International Journal of Multiphase Flow 000 (2017) 1–18

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

journal homepage: www.elsevier.com/locate/ijmulflow

A deterministic and viable coalescence model for Euler–Lagrange simulations of turbulent microbubble-laden flows

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ARTICLE INFO

Article history:
Received 16 June 2017
Revised 25 September 2017
Accepted 18 October 2017
Available online xxx

Keywords:
Coalescence
Film drainage
Clean and contaminated bubbles
Microbubbles
Bubble-laden turbulent flows
Bubble-induced turbulence
Euler–Lagrange

ABSTRACT

The topic of the paper is the development of an enhanced film drainage model for the prediction of bubble coalescence in the context of the Euler–Lagrange approach relying on large-eddy simulations. The starting point is the coalescence model by Jeelani and Hartland (1991), which compared to other often used models has several benefits: (1) A temporally evolving contact surface is considered avoiding the strong simplification of a constant contact area. (2) For contaminated bubbles an initially inertia-dominated process followed by a viscous-controlled regime are distinguished. (3) The contact time of the bubbles results as a side product of the modeling assumptions and thus is consistent with the film drainage concept. The main reason why this improved coalescence model was not applied in the past is the specific circumstance that the implicit equation for the determination of the transition time between the two phases (inertial and viscous) cannot be determined analytically. This problem is eliminated in the present study by numerically solving this equation. However, to avoid a time-consuming procedure for each individual bubble collision, a regression function is set up for a pre-defined range of bubble diameters and relative collision velocities. This renders the coalescence model feasible for flows with a huge number of bubbles. In a first step, the new coalescence model is validated against the experiments of single bubble coalescence with a free surface by Zawala and Malysa (2011) and Kosior et al. (2014). For the different cases considered the coalescence model yields reasonable agreement with the experiments. Furthermore, it is demonstrated that the results are improved compared to more popular but simpler models available in the literature. Afterwards, the coalescence model is applied to four-way coupled Euler–Lagrange simulations of a bubble column with clean and contaminated bubbles considering two different sizes. Significant deviations are found between the different cases, which can be traced back to varying collision frequencies and the different coalescence mechanisms in effect. Thus, it is shown that on the one hand the enhanced coalescence model leads to reasonable results and on the other hand is highly efficient allowing to take a huge number of bubble collisions deterministically into account.

1. Introduction and literature overview

Turbulent flows containing dispersed bubbles are encountered in many industrial and natural processes. Prominent examples are bubble column generators used in the chemical industry or the approach of skin friction reduction by the generation of small bubbles around ship hulls. One important feature of turbulent bubble-laden flows is the possibility of bubbles to collide with each other partially leading to coalescence of the bubbles altering the total number of bubbles and the bubble size distribution, thus, affecting the turbulent bubble-laden flow. For example, Hara et al. (2011) demonstrated that frictional-drag reduction by microbubbles in a horizontal channel flow reduces downstream of the bubble-producing electrode. This effect is explained by the coalescence of the bubbles leading to fewer but larger bubbles downstream of the electrode, which interact less with the vortices near the wall. The influence of changing bubble size distributions on chemical reactions is also obvious.

Consequently, numerical predictions of turbulent two-phase flows are required to consider collisions and coalescence in order to provide accurate results. The modeling of the bubble coalescence in a turbulent flow is a challenging task, since the physical processes are highly complex involving the interaction of the participating bubbles and the fluid trapped between the bubbles. Typically, the length and time scales of the involved processes span several orders of magnitude. Therefore, direct numerical simulations (DNS) resolving both the fluid structures and the deformable gas–liquid interface are highly challenging. Several tech-

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https://doi.org/10.1016/j.ijmultiphaseflow.2017.10.009

niques capable of treating deformable bubbles in turbulent flows are available in the literature, for example the level-set method (see, e.g., Osher and Fedkiw, 2001; Mitchell, 2008), the volume-of-fluid method (see, e.g., Meier et al., 2002; Albert et al., 2012) or the immersed boundary method (see, e.g., Tryggvason et al., 2007; Kempe and Fröhlich, 2012; Sotiropoulos and Yang, 2014; Schwarz et al., 2016; Tschisgale et al., 2017). Other methods based on the Euler–Euler or the Euler–Lagrange framework, which do not fully resolve the bubbles, require the modeling of the collision and coalescence process.

