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Validation of closure models for interfacial drag and turbulence in numerical simulations of horizontal stratified gas–liquid flows

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ABSTRACT

The development of general models closer to physics and including less empiricism is a long-term objective of the activities of the HZDR research programs. Such models are an essential precondition for the application of CFD codes to the modeling of flow related phenomena in the chemical and nuclear industries. The Algebraic Interfacial Area Density (AIAD) approach allows the use of different physical models depending on the local morphology inside a macroscale multi-fluid framework. A further step of improvement of modeling the turbulence at the free surface is the consideration of sub-grid wave turbulence that means waves created by Kelvin–Helmholtz instabilities that are smaller than the grid size. In fact, the influence on the turbulence kinetic energy of the liquid side can be significantly large. The new approach was verified and validated against horizontal two-phase slug flow data from the HAWAC channel and smooth and wavy stratified flow experiments of a different rectangular channel. The results approve the ability of the AIAD model to predict key flow features like liquid hold-up and free surface waviness. Furthermore an evaluation of the velocity and turbulence fields predicted by the AIAD model against experimental data was done. The results are promising and show potential for further model improvement.

1. Introduction

In the last decade, applications of Computational Fluid Dynamic (CFD) methods for industrial applications received more and more attention, as they proved to be a valuable complementary tool for design and optimization. The main interest towards CFD consists in fact in the possibility of obtaining detailed 3D complete flow-field information on relevant physical phenomena at lower cost than experiments.

Stratified two-phase flows are relevant in many industrial applications, e.g. pipelines, horizontal heat exchangers and storage tanks. Special flow characteristics as flow rate, pressure drop and flow regimes have always been of engineering interest. Wallis and Dobson (1973) analyzed the onset of slugging in horizontal and near horizontal gas–liquid flows. Flow maps which predict transitions between horizontal flow regimes in pipes were introduced, e.g. by Taitel and Dukler (1976) and Mandhane et al. (1974). The most important flow regimes are smooth stratified flow, wavy flow, slug flow and elongated bubble flow. Taitel and Dukler (1976) explained the formation of slug flow by the Kelvin–Helmholtz instability. They also proposed a model for the frequency of slug initiation (Taitel and Dukler, 1977). The viscous Kelvin–Helmholtz analysis proposed by Lin and Hanratty (1986) generally gives better predictions for the onset of slug flow.

Typically free surfaces manifest as stratified, wavy or slug flows in horizontal flow domain where gas and liquid are separated by gravity. The simulation of slug formation is a sensitive test case for the model setup regarding the quality of the models for interfacial friction respectively momentum transfer. A general overview on the phenomenological modeling of slug flow was given by Hewitt (2003) and Valluri et al. (2008). Various multidimensional numerical models were developed to simulate stratified flows: Marker and Cell (Harlow and Welch, 1965), Lagrangian grid methods (Hirt et al., 1974), Volume of Fluid method (Hirt and Nichols, 1981) and level set method (Osher and Sethian, 1988). These methods can in principle capture accurately most of the physics of the stratified flows. However, they cannot capture all the morphological formations such as small bubbles and droplets, if the grid is not sufficiently small. One of the first attempts to simulate mixed flows was presented by Cerne et al. (2001) who coupled the VOF method with a two-fluid model in order to bring together the advantages of both formulations.

Mouza et al. (2001) were numerically investigating the characteristics of horizontal wavy stratified flow in circular pipes and

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rectangular channels. They used the CFD code CFX for a simulation of the gas and liquid flow in separate domains, setting the time averaged values of interfacial velocity and shear as boundary condition at the free surface. They used the data set by Fabre et al. (1987) as test case for rectangular channel flows. In a validation study for a preliminary version of the NEPTUNE_CFD code, Yao et al. (2003) conducted 2D-simulations of the experiments by Fabre et al. (1987) as one of three test cases. They report a qualitatively good agreement of the calculated profiles of velocity, turbulence kinetic energy and turbulent shear stresses for the cases with zero and medium gas velocity. But some quantitative deviations occur. In the case with high gas velocity (case 400), the code fails in predicting the turbulence parameters, which they account to the inability of the 2D-model to capture the transverse flow reported for that experiment. Terzuoli et al. (2008) used the data set as test case for a cross-code comparison of three different CFD codes and to validate the free surface flow models of the respective codes. They compared the scientific code NEPTUNE_CFD and the commercial codes ANSYS CFX and FLUENT. By comparing 2D and 3D simulations with the experiments they found that three-dimensional effects should not be neglected. Furthermore they pointed out the fundamental role of the drag modeling at the free surface. A series of five different experiments were used by Coste et al. (2012) for the validation of the NEPTUNE_CFD code, the experimental cases 250 and 400 from Fabre et al. (1987) being among them. They were able to achieve a good agreement of their numerical data with the experimental data for velocity and turbulence in case 250. For case 400 they found a significant deviation between their simulations and the experiment, which they account to the inability of the NEPTUNE_CFD code to predict the transverse flows occurring in case 400.

