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Technical Note

General guideline for closure model development for gas-liquid flows in the multi-fluid framework

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Abstract

The two- or multi-fluid approach is frequently used for Nuclear Reactor Safety (NRS)-related simulations of gas-liquid flows. To enable reliable predictions the closure models have to reflect the involved local physical phenomena at the non-resolved scale properly. To consolidate the CFD-modelling in the frame of the multi-fluid approach the so-called baseline model strategy was recently proposed (Lucas et al., Nucl.Eng.Des, 299, 2-11, 2016). The present technical note discusses a long-term strategy for the baseline model development and ways to obtain or improve closure models. Guidelines for the model development are given by listing requirements for appropriate closure models as well as frequently made mistakes. This is illustrated by examples for recent developments done for HZDR baseline models for poly-disperse bubbly flows.

Keywords: CFD, multi-fluid model, closure models

1. Introduction

CFD is increasingly used for nuclear reactor safety (NRS) relevant investigations. Following the requirement to keep NRS research always on state of the art it can be expected that the importance of reliable CFD-simulations will increase in the future. Accordingly, a solid strategy for model development and modelling framework is required.

There is a wide spectrum of NRS-relevant flow situations depending on the reactor type (e.g. PWR, BWR, Gen IV reactor concepts) and the components considered (e.g. primary and secondary circuit, passive systems, containment). Single phase and multiphase flow situations can occur. In this technical note, we discuss the status and further developments of CFD approaches for gas-liquid flows with some focus, but not exclusively on the primary circuit of PWRs and BWRs and corresponding passive systems. For such flows the two- or multi-fluid approach (Euler-Euler) is most frequently applied and often the only feasible one. Accordingly, this note is restricted to the application of the Euler-Euler approach and the strategy for its further development.

In real flows as well as in scale-resolved simulations at one position in space and time either gas or liquid is present. Contrarily, in the multi-fluid approach (see e.g. Ishii & Hibiki, 2006) the phases are represented by interpenetrating fields, which occur everywhere with a certain probability. By the averaging procedure that leads to the basic balance equations for mass, momentum and energy, all information on the gas-liquid interface reduces to integral transfer terms between the phases without explicit description of the local structure of the interfaces. However, interactions between the phases strongly depend on the structure of the interface. In consequence phase interactions and information that are characterizing the interfacial structure have to be considered by closure models. As recently discussed by Lucas et al. (2016) there is not yet a consensus in the community regarding the most appropriate closures what limits the reliability of CFD-simulations using the Euler-Euler approach. Since the closure models have to reflect the local phenomena a case by case tuning is not meaningful and instead a fixed set of closure models should be defined for certain flow conditions and applied to different cases without any modification. Accordingly, a so-called baseline model strategy was proposed by Lucas et al. (2016).

For NRS with the above mentioned focus, steam-water flows are most relevant. Different flow morphologies as bubbly flows, droplet flows and segregated flows with large interfaces can be distinguished. Each flow morphology requires separate closure models. They may occur simultaneously in one flow domain and transitions between these morphologies can be of importance. In addition for poly-disperse bubbly flows, it may be necessary to divide the gas phase into sub-phases reflecting bubbles of different size respectively. At HZDR a baseline model for poly-disperse bubbly flows basing on the inhomogeneous MUSIG (iMUSIG) approach (Rzehak and Krepper, 2015) and a model for segregated flows basing on AIAD (Algebraic interfacial area density, Porombka and Höhne, 2015) have been established. Especially the baseline model for poly-disperse flows with fixed model formulations and model parameters was validated on a large number of experiments (more than 150) for different flow geometries, flow rates and material systems (Liao et al., 2018 & 2019). In many flow situations, interfaces within a wide range of scales may occur, combining dispersed and segregated morphologies (Hänsch et al., 2012). To handle such flows, the innovative GENTOP (Generalized two-phase flow) concept was developed. It combines the iMUSIG and AIAD approaches and allows also simulating transitions between the different morphologies. The well validated baseline models are thus part of GENTOP. Recently, the concept was applied for a simulation of a boiling pipe, which includes flow pattern transitions (Höhne et al., 2017).

