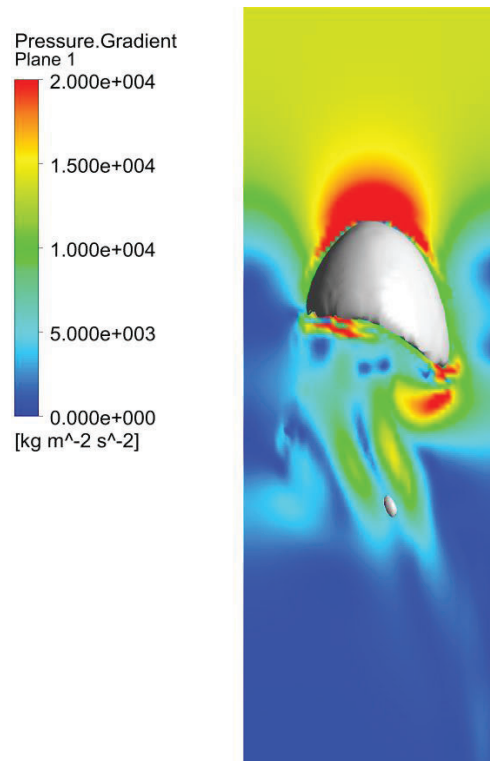
Experimental data for dense flows with required detailedness are rare or even not existing. There are clear limitations in measuring techniques for such flows. To get the required information on the gas-liquid interface in dense air-water and steam-water flows new innovative measuring techniques as wire-mesh sensors and ultrafast X-ray tomography were developed at Helmholtz-Zentrum Dresden - Rossendorf (HZDR) and extensively used to establish comprehensive databases (Lucas et al., 2005, 2010, 2013). Beside the detailed information on the interface they provide information on the velocity of the interfaces, but not on the velocity of the liquid phase or on turbulence parameter.

In the two- or multi-fluid model no single bubbles are considered, but interpenetrating phases and the interaction between the phases have to be modelled. In case of adiabatic flows without mass and energy transfer we finally have to model only momentum transfer. However, we have to distinguish between a resultant force which has to be considered as source terms in the averaged momentum equations of both phases and statistically fluctuating momentum transfer or energy dissipation at the interface which influences the turbulence within both phases. The resultant momentum transfer is usually modelled by

bubble forces. The momentum transfer and, therefore, all bubble forces sensitively depend on the bubble sizes. Consequently, the local bubble size distribution is required in an adequate simulation. Hence, this requires the modelling of bubble coalescence and breakup. These effects as well as some special problems are discussed in the next sections followed by the extra phenomena that have to be considered for flows with phase transfer.

## 2.1. Momentum transfer between the phases

Because of the density difference between gas and liquid phase pressure gradients generate a motion of the bubbles relative to the surrounding liquid. For many flows buoyancy is the most important reason for relative motion caused by the vertical gradient of the hydrostatic pressure. This body force effect is implicitly considered in the momentum equations of the two- or multi-fluid model. However extra sources terms are required to model the momentum transfer at the interface. The surface integral on the pressure distribution and local shear stresses (Fig. 1) should determine this source term. Since the bubble interface is not resolved in the simulation the local pressure distribution is unknown and closure models are needed to reflect this integral. They base on the consideration of some general phenomena which have to be expected. The resulting bubble forces which will be discussed below are summed up to form a source term in the momentum equation, i.e. a superposition of these effects is assumed. There is no proof that such a superposition is justified. Interactions between these effects could be expected from the above mentioned consideration of the integral over the pressure distribution at the bubbles surface.



**Fig. 1:** Pressure field around a single bubble in an upward flow field in a pipe

### Drag force

The motion of the bubble increases the pressure in front of it and reduces the pressure in the rear. The integral of the pressure resulting from this effect is reflected by the drag force. It is obvious that it

depends at least on the bubble size, on the bubble shape, on the mobility of the interface, on material parameter of the liquid, and on the local liquid flow field around the bubble which may be influenced e.g. by other bubbles. The drag force can be expressed by

$$\mathbf{F}^{drag} = -\frac{3}{4d_B} C_D \rho_L \alpha_G |\mathbf{u}_G - \mathbf{u}_L| (\mathbf{u}_G - \mathbf{u}_L) \quad (1)$$