Due to the complex nature of the involved processes, all coalescence models available in the literature apply a certain number of simplifications in order to make an estimation feasible. Note that most of these models are derived in the context of Euler–Euler predictions. Hence, the corresponding coalescence criteria are inserted into probability density functions, which are used to estimate the number of coalescence processes at each Eulerian grid point. However, those models can be transferred to the framework of Euler–Lagrange predictions by applying the derived coalescence criteria directly to the occurring bubble collisions.

The existing models describing the coalescence of bubbles can be divided into three categories, i.e., *energy-based* models, *critical velocity* models and *film drainage* models (Liao and Lucas, 2010). Among the energy-based models the one by Sovová (1981) is the most prominent example. The idea is to compare the kinetic energy of the relative motion of the collision partners with the combined surface energy of the bubbles. If the kinetic energy of the collision exceeds the surface energy, the bubbles coalesce, otherwise a rebound occurs. Consequently, high approach velocities are favorable for the occurrence of coalescence. However, there exist experimental investigations of bubble coalescence describing the opposite phenomenon. Several authors (Doubliez, 1991; Kirkpatrick and Lockett, 1974; Kosior et al., 2014; Zawala and Malysa, 2011) investigating the impact of a rising bubble with a free surface reported that higher impact velocities led to rebounds of the bubbles rather than coalescence. It has to be noted that the free-surface case is not exactly similar to the case of two bubbles colliding in a turbulent flow. However, the results are supported by the experiments of Lehr et al. (2002), which are described in more detail below, investigating binary collisions of bubbles in a channel flow. A possible explanation for the discrepancy between the prediction of energy-based models and the results of the above mentioned experiments is that the energy-based approaches originally consider the coalescence of droplets and not bubbles (Sovová, 1981). Droplets may be subject to different physical mechanisms, although it is often stated that droplet and bubble coalescence are equivalent (Chesters, 1991; Liao and Lucas, 2010).

The second group of coalescence models are the critical velocity models, which decide on the occurrence of coalescence by comparing the collision velocity with a certain critical velocity. Here, the empirical model of Lehr et al. (2002) is mentioned. The authors experimentally investigated the coalescence of bubbles by a high-speed recording of a bubble swarm dispersed in a downward channel flow of distilled water. The flow velocity was adjusted in a way to keep the bubbles at the same vertical position, thus, allowing to analyze the influence of the collision velocity ranging below 0.30 m/s and the bubble diameter ranging between 3 mm to 8 mm on the occurrence of coalescence. Based on these results (Lehr et al., 2002) concluded that irrespective of the diameter bubbles coalesce if the collision velocity is below the critical velocity of $u_{\mathrm{crit}} = 0.08\,\mathrm{m/s}$. The application of the model of Lehr et al. (2002) to general turbulent flows with differing bubble parameters and fluid properties may be difficult, since the experimental results are based on a limited range of bubble diameters and collision velocities and are restricted to clean water.

The third type of models are the film drainage models making up the largest group of coalescence models with a vast amount of literature available describing the models and their applications. Nevertheless, many of these models apply strong simplifications, thus, only being valid in the restricted framework of their derivations. This is due to the complex physics of the coalescence process yielding a general approach incorporating all physical mechanisms impossible. In the framework of the film drainage model coalescence is usually described by the following three-step process:

1. Bubbles approach each other and collide with a certain relative velocity. Thereby, the surfaces of the bubbles deform, trapping a small amount of liquid between them.
2. The liquid in the film is forced out of the gap by a pressure gradient, thus, decreasing the film thickness.
3. If the film thickness reaches a critical minimum after a certain time, the film ruptures instantaneously and the bubbles coalesce. If this critical minimum thickness is not reached, the deformed bubbles separate from each other by restoring their original form.

Based on these assumptions coalescence is typically modeled by comparison of two characteristic time scales of the coalescence process, i.e., the time t_{c} the bubbles are in contact during the collision and the time t_{d} it takes to drain a sufficient amount of fluid trapped between the bubbles for the film to rupture. Alternatively, it is possible to compare the final film thickness h_{f} obtained during the contact time t_{c} with a certain critical film thickness at which rupture of the film occurs. Both approaches are equivalent though the comparison of the time scales is the more prominent one in the literature.

The film drainage models are usually further divided into approaches considering the coalescence of clean bubbles and