The baseline model concept (Lucas et al., 2016) was inspired by the fact that in many papers presenting CFD-simulations a "result-oriented" selection of closure models and coefficients is done, finally leading to an acceptable agreement with experimental data obtained in a single or few experimental runs. However, such model setups are usually not transferable to other flow situations and the capabilities for predictions are strongly limited. This technical note focuses on the questions how an improvement of closure models can be obtained to achieve more generality of the model setups and improve the predictive capabilities of CFD in the multi-fluid framework.

2. General requirements for closure models

The closure models used in an Euler-Euler CFD-simulation should reflect the **local physical phenomena** occurring on the non-resolved scale (non-resolved interfaces and non-resolved turbulent fluctuations - different filters may apply here depending on the turbulence model and the flow morphology). This has several consequences:

- More detailed understanding and knowledge on the physics of such local flow phenomena is required.
- The closure models have to reflect the physics of all important local phenomena properly, including their dependency on material parameter and on different local flow characteristics.
- The set of closure models used in a CFD-simulation should not be defined based on the global flow situation, but based on the expected local flow phenomena and local flow characteristics.

Such local flow characteristics may be very similar, e.g. in different bubbly flow configurations as bubbly pipe flows, bubble columns, air-lift reactors or boiling flows in passive systems. For this reason a unified setup should be applicable for such flows. This justifies that the baseline strategy proposed by Lucas et al. (2016) should be applicable. The strategy should not be repeated in detail, but the main ideas are as follows:

- include closure models for all phenomena that may occur in the specific flow situation (if the model reflects the physics well it should blend out automatically in case of local non-importance),

- define a set of closures that reflect the physics in the best way according to our present knowledge,
- fix all open parameters depending on experiences from previous simulations,
- apply the fixed model setup under consideration of the Best Practice Guidelines (BPG, see e.g. Bestion, 2012) to a large number of different flow configurations and material systems,
- try to include flow situations for which the single phenomena are of different importance and might be negligible,
- identify the most severe shortcomings of the model,
- figure out an improved model,
- update the baseline model (only) in case there is an overall improvement or the new model definitely reflects the local phenomenon in a more physical way.

This strategy could also be helpful to avoid frequently made mistakes as:

- case by case tuning of models,
- modifying more than one sub-model at the same time – it will be not clear from which modification the observed differences in the results originate from, or
- closure model development based on integral data without consideration of the local physical phenomena, e.g. deriving correlation of the lift force coefficient based on gas volume fraction profiles.

It has to be considered that the simulation results arise from a complex interaction between all sub-models. In case of closure model development based on integral data, the derived model will combine in itself all uncertainties of the whole setup. It cannot be expected that such a model is universal and transferrable to another flow situations as the one it was derived from.

Also, it should always be considered that experimental data have uncertainties which are often not well specified. Beside statistical errors, which usually can be well evaluated, also possible systematic errors resulting from the experimental setup as well as from the measuring technique may be of importance. The agreement between simulation results and experimental data is definitely no single measure for the scientific quality of a work done. Much more important is to have a well-based model and numerical setup, a consequent consideration of the BPG, and a throughout analysis of the results including a sound interpretation of reasons for observed deviations.

The discussion above directly leads to the question how a local flow situation can be characterized. Basic parameters which determine the local physical phenomena of multiphase flows like phase interactions, turbulence production and dissipation and which consequently could be used as input parameters for a closure model are:

- parameters characterising the continuous phase:
    - shear rate and vorticity of the continuous phase,
    - turbulence parameters of the continuous phase (e.g. Reynolds stresses, turbulent kinetic energy, dissipation rate of the turbulent kinetic energy, turbulent viscosity),
- parameters characterizing the local situation regarding the phases:
    - phase fractions,
    - interface morphology (e.g. characterized by a local bubble or drop size distribution, bubble shape or aspect ratio),
    - relative velocities of the phases,
- specific parameters for inclusion of equations for energy and species:
    - temperatures or any variables characterizing the local energy of the phases,
    - species concentrations in the phases,
- parameters specifying the necessity for a special treatment at boundaries:
    - distance from the wall in the region near the wall,
    - distance from a large interface in the region near the interface.