For a single non-deformable rigid sphere in stagnant liquid at very low particle Reynolds numbers the drag coefficient  $C_D$  equals to  $24/Re$  ( $Re$  is the bubble Reynolds number) which corresponds to the Stokes law. However for poly-disperse bubbly flows we have to consider all the influences mentioned above. Usually this is done by modifications of  $C_D$ . Accordingly many different correlations for  $C_D$  can be found in literature, most of them basing on experimental observations of single bubbles. These correlations usually base on bubble Reynolds and/or Eötvös numbers. There is an implicit consideration of an average bubble shape assuming that it is related to the bubble size. The validity of most of the correlations is limited to one bubble regime. The correlation by Ishii and Zuber (1979), which is also used in the HZDR baseline model for poly-disperse bubbly flow, combines correlations for the spherical, elliptical and cup bubbles regimes and seems to be applicable over a wide range as required for modelling of poly-disperse flows. The shape effect on bubble terminal velocity is discussed in more detail by Tomiyama (2004). It is shown that especially the curvature at the bubble nose has an important influence on the bubble terminal velocity, i.e. also on the drag. It sensitively depends on impurities of the fluid leading to a different drag as it is well known from the diagram of Clift et al. (1978). It shows the variation of terminal bubble velocities for clean and contaminated systems, which is of special importance for bubbles with sphere equivalent diameters between 1 mm and 6 mm for air-water flows. Contaminations modify the bubble shape and the mobility of the interface. The bubble shape as well as the liquid velocity distributions close to the bubble may also be modified by other bubbles. Some modifications are proposed by using so-called swarm factors.

Although there are many phenomena which influence the drag force and cannot be reflected in detail by the available  $C_D$ -correlations. However, CFD-simulations using the baseline model with carefully measured bubble size distributions show already satisfying results regarding average bubble velocities and void fraction which are strongly influenced by the drag force. In any case it is important to consider the bubble size or the bubble size distribution in the simulation. Uncertainties regarding the drag force may mainly result from the following effects which are reflected only with rather rough approximations in the existing models:

- transient bubble deformation (wobbling),
- contaminations which modify the bubble shape and mobility of the interface,
- bubble-bubble interactions which may modify the liquid flow field around a bubble and the bubble shape (swarm effects).

#### Lateral lift force

When the bubble rises in a liquid shear flow, different relative velocities at both sides of the bubble also cause a pressure difference which leads to bubble migration which is perpendicular to the bubbles relative velocity. This reflected by the so-called lateral lift force which is calculated according to:

$$\mathbf{F}^{lift} = -C_L \rho_L \alpha_G (\mathbf{u}_G - \mathbf{u}_L) \times rot(\mathbf{u}_L). \quad (2)$$

It was shown by Tomiyama et al. (2002) as well as in several numerical simulations (Ervin and Tryggvason, 1997; Bothe et al., 2006) that the lift force sensitively depends on the bubble shape. For deformed bubbles it even changes its sign. From experiments with single bubbles in a high viscos laminar

linear shear flow, Tomiyama et al. (2002) developed the well-known correlation for the lift force coefficient. In this correlation there is a change of the sign of the lift force coefficient at a critical bubble diameter. For air-water flows at ambient conditions this critical diameter is about 5.8 mm sphere equivalent bubble diameter. For steam-water flows it drops down to about 3 mm at saturation conditions for at 7 MPa, which is the most relevant pressure for LOCA-scenarios. A comprehensive evaluation of data obtained for various vertical pipe flows at the TOPFLOW-facility of HZDR showed that at least this critical diameter is in accordance to the correlation also for turbulent air-water and steam-water flows with medium void fraction (Lucas and Tomiyama 2011). Also in investigations of boiling tests using a refrigerant (e.g. DEBORA using R12) the usefulness of this correlation could be shown (Krepper et al., 2013, see Fig. 2). The Tomiyama correlation is frequently used in CFD-simulations and the experimentally observed separation of small and large bubbles can be well captured by using this model. It seems to be the best model which is presently available and for this reason it is also used in the HZDR baseline model. However it should be kept in mind that it was obtained for completely different conditions. Similarly to the drag force, the consideration of the bubble size distribution is essential for simulations. Moreover, several gas momentum equations are needed to simulate the bubble size depending migration of the bubbles. Uncertainties may result mainly from:

- the extrapolation from laminar to turbulent flows,
- the extrapolation from high viscous glycerol-water mixtures to low viscous water,
- bubble-bubble interactions which may modify the liquid flow field around a bubble and the bubble shape (swarm effects),
- near wall effects.