In general, CFD simulations for free surface flows require the modeling of the non-resolved scales. For modeling of interfacial transfers it is necessary to select the adequate interfacial transfer models and to determine the interfacial area. The numerical solution can resolve the statistically averaged motion of the free surface (including waves) which may not be too small relatively to the channel height and to the characteristic length of the spatial discretization. However, the detailed structure of interacting boundary layers of the separated continuous phases and surface ripples cannot be resolved. Instead, its influence on the average flow must be modeled.

Non-resolved small scale structures of the interface have influence on mass, momentum and heat transfer between the phases. The type of required models depends on the general modeling approach used. To model the momentum transfer, e.g. in the frame of the two-fluid model the correlations for the interfacial drag are used. In the past due to the lack of appropriate models often drag correlations valid for bubbly flows or correlations developed for 1D codes were used to simulate the interfacial momentum transfer at the free surface. Such approaches do not properly reflect the physics of the phenomena.

From this point of view, in the framework of the two-field model, it is interesting to consider, close to the interface, an anisotropic momentum exchange between liquid and gas. This is done for the Algebraic Interfacial Area Density (AIAD) model (Höhne and Vallée, 2010; Höhne et al., 2011) which allows using different models to calculate the drag force coefficient and the interfacial area density for the free surface and for bubbles or droplets.

A further step of improvement of modeling the turbulence is the consideration of non-predicted free surface waves or so called "sub-grid waves" that means waves created by Kelvin–Helmholtz instabilities that are smaller than the grid size. So far in the present code versions they are neglected. However, the influence on the turbulence kinetic energy of the liquid side can be significantly large. A region of marginal breaking is defined according Brocchini and Peregrine (2001). In addition turbulence damping functions should cover all the free surface flow regimes, from weak to strong turbulence.

2. Modeling free surface flows

2.1. The CFD approaches applicable to free surface flow

The three main types of two-phase CFD, namely the RANS approach, the space-filtered approaches (such as LES methods), and the pseudo-DNS approaches are in principle applicable to free surface flow (see Bestion, 2010a,b). Table 1 shows the main characteristics of these methods. If only two continuous fields (continuous liquid and continuous gas) exist in the flow without any bubble below the free surface and without any droplet in the gas flow, a one-fluid approach (homogeneous model) is applicable together with an Interface Tracking Method (ITM) to predict the free surface.

Since there may be some bubble entrainment below the free surface, a two fluid approach was also used to be able to deal with various types of interface configurations including both large interfaces (free surface) and interface of dispersed fields (bubbles, droplets). Detailed derivation of the two-fluid model can be found in the book of Ishii and Hibiki (2006).

On both sides of the free surface, shear layers are expected which require a specific attention since complex phenomena with turbulent transfers coupled to possible interfacial waves take place. It was found necessary to be able to track the interface position in order to treat this zone in a similar way as a wall boundary layer using wall functions. When trying to use a two fluid approach, the development of an interface recognition method was found necessary.

The AIAD method belongs to the third time and space filtering type. Because the model can be directly applied for industrial cases it is classified as a macroscale model (Fox, 2013). A different approach in this group for instance is done in the NEPTUNE code (see Coste et al., 2007; Coste and Laviéville, 2009).

Table 1
Time and space filtering of the methods applicable to free surface flow (Bestion, 2010a).

Type of model	Pseudo-DNS	Filtered approaches LES (VLES, LEIS)	RANS (URANS, TRANS)
Time or ensemble averaging	No	No	Yes
Space filtering	No	Yes	No
Treatment of eddies	All eddies simulated	Large eddies simulated Small eddies modeled	No eddy simulated
Treatment of free surface waves	All wavelength simulated	Large wavelength simulated Small wavelength modeled	No wavelength simulated
Required turbulence models	No model	Sub-grid turbulent diffusion for momentum and energy	Reynolds stress tensor Turbulent diffusion of energy
Required closure models at free surface	No model	Interfacial friction Effects of sub-grid wavelength on interfacial transfers	Interfacial friction Effects of non-predicted free surface waves