Combinations of these parameters among each other and with material properties as, e.g. bubble Reynolds number, Morton number or Eötvös number may be used in closure models. In contrast parameters like a pipe diameter or superficial velocities are not appropriate to be used in closure models. The above mentioned parameters span a multi-dimensional matrix to build closure models. Even if for some phenomena only a few of these parameters might be important, an ideal closure model considering all the remaining dependencies is difficult to derive. Indeed the available closure models are far away from having this generality. For this reason, neglecting such dependencies should be considered as a source of uncertainty as soon as the parameter deviates from the conditions the closure model was derived for. The limited knowledge on local flow phenomena caused by limitations in currently available measurement techniques is the most important reason for the present shortcomings of the existing closure models.

Appropriate closure models clearly differ for different flow morphologies that are involved in gas-liquid flows. Here at least bubbly flows, droplet flows and segregated flows, which are characterized by a large interface, should be distinguished. One long term goal is to have a model setup which can cover all these flow morphologies including transitions between them. One possible way to construct such a model was presented some years ago by the introduction of the GENTOP-approach (Hänsch et al., 2012). Baseline models for different ranges of applicability can be brought together in such a framework. However, it has clearly to be stated that the present state of CFD in the multi-fluid approach is far away to reach this goal. Still we are struggling to establish baseline models for special flow morphologies with a limited range of applicability regarding the above listed values characterizing the local flow situation.

3. Ways to improve closure models

For the improvement of existing closure models or the development of new ones, it is essential to separate effects, i.e. to exclude or at least minimize the influence of other phenomena on the one under consideration. Generally there are three ways to improve or to establish closure models: 1) theoretical considerations, 2) dedicated experiments and 3) dedicated Direct Numerical Simulations (DNS). For some model adaptions also Large Eddy Simulations (LES) may be applicable.

The derivation of theoretical models and analytical solutions is usually only possible for strongly simplified flow situations. Most of the closures used are semi-empirical, i.e. the structure of the model is obtained from theoretical considerations, while coefficients are adapted on experimental results.

The baseline model for poly-disperse bubbly flows was established over several years. It defines the closure models for basic hydrodynamics as momentum exchange between the phases (bubble forces), the turbulence modelling in the RANS framework including models for bubble-induced turbulence (BIT) and also model for bubble coalescence and breakup (Liao et al., 2015). It has to be considered that e.g. the definition of bubble forces results from theoretical considerations of different phenomena, but the migration of the bubbles, which finally can be observed in a flow, results just from the sum of these forces. There are several papers defining the closure models and presenting validation examples (Rzehak et al., 2017; Ziegenhein et al., 2017; Liao et al., 2018; Liao et al., 2019). Extensions for flows with phase transfer are also available including a few validation cases (Liao and Lucas, 2016). Depending on the flow situation fixed-mono-disperse cases, fixed poly-disperse cases, and cases which require the consideration of bubble coalescence and breakup have to be distinguished. “Fixed” means that the bubble size distribution does not considerably change along the flow path or only changes caused by pressure changes. In consequence bubble coalescence and breakup can be neglected. Mono-disperse flows are characterized by a narrow bubble size distribution and the fact that almost all bubbles are smaller than the critical bubble diameter where the lateral lift force changes it sign. In case of poly-dispersity usually a mixture of bubbles smaller and larger than this critical diameter occur and, consequently, the iMUSIG approach (Krepper et al., 2008) should be applied by considering at least two velocity groups. Up to now the baseline model for poly-disperse flows was validated on more than 150 experiments including different geometries, flow parameter and material systems. Details on the validation can be found in papers by Rzehak & Krepper, (2013a); Liao et al., (2015); Ziegenhein et al., (2015); Rzehak & Krepper, (2015); Rzehak et al., (2015); Liao et al., (2016); Rzehak et al., (2017); Ziegenhein et al., (2017); Liao et al. (2018), Liao et al. (2019). This large number of validation cases overall show that the model already provides good results for many cases, but there are clear deviations for others. It is a scientific challenge to figure out the reasons for the deviations and to improve the modelling accordingly. Examples for recent and ongoing research to improve the baseline model for poly-disperse bubbly flows will be presented in the following.