#### Turbulent dispersion force

The local instantaneous pressure field at the bubble surface may also be influenced by non-resolved turbulent eddies. This leads to a superposed random bubble migration. If a LES model is used in the simulation the resulting bubble dispersion should be a result of the simulation without additional models. For RANS models however the turbulent fluctuations are not resolved and an additional model is required to capture this effect. From a Favre averaging of the drag force Burns (2004) obtained the following expression, which is used also for the HZDR baseline model:

$$\mathbf{F}^{disp} = -\frac{3}{4} C_D \frac{\alpha_G}{d_B} |\mathbf{u}_G - \mathbf{u}_L| \frac{\mu_L^{turb}}{\sigma_{TD}} \left( \frac{\text{grad } \alpha_G}{\alpha_G} - \frac{\text{grad } \alpha_L}{\alpha_L} \right) \quad (3)$$

Of course here the same sources of uncertainty are involved as mentioned above for the drag force coefficient since it is part of the equation above. An additional source of uncertainty is the value of the Schmidt number  $\sigma_{TD}$  which is usually set to 0.9. There is no check about the validity of this number for poly-disperse bubble flows.

#### Wall force

In the near wall region the lift force discussed above is modified because of thin liquid film which may exist between the bubble and the wall. There are several formulations for such a wall force in literature, e.g. basing on the lubrication theory. The general expression for the wall force is given by

$$\mathbf{F}^{wall} = \frac{2}{d_B} C_w \rho_L \alpha_G |\mathbf{u}_G - \mathbf{u}_L|^2 \hat{\mathbf{y}} \quad (4)$$

A correlation for the wall force coefficient based on experimental observations of the bubble path close to the wall was obtained by Hosokawa et al. (2002). This formulation is also part of the HZDR baseline model (Rzehak et al., 2012). However, such a correlation is only valid as long the bubble rises without



direct wall contact. If the bubble is pushed closer to the wall it is deformed and a deformation force has to be considered. Basing on the consideration of the increase of surface energy by this deformation an expression for such a deformation force was derived by Lucas et al. (2007). It was used for simulations with a simplified in-house test solver, but it cannot be directly applied in a usual Euler-Euler simulation since here the spatial extension of the bubble has to be considered. The two- or multi-fluid Euler/Eulerian approach in general allows to simulate bubbles which are larger than the mesh size. This is frequently done since in poly-disperse flows we have to consider bubbles sizes at least up to about 10 mm sphere equivalent bubble diameter and we should have a much finer mesh in the near wall region. That however means that the gas volume fraction distribution in the near wall region is influenced by the bubble shapes. The wall forces as discussed above are valid for the bubble centre of mass. The above mentioned deformation force avoids that the bubble centre of mass approaches too close to the wall. Using it as a bubble force in a usual CFD-simulation would lead accordingly to a gas free region close to the wall which beside others depends on the bubble size. One way to overcome this problem would be to convolute such a bubble centre related gas volume distribution with an assumed bubble shape. This was the way used in the above mentioned test solver. In common CFD code implementations the above mentioned wall force models are extrapolated for all cells close to the wall. Furthermore this formulation causes convergence problems for too fine grids in the near wall region and doesn't yield a grid resolution independent solution. Beside the uncertainties of the wall force formulations itself which are the same as mentioned above for the lift force, also this non-physical treatment of the near wall behaviour for bubbles larger than the mesh size in the near wall region are an source of uncertainties in the simulations. Obvious here a revision of the near wall treatment considering all bubble forces and turbulence is necessary.

#### Virtual mass force

The pressure distribution at the bubble interface discussed for the drag force also feeds back to the liquid. For this reason it has to be assumed that the bubble moving relative to the liquid always carries a part of liquid with it. The inertia of the gas phase is considered in the momentum balance; however the acceleration of this attached liquid part has to be added to the corresponding mass. Because of the much larger density of the liquid this part of the inertia in case the acceleration of the bubble is usually larger as the one caused by the gas mass itself. The expression for the virtual mass is

$$\mathbf{F}^{VM} = -C_{VM} \rho_L \alpha_G \left( \frac{D_G \mathbf{u}_G}{Dt} - \frac{D_L \mathbf{u}_L}{Dt} \right) \quad (5)$$

and the only open question is here the amount of water which is carried with bubble. For isolated bubble in creeping flows it can be obtained to be half of the bubble volume leading to  $C_{vm} = 0.5$ . Usually this value is taken in the simulations, as e.g. in HZDR baseline model. Some investigations show that it may be clearly larger for deformed bubbles (Simcik et al., 2014).

