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TOPIC ②

MECHANICS

2.1 Thermal-hydraulics

2.1.2 Two phase flow modelling and simulation

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1. Introduction

Computational fluid dynamics (CFD) is to an increasing extend being adopted in nuclear reactor safety analyses as a tool that enables specific safety-relevant phenomena occurring in the reactor coolant system to be better described (Smith and Hassan, 2008; Smith et al. 2010). CFD has the potential to handle 2D/3D geometries of arbitrary complexity and has, for single-phase flows, already reached a certain level of maturity. For two-phase flows, Bestion (2010) lists 26 nuclear reactor safety issues that could benefit from investigations at the CFD scale.

Gas-liquid flows appear in quite different topological or morphological configurations (flow regimes). The special significance of the flow regime arises from the fact that the various physical transfer processes taking place across the interface strongly depend on the flow regime. Therefore, the selection of adequate numerical methods and physical models for interfacial transfer requires the identification of the flow regime first. While disperse flows can now be well described, trustworthy closure relations for other flow regimes are still missing.

In this lecture we give an introduction into the most popular CFD methods for general multiphase flows (all are based on the concept of interpenetrating continua, see below). We highlight the assumptions underlying these methods as well as their achievements and limitations and also discuss some trends in advancement of the modeling capabilities of the two-fluid model. For comprehensive overviews on methods and models for CFD of multiphase flows we refer to textbooks (Ishii and Hibiki, 2006; Crowe et al. 2011).

2. Averaged balance equations

The starting point for any mathematical or computational description of fluid flow is given by the local conservation equations for mass, momentum and energy. These equations are valid in each bulk phase while at the interface, which separates the two phases, so-called jump conditions apply. While these equations are well known, it is often neither possible nor reasonable to solve them for technical two-phase flow problems. This is in particular true for nuclear applications where the length scales range from the diameter of the smallest bubble to (e.g.) the diameter of the reactor pressure vessel. Instead of solving directly the local equations, which would require to resolve all these scales by a direct numerical simulation, an averaging procedure is introduced which smears out details of the flow and interfacial structure. Common averaging procedures employ time, volume or ensemble averaging (Drew and Passman, 1999). Here, we consider volume averaged equations but note that time or ensemble averaging yields formally similar equations. The resulting averaged fields are smoothed and the respective equations can be solved on grids that are much coarser than the ones required for the local equations. Unlike the local equations, the volume averaged equations are valid in the entire computational domain and the phases constitute so-called interpenetrating continua (fields). However, the set of averaged equations is not closed (i.e. there are more unknowns than equations). To reduce the number of unknowns it is commonly assumed that both phases share the same pressure field. For the unknown turbulent stresses a turbulence model is applied (a topic that is not covered here). The remaining equations needed for closure are provided by so called constitutive laws.

3. Models for interpenetrating continua

Two-phase flows usually involve some relative motion of one phase with respect to the other. Within the continuous field approach, there are three main modeling concepts to describe this relative motion and to close the set of equations. These concepts differ in their complexity and therefore have different ranges of applicability. We introduce these models in increasing order of complexity and discuss first the homogeneous Model (HM), then the algebraic slip model

(ASM) and the closely related drift-flux model (DFM) and finally the most general two-fluid model (TFM) as well as some of its modern extensions.

3.1 Homogeneous model

The homogeneous model (HM) is the simplest model within the continuous field approach. It assumes *mechanical equilibrium* which means that there is no relative velocity of the phases within the averaging volume so that both phases move with the same velocity. An equivalent assumption for closure of the two interpenetrating energy equations is thermal equilibrium which means that both phases have the same temperature. Then, the homogeneous model involves four conservation equations, namely those for the mass of both phases and for the momentum and energy of the mixture.

From computational point of view, the assumption that the two phases share the same velocity field is reasonable for two remarkably distinct situations. The first one refers to dispersed flow, while the second corresponds to flows were the phases are well separated. Computationally, the distinction between dispersed and separated phases is mainly a matter of the length scale down to which the flow is resolved, i.e. a matter of the size of the averaging volume. This length scale of averaging is itself usually related to the grid size chosen in a computation.

An example for application of the homogeneous model for separate flows is given by flows under strong influence of gravity such as stratified or wavy flow in a horizontal duct. In this case, the volume fractions of the phases are equal to one or zero everywhere except at the interface. In this situation it is meaningful to use a single velocity field. Because the interface is well resolved by the grid the surface tension force needs to be considered in principle. However, within the homogeneous model it is usually neglected. The homogeneous model may also be used for disperse flow supposed the phases have similar density and buoyancy forces may be neglected.

3.2 Algebraic slip and drift-flux model

The algebraic slip model and drift-flux model can be considered as a generalization of the homogenous model. Both models do not assume that the phases are in mechanical equilibrium. So the phase velocities are allowed to differ from each other and consequently also differ from the mixture velocity. The main assumption of both models is that the relative velocity between the phases (respectively the drift velocity of one phase) can be approximated by an algebraic expression. The drift-flux model is usually applied in its one-dimensional form (where the average is over the channel cross-section).