Recently a new model for bubble-induced turbulence (BIT) was developed in co-operation with TU Dresden based on DNS data for a bubbly channel flow with up to 2880 spherical bubbles (Santarelli et al., 2016). There is a background liquid flow causing some shear-induced turbulence, but BIT is dominant. Based on the spectrum of the turbulent kinetic energy a suitable time scale for the dissipation rate was defined. From the budgets of the turbulent kinetic energy and the dissipation rate coefficients for the source terms in the SST-k-ω model were derived. A special procedure described by Ma et al. (2017) was developed to determine these coefficients for the RANS model from the DNS data. In the RANS simulations other models (as e.g. for the drag and lift force) were adapted to meet the DNS data and thus to minimize their influence on the derived model. Finally a new BIT model was established (Ma et al., 2017). It was tested by replacing the previous BIT model (Rzehak & Krepper, 2013b) in the baseline setup for a large number of the test cases. The overall comparison showed similar results for most cases and an improved agreement with experimental results for a few cases (Fig. 1). Based on the fact that it leads to a (slight) overall improvement, but particularly due to the better physical substantiation and the fact that the new model does not have undetermined constants like the previous one, it was decided to update the baseline model by this new BIT-model of Ma et al., 2017. Comparisons of simulations results obtained by the new baseline model with experimental data are presented by Liao et al., 2018 and 2019.

It should be noted that also this model has limitations. It bases only on few datasets and includes the assumption of spherical bubbles. An extension or revision of the model based on dedicated experimental data and DNS data for deformable bubbles will be necessary in future. It can be expected that increasing DNS capabilities as well as improved measuring techniques will give an improved input in future.

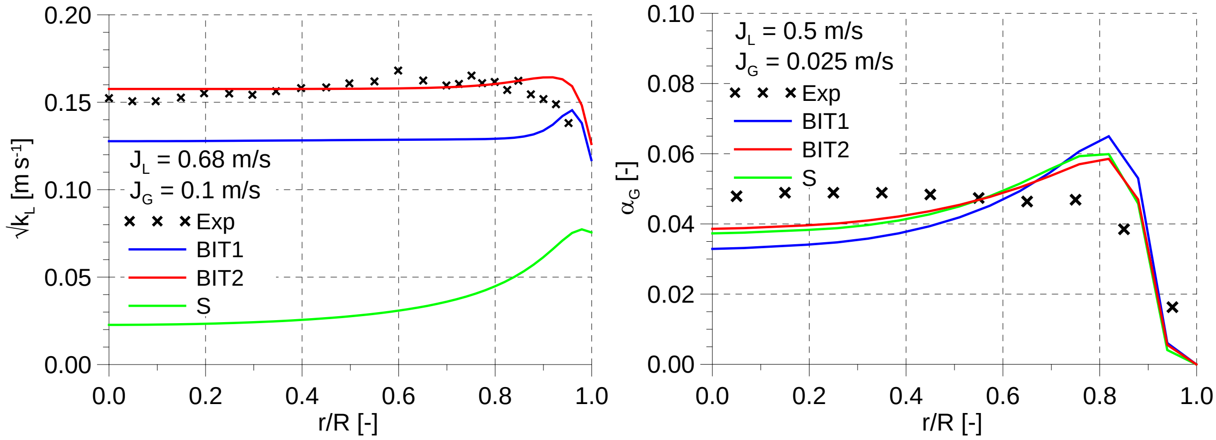

Fig. 1: Comparison of different BIT models (BIT 1 - Rzehak & Krepper, 2013b; BIT 2 Ma et al., 2017; S - Sato et al., 1981) a) Measured and calculated turbulent kinetic energy for the experiment by Shawkat et al. (2008), b) Measured and calculated gas volume fraction for the experiment of Hosokawa et al. (2007)