#### Other effects

From a single bubble rinsing in stagnant liquid it is well known that the bubble moves on a zig-zag or helical trajectory depending on the bubble size and the resulting deformation. Such effects cannot be considered in a two- or multi-fluid simulation since they are influenced by the shape of the bubble surface. Also Basset force and turbophoresis are not considered in the present modelling.

## **2.2 Turbulence**

Turbulence modelling is one of the most challenging issues in flow simulations. There are even several open issues for single-phase flows and the modelling for two-phase flows is rudimentary. In most studies, turbulence is treated differently for the different phases. The turbulence in the dispersed gas phase is of little relevance, because of the density of the gas and the low volume fraction. For the liquid phase, there

are several controversy papers in literature proposing different models for bubble induced turbulence (BIT) and its combination with shear induced turbulence (SIT). When bubbles move with a relative velocity through the liquid, the replacement of the liquid by the bubble leads to velocity fluctuations. This is no effect of turbulence and for this reason it is often called pseudo-turbulence. Also the fluctuating flow in the bubble wakes differs from the usual characteristics of turbulence. From open bubble wakes fluctuations are generated and interact with the shear induced turbulence. On the other hand the bubbles may enhance the dissipation of turbulent energy. In many CFD-simulations on bubbly flow a superposition of SIT and BIT is assumed, e.g. using the model by Sato et al. (1981) to increase the turbulent viscosity. In other approaches an extension of the two-equation single phase turbulence models by adding source terms for BIT is proposed. In the HZDR baseline model the SST-model by Menter (2009) with additional source terms is used:

$$\frac{\partial(\alpha_L \rho_L k_L)}{\partial t} + \nabla \cdot (\alpha_L \rho_L \mathbf{u}_L k_L) = \nabla \cdot \left( (\mu^{mol} + \mu^{turb} / \sigma_k^*) \nabla k \right) + P_k - D_k + S_k \quad (6)$$

$$\frac{\partial(\alpha_L \rho_L \omega_L)}{\partial t} + \nabla \cdot (\alpha_L \rho_L \mathbf{u}_L \omega_L) = \nabla \cdot \left( (\mu^{mol} + \mu^{turb} / \sigma_\omega^*) \nabla \omega \right) + C_\omega + P_\omega - D_\omega + S_\omega \quad (7)$$

with  $S_L^k = \mathbf{F}_L^{drag} \cdot (\mathbf{u}_G - \mathbf{u}_L)$  and  $S_L^\varepsilon = C_{\varepsilon B} \frac{S_L^k}{\tau}$ ,  $\tau = d_B / \sqrt{k_L}$ . The constant  $C_{\varepsilon B}$  is set equal to one. The source term for the  $\omega$ -equation, to which the SST-model blend in the wall region can be transformed according to:

$S_L^\omega = \frac{1}{C_\mu k_L} S_L^\varepsilon - \frac{\omega_L}{k_L} S_L^k$ . The turbulent and total viscosity is calculated with the usual relations.

A detailed discussion on this approach and comparisons with other models are given by Rzehak and Krepper (2013, 2013a).

Uncertainties of the turbulence modelling may arise from

- limited representation of the BIT by the source terms described above, in particular the one in the  $\varepsilon$ -or  $\omega$ -equation, respectively,
- the direct dissipation due to deformation of the bubble surface interacting with a turbulent eddy (Kataoka et al. 1993),
- different structures of shear- and bubble-induced turbulence which may require separate equations both effects (e.g. Cahed et al. 2003),
- lack of a well-established two-phase turbulent wall function although some attempts can be found in the literature (Marie et al. 1997, Troshko and Hassan 2001).

### 2.3 Bubble coalescence and breakup

Simulations with a fixed bubble size should only be applied on diluted bubbly flows. As gas volume fraction reaches c.a. 3%, collision and coalescence between bubbles becomes important. Depending on surrounding hydrodynamic conditions bubbles larger than some value begin to deform and breakup. The opposite phenomena lead to a dynamic change of bubble size or bubble size distribution. Detailed reviews on bubble coalescence and breakup phenomena as well as on corresponding models can be found in the review papers by Liao and Lucas (2009 and 2010). Different mechanisms may lead to bubble coalescence and fragmentation. A new model which considers the combination of these mechanisms was proposed by Liao et al. (2011). However it contains a number of model constants which are fixed in frame of the HZDR baseline model (Liao et al., 2015), but which are not jet well justified. Difficulties mainly come from:

- definition of critical conditions as the critical film thickness which is required in the film drainage models to calculate the coalescence efficiency, or the critical Weber number for breakup,
- description of relative motion between bubbles in case one or two velocity fields shared by all bubbles,
- superposition of various mechanisms,
- breakup in more than two daughter bubbles.