3.3 Standard two-fluid model (Euler-Euler model) and its advanced variants

The mathematical basis of the two-fluid model is given by the volume-averaged conservation equations of mass, momentum and energy for both phases (or by the time-averaged counterparts, respectively). Thus the two-fluid model consists of six partial differential equations (six equation model). The momentum/energy equations of the two phases are coupled through interfacial transfer terms which need to be modeled to close the system of equations. Mathematically, the interfacial momentum transfer terms are given by the integral of the dynamic pressure and viscous stress distribution over that part of the interface that lies within the averaging volume. In analogy to a rigid spherical particle moving in creeping flow (where these integrals can be solved analytically) the interfacial momentum transfer terms are modeled as a linear superposition of a drag force (the most important hydrodynamic force), a virtual mass force and a history force (which is usually neglected) as well as further forces such as a transversal lift force, turbulent dispersion force and a wall-lubrication force. For the

drag coefficient various relations have been proposed in literature and for the lift force a generally accepted model is still missing. Nevertheless, is can be noted that for disperse flows the two-fluid model has reached a certain level of maturity and can be applied with confidence. The same is, however, not true for other flow regimes (wavy flow, slug flow, churn-turbulent flow) where reliable multi-dimensional closure relations for the interfacial forces are often missing. As an example for application of the two-fluid model we consider the investigation of mixing phenomena in a large-scale bubble plume (Dhotre and Smith, 2007), a topic that is related to the issue of pressurized thermal shocks in pressurized water reactors.

One important assumption of the two-fluid model for disperse flows is that the particle diameter is small as compared to the averaging volume (i.e. the mesh cell). Another assumption of the standard two-fluid model is that the flow is mono-disperse (i.e. all particles have the same size). The latter assumption is rather restrictive since in gas-liquid flows breakup and coalescence are quite common and lead to a spectrum of bubble diameters. To overcome the restriction of mono-disperse flow, different conceptual extensions of the two-fluid model have been proposed. In the following, we discuss three of them.

The **four-field two-fluid model** (Lahey and Drew, 2001) considers two fluids or phases, which are denoted here as "liquid" and "vapor". The basic idea is that each phase may be continuous in some regions of space while it may be disperse in some other regions of space. Typical examples are given by the slug flow and annular flow regimes. In the four-field two-fluid model the four fields are given by continuous liquid, continuous vapor, disperse liquid and disperse vapor. For each of these four fields separate transport equations for mass, momentum and energy are solved (i.e. 12 equations in total). Similar to the two-fluid model these equations are coupled by mass/momentum/energy transfer terms which must be modeled.

Another promising concept to overcome the mono-disperse flow limitation of the standard two-fluid model flow is based on the introduction of size groups and **population balance modeling**. In this approach the disperse phase is divided in M classes. Each class covers its own range of bubble volume (respectively volume equivalent diameter) and is treated as a separate field. For each class a mass balance equation and a momentum equation is solved leading in total to M+1 coupled continuity as well as momentum equations. Depending on M this approach can consume extensive computer resources. To limit the computational costs, Lo (1999) proposed the so-called Multiple Size Group (MUSIG) model. MUSIG assumes that all the velocities of the different particle classes can be algebraically related to the average velocity of the disperse phase. Therefore, only one momentum equation is solved for the disperse phase. Recently, Frank et al. (2008) proposed the inhomogeneous MUSIG model which solves for M bubble classes N momentum equations. It is $N < M$ which means that some bubble classes share the same velocity field.

The third approach is based on the intuition that in a two-phase flow not only the volumetric concentration of the phases is important, but also the interfacial area concentration (Ishii and Mishima, 1981). The available interfacial area influences not only the viscous and form drag but is also of special relevance when heat or mass transfer processes take place at the interface. Ishii (1975) proposed to determine the interfacial area concentration by solution of an **interfacial area transport equation** (IATE). Then, the bubble diameter needed for the specification of the drag force and particle Reynolds number is no more a global quantity (like in the standard two-fluid model) but a local one which can vary in space. The interfacial area transport equation can be derived by considering the fluid particle number density equation analogous to Boltzmann's transport equation (Kocamustafaogullari and Ishii, 1995). The major problem in development of the IATE is the development of adequate models for the source/sink terms due to breakup and coalescence.

With one transport equation for the interfacial area concentration a change of the particle size can be modeled but not a change of the particle shape. To overcome this limitation the concept of two-group interfacial area transport has been proposed (Ishii et al., 2003). In this approach the bubbles are treated in two groups and for each group a separate transport equation for the interfacial area concentration is solved. The first group represents spherical and distorted (e.g. ellipsoidal) bubbles while the second group represents cap-type bubbles and elongated bubbles which are typical for slug flow. It is hoped that this approach can replace the traditional flow regime maps and regime transition criteria that do not dynamically represent the changes in the interfacial structure. However, at present the one-group and two-group IATE model is most often applied in its one-dimensional form.

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