Many discussions can be found in literature on the lateral lift force (e.g. Dijkhuizen et al., 2010, Aoyama et al., 2017, Hessenkemper et al., 2019). The widely used correlation by Tomiyama et al. (2002) is part of the baseline model. It was obtained based on experiments with single bubbles in a laminar linear shear field in highly viscous liquid. i.e. atlarge Morton number. Nevertheless, air-water and steam-water experiments, with a Morton number several orders of magnitude lower, showed a good agreement of this correlation at least for the critical diameter where the lift force changes its orientation with respect to shear rate (Lucas & Tomiyama, 2011). Also the baseline model validation suggests that the model performs well even for turbulent, low viscous systems with dense bubbly flow. Nevertheless, the results are for some reason quite sensitive, especially with regard to the critical diameter. Shifting the critical diameter slightly may lead to a considerable change of the fraction between large and small bubbles in cases for which the peak of the bubble size distribution is close to this diameter. To account for this, dedicated experiments on lift force for low viscous systems (air-water and air-water + additions) are conducted. For this aim a new methodology was developed (Ziegenhein et al, 2018). The preliminary results show that the Tomiyama correlation agrees well also for such conditions in case the modified Eötvös number is calculated based on the bubbles major axis (Fig. 2). However, in case of clean systems as in most air-water and steam-water experiments the major axis should not be calculated by the Wellek correlation (Wellek et al., 1966) as frequently done in connection with the lateral lift force. The Wellek correlation is only applicable to contaminated systems. A bubble shape correlation, which fits for many experimental air-water data was published by Ziegenhein et. al. (2017). In consequence of this shape function the critical diameter shifts from about 5.8 mm down to about 5.2 mm which already may have an influence on the above mentioned cases. A comprehensive experimental series with some further improvements of the methods led to better statistics compared to the results shown in Fig. 2 (Hessenkemper et al., 2019). It is planned to update the baseline model after finishing the validation for the above mentioned database.

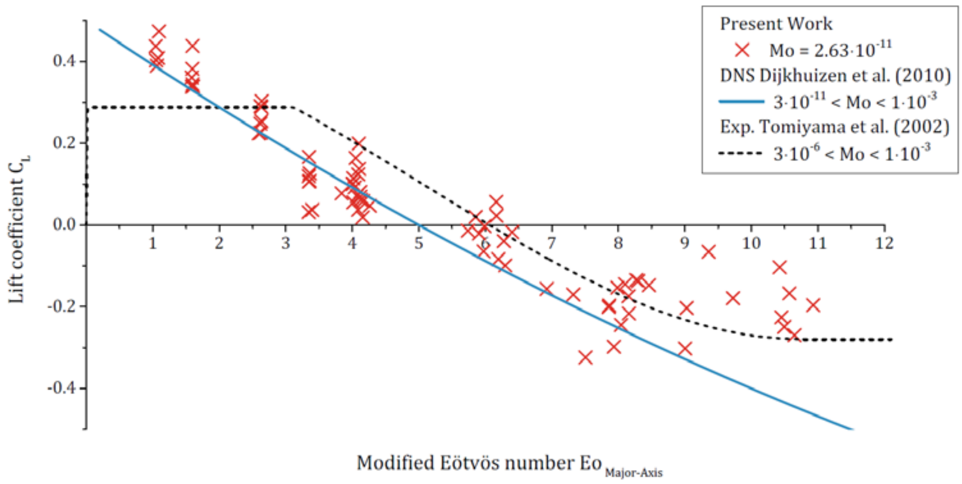

Fig. 2: Experimental determined lift force coefficient for air water-system (x) based on the modified Eötvös number in comparison with DNS results obtained by Dijkhuizen et al. (2010) and the Tomiyama correlation (from Ziegenhein at al., 2018).