Uncertainties also result from the modelling of two-phase turbulence. Turbulence strongly influences bubble coalescence and breakup and accordingly the dissipation rate of turbulent energy is an input parameter for bubble coalescence and breakup models. Possibly there is a high sensitivity to material properties. Impurities may play a role especially for the thinning and rupture of the liquid film that forms between two bubbles after their collision. More detailed models for the coalescence efficiency seem to be necessary to consider such effects. In addition, the coalescence and breakup of large irregular gaseous structures might be different from that of the spheres.

## 2.4 Phase transfer

For existing gas-liquid interfaces the dynamics of evaporation and condensation processes are mainly determined by the heat transfer from or to the interface to or from the bulk liquid. Since the heat capacity of the gas is much lower compared that of the liquid the heat flux in the gas phase can often be neglected and replaced by the assumption that gas phase is on saturation temperature as long as the phase transfer rates are not too high. In laminar flows the heat transfer is determined by heat conduction. In case of turbulent flows the heat transfer is enhanced by turbulence. This is expressed by the Nusselt number. There are several correlations available in literature to calculate the Nusselt number mostly basing on Reynolds and Prandtl numbers. The definition of these dimensionless numbers for the simulation of local flow properties has to be carefully checked. In general, two types of correlations are available in literature. One is obtained by fitting experimental data while the other by performing DNS or LES simulations. The former is usually correlated with particle Reynolds number, where bubble size and velocity relative to surrounding fluids are used as characteristic length and velocity, respectively. The latter is correlated with turbulent Reynolds number basing on turbulence length scale and fluctuation velocity. The latter one is more phenomenological. However, its application to RANS simulation is dangerous due to the low accuracy of predicted turbulence parameters. Also the correlations are valid only for small bubbles, but often extrapolated to larger ones without any proof. The phase transfer is proportional to the interfacial area of a bubble. However usually in an Euler/Eulerian CFD simulation bubble deformation is not considered, i.e. a spherical shape is assumed. This may lead to an underestimation of the heat transfer. On the other hand there is a large uncertainty of the available correlations for the Nusselt number which may limit the importance of this effect.

Probably phase transfer leads to modifications on all the phenomena discussed in previous sections. Thus a modification of the pressure distribution at the surface of the bubble can be expected due to phase transfer. Also the local turbulence fields will be modified. Evaporation of the thin liquid film between collided bubbles may enhance bubble coalescence. There might be more effects. Nevertheless in the present state of the art of modelling phase transfer processes are just modelled as a superposition to adiabatic flow processes.

Besides sound models for the heat transfer to the gas-liquid interface also nucleation has to be considered. It can be assumed that wall boiling is most important. Several models exist here. A detailed discussion on wall boiling models can be found in Krepper and Rzehak (2013). In the case of evaporation caused by pressure decrease (flashing flows) a nucleation in the bulk may be also important as shown by Janet and Liao (2015).



State of the art in CFD modelling for bubbly flows with phase transfer is the assumption of a fixed bubble number density or a fixed bubble size. Both assumptions are not sufficient to reflect the physics behind. In case of boiling flows nucleation and growth of existing bubbles has to be handled in parallel.

### **3. CFD-MODELLING OF POLY-DISPERSE FLOWS IN FRAME OF THE MULTI-FLUID MODEL**

Depending on the flow situation under investigation all or only some of the phenomena discussed above have to be considered in a CFD-simulation basing on the multi-fluid approach. One important point for the model setup is the fact that closure models for bubble forces as well as BIT depend on the bubble size. For monodisperse flows a two-fluid approach with one gas and one liquid phase can be applied with the bubble diameter as a parameter. However for poly-disperse flows this is clearly not sufficient. If bubbles in the range of several mm are considered especially the change of the sign of the lift force has to be considered. There are several approaches to couple CFD with population balances. Beside the introduction of discrete bubble size classes as in the MUSIG model also different methods basing on transport equations for moments of the bubble size distribution can be found in literature. In the following the discussion focuses on the inhomogeneous MUSIG model (Krepper et al., 2008), but in general similar setups can be defined also for the methods of moments approaches.

As mentioned above a baseline model for adiabatic poly-disperse bubbly flows has been defined at HZDR as a basis for the further model development. The closure models used were mentioned in the previous chapter together with the uncertainties and shortcomings of these models. Although the models base on quite coarse approximations the validation results for the baseline model obtained so far look rather promising. Bubble columns and pipe flows with different geometries and a wide range of flow rates and bubble sizes were considered in this validation. The validation is done from most simple towards more complex cases which in general can be classified as:

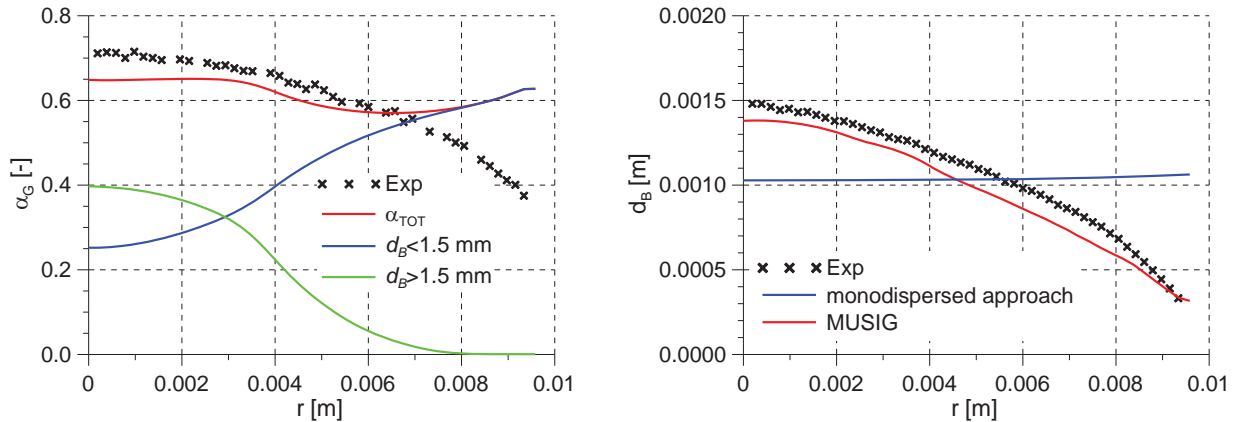
- adiabatic fixed mono-disperse (small bubbles, narrow bubble size distribution which does not significantly change along the flow path)
- adiabatic fixed poly-dispersed (small and large bubbles, but no significant change of the bubble size distribution along the flow path)
- adiabatic poly-dispersed with bubble coalescence & breakup
- flows with phase transfer (evaporation & condensation, chemical reaction).

Here small and large bubbles are defined according to the change of the sign of the lateral lift force according to the Tomiyama correlation.

While only one gas phase is considered in the case of fixed mono-disperse flows, for the other cases two gas phases (velocity groups) are considered in frame of the inhomogeneous MUSIG model. A larger number of MUSIG groups is used to reflect the bubble size distribution in a sufficient manner. Simulations results in comparison with experimental data can be found in the papers by Rzehak et al. (2013, 2014, 2015), Ziegenhein et al. (2015), Liao et al. (2015), Kriebitzsch et al. (2015). For the comparison with experimental data it is important to keep in mind that uncertainties exist not only for the simulations, but also for the experimental data.

The simulations clearly show that for poly-disperse flows one gas phase is not sufficient to reflect the characteristics of the flow as the separation of small and large bubbles due to the lateral lift force (Fig. 2). This was already shown in the paper by Krepper et al. (2005, 2008) and many others later on. Because of the demanding computational resources for the introduction of more than 2 bubble size groups most simulations done up to now stuck to this approximation. However simulation results seem to be quit sensitive to the bubble size at which the division for these groups is done. Only the average Sauter

diameter for each of the two groups is used in the closures discussed above, respectively. As some recent simulations show, this may be not sufficient for all cases.



**Fig. 2:** Application of the inhomogeneous MUSIG model to the test of subcooled boiling flow DEBORA: Without this approach the core peak cannot be described (Krepper et al. 2013)

There are many other effects which have to be considered to set up a proper CFD-simulation for poly-disperse bubbly flows. Among them there are effects of the numerical grid. Of course the grid independency has to be shown according to best practice guidelines (see e.g. Bestion 2010). Special attention has to be paid to the influence of cell sizes close to the wall. For transient simulation the time step should be small enough to keep the Courant–Friedrichs–Lewy number should be kept below 1 even for implicit schemes. In addition convergence has to be checked carefully. Considering all these issues together with a well-established and validated baseline models setup a consolidation of multiphase CFD allowing reliable predictions can be achieved in near future.

#### 4. CONCLUSIONS

The CFD-modelling of poly-disperse bubbly flows is challenging task. Still many phenomena on the local scale are not yet well understood which results from limits in measuring techniques for dense bubbly flows. For flows without chemical reactions and heat and mass transfer at least the momentum transfer between the phases, the modulation of the liquid phase turbulence and bubble coalescence and breakup have to be considered. These phenomena again result from different mechanisms for which different models are available in literature. Most of these closure models depend on the bubble size, i.e. a coupling of the transport equations with a population balance is required to provide the information on the local bubble size distribution. Most of the correlations for the bubble forces which reflect the momentum transfer were obtained from investigations on small to medium sized single bubbles. Often these correlations are extrapolated to situations with dense bubbly flows and to bubbles much larger than the original range of validity.

A more systematic investigation on the applicability of such closures seems to be necessary. Because of the high number of options as well as undetermined tuning parameters published simulation results are often hardly comparably to each other. For this reason a small number of baseline models should be established and applied to a larger number of experiments. Baseline model means that all closures including tuning parameters are fixed and applied to different cases without any change. This strategy was presented by Lucas (2014) and seems the only way to obtain some consolidation for the CFD-modelling in frame of the two- or multi-fluid model approach. Such a baseline model was formulated at HZDR for poly-disperse bubbly flows and published in several papers investigating different aspects of the model as

well as presenting validation on different cases. The validation shows a good agreement with many experimental data, but for some flow conditions also clear deviations occur. The identification of the shortcomings in the model which are responsible for these deviations is a challenging scientific task. This paper discusses the limitations of the present models in order to support this discussion.

Already now CFD for multiphase flows can provide valuable insights into flow phenomena and it can be used with some care to investigate the influence of variations of geometrical boundaries or flow conditions. The next step which has to be done now is to consolidate multiphase CFD to enable reliable predictions. CFD-grade experiments which not only provide data with high resolution in space and time but also comprise all relevant local parameter as gas volume fraction, velocity fields, turbulent fluctuations for all directions, bubble size distributions and in case of non-adiabatic flows temperature fields are required for the validation of the baseline models and later on to establish blind benchmark exercises.

## REFERENCES

1. D. Bestion, “Applicability of two-phase CFD to nuclear reactor thermalhydraulics and elaboration of Best Practice Guidelines”, *Nucl. Eng. Des.*, **253**, 311-321, (2012).
2. D. Bothe, M. Schmidtke, H.-J. Warnecke, “VOF-simulation of the lift force for single bubbles in a simple shear flow”, *Chem. Eng. Technol.*, **29**, 1048–1053, (2006).
3. J. Chahed, V. Roig, and L. Masbernat, “Eulerian–Eulerian two-fluid model for turbulent gas–liquid bubbly flows”, *Int. J. Multiphase Flow*, **29**, 23 (2003).
4. Ervin, E.A., Tryggvason, G., 1997. The rise of bubbles in a vertical shear flow. *J. Fluids Eng.* 119, 443–449.
5. Th. Höhne and J.P. Mehlhoop, “Validation of closure models for interfacial drag and turbulence in numerical simulations of horizontal stratified gas-liquid flows”, *Int. J. Multiphase Flow*, **62**, 1-16, (2014).
6. S. Hosokawa, A. Tomiyama, S. Misaki, T. Hamada, “Lateral Migration of Single Bubbles Due to the Presence of Wall”, *Proc. ASME Joint U.S.-European Fluids Engineering Division Conference (FEDSM2002)*, Montreal, Quebec, Canada, 2002.
7. J. Janet, Y. Liao, D. Lucas, “Heterogeneous Nucleation in CFD Simulation of Flashing Flows in Converging-Diverging Nozzles”, *Int. J. Multiphase Flow*, submitted, (2015)
8. I. Kataoka, A. Serizawa, A., D. Besnard, “Prediction of turbulence suppression and turbulence modeling in bubbly two-phase flow”, *Nucl. Eng. Des.*, 141, 145, (1993).
9. E. Krepper, R. Rzehak, C. Lifante, T. Frank, “CFD for subcooled flow boiling: Coupling wall boiling and population balance models”, *Nucl. Eng. Des.*, 255, 330– 346, (2013).
10. Y. Liao, and D. Lucas, “A literature review of theoretical models for drop and bubble breakup in turbulent dispersions”, *Chem. Eng. Sci.*, 64, 3389-3406, (2009)
11. Y. Liao, and D. Lucas, “A literature review on mechanisms and models of the coalescence process of fluid particles”, *Chem. Eng. Sci.*, 65, 2851-2864, (2010)
12. Y. Liao, D. Lucas, E. Krepper, M. Schmidtke, “Development of a generalized coalescence and breakup closure for the inhomogeneous MUSIG model”, *Nucl. Eng. Des.*, **241**, 1024 -1033, (2011)
13. Y. Liao, R. Rzehak, D. Lucas, E. Krepper, “Baseline closure model for dispersed bubbly flow: bubble coalescence and breakup”, *Chem. Eng. Sci.*, **122**, 336-349, (2015)
14. D. Lucas, E. Krepper, H.-M. Prasser, “ Development of co-current air-water flow in a vertical pipe”, *Int. J. Multiphase Flow*, **31**, 1304-1328, (2005).
15. D. Lucas, M. Beyer, L. Szalinski, P. Schütz, “A new database on the evolution of two-phase flows in a large vertical pipe”, *Int. J. Therm. Sci.*, **49**, 664-674, (2010).

16. D. Lucas and A. Tomiyama, "On the role of the lateral lift force in poly-dispersed bubbly flows", *Int. J. Multiphase Flow*, **37**, 1178-1190, (2011).
17. D. Lucas, M. Beyer, L. Szalinski, "Experimental database on steam-water flow with phase transfer in a vertical pipe", *Nucl. Eng. Des.*, **265**, 1113-1123, (2013).
18. D. Lucas, "A Strategy for the qualification of multi-fluid approaches for nuclear reactor safety", *CFD4NRS-5 Application of CFD/CMFD Codes to Nuclear Reactor Safety and Design and their Experimental Validation*, OECD/NEA & International Atomic Energy Agency (IAEA) Workshop, September 9–11, 2014, Zurich, Switzerland, (2014).
19. J.L. Marie, E. Moursali, S. Tran-Cong, "Similarity law and turbulence intensity profiles in a bubbly boundary layer at low void fractions", *Int. J. Multiphase Flow*, **23**, 227, (1997).
20. R. Rzehak, E. Krepper, C. Lifante, "Comparative study of wall-force models for the simulation of bubbly flows", *Nucl. Eng. Des.*, **253**, 41 (2012).
21. R. Rzehak and E. Krepper, "Closure Models for turbulent bubbly flows: A CFD study", *Nucl. Eng. Des.*, **265**, 701-711, (2013).
22. R. Rzehak and E. Krepper, "CFD modeling of bubble-induced turbulence", *Int. J. Multiphase Flow*, **55**, 138, (2013a).
23. R. Rzehak, E. Krepper, Th. Ziegenhein, D. Lucas, "A Baseline Model For Monodisperse Bubbly Flows", 10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries (CFD2014), Trondheim, Norway, (2014).
24. R. Rzehak and E. Krepper, "Bubbly flows with fixed polydispersity: validation of a baseline closure model", *Nucl. Eng. Des.*, submitted, (2015).
25. A. Tomiyama, H. Tamai, I. Zun, S. Hosokawa, "Transverse migration of single bubbles in simple shear flows", *Chem. Eng. Sci.*, **57**, 1849-1858, (2002).
26. A.A. Troshko and Y.A. Hassan, "A two-equation turbulence model of turbulent bubbly flows", *Int. J. Multiphase Flow*, **27**, 1965 (2001).
27. M. Schmidtke, M., "Investigation of the dynamics of fluid particles using the Volume of Fluid Method", PhD-Thesis University Paderborn (in German), (2008).
28. M. Simcik, M. Puncochar, M.C. Ruzicka, "Added mass of a spherical cap body", *Chem. Eng. Sci.*, **118**, 1-8. (2014).
29. T. Ziegenhein, R. Rzehak, D. Lucas, "Transient simulation for large scale flow in bubble columns", *Chem. Eng. Sci.*, **122**, 1-13, (2015).