It has to be pointed out that also the new C_L-correlation and shape function will be obtained under low turbulence condition on single bubbles. Influences of turbulence, high shear rates, gas volume fraction a.s.o. have to be further investigated by dedicated experiments or DNS. Probably, such dependencies can be added as correction factors or modifications to existing correlations. It is not meaningful to develop correlations that focus on these dependencies without considering that they should collapse in the limit of diluted, low turbulent flows with the aforementioned correlation.

Another clear limitation of the present baseline model is the near wall treatment. As pointed out by Lucas et al. (2007) the bubble dimension becomes important at the wall as soon as they become larger than the cell size. The near wall gas volume distribution is strongly influenced by the bubble dimension and shape. In the 1D model of Lucas et al. (2007) a deformation force was introduced, which keeps the bubble centre of mass away from the wall. Form the balance equations a bubble centre of mass volume fraction profile is obtained which can be transferred by a convolution with a bubble shape function to the gas volume fraction profile. It is quite difficult to apply such a procedure to a general purpose CFD-code on unstructured grids. A good compromise may be the procedure proposed by Lubchenko et al. (2018) who use the structure of the turbulent dispersion force to ensure that the gas volume fraction near the wall fits the one resulting from the bubble geometry. It seems to be worth to test this methodology in frame of the baseline model. Independently a more throughout modelling of near wall effects remains an important task.

Further requirements for improvement of the baseline model for poly-disperse flows result from the insufficient consideration of swarm effect on all the bubble forces and the still non-satisfying generality of the models for bubble coalescence and breakup.

As last point a limitation should be mentioned, which may be important for the simulations of bubbly flows in core cooling channels. For pipe flows with high liquid superficial velocities, e.g. for the 4 m/s liquid superficial velocity cases in a 51.2 mm (inner diameter) pipe, intermediate peaks of the gas volume fraction are observed (see, e.g. Figs. 7 & 8 in Lucas et al., 2007). Similar observations were made by other researches. In contrast, due to the large velocity gradients and the occurrence of small bubbles (the regime is usually called finely dispersed flow) the models lead to predictions of a pronounced wall peak. Here, obviously other effects, which are not well understood and accordingly not part of the model play a role and surpass the lift force. It can be speculated that large vortex structures maybe the reason, but to our knowledge there is no throughout explanation or model for this observation. Similar phenomena, which are not consistent with the present modelling, were observed in flows around an obstacle, see Krepper et al. (2009). In consequence, the baseline model for poly-disperse bubbly flows (as all other non-tuned models) should be applied with care for flows with very high turbulence and/or shear rates.

4. Conclusions

A considerable progress was achieved on CFD-models in the multi-fluid context during the last 25 years. By applying different closure models for the single non-resolved phenomena comprehensive knowledge on perspectives and limits of the modelling was obtained. To go beyond this stage a consolidation of multiphase CFD is required. The only possible way seems to be the baseline model strategy. The corresponding fixed model setup(s) have to be improved step by step. This only can be achieved by new or improved closure models on a sound physical basis. They should be valid for a certain range of local flow parameters listed in the paper. The main difficulty results from limitations in knowledge on local phenomena caused by limitations of the current available measurement techniques. CFD-grade experiments (Manera and Petrov, 2019) which include information on these flow parameters in high resolution in space and time are required beside dedicated DNS databases as basis for the further development.

The recent, ongoing and planned activities on the HZDR baseline models illustrate some ways for such model developments. They are very challenging and time-consuming. It would be wishful to go ahead with joint effort to solve the comprehensive tasks. The paper aims to establish a guideline how such developments should be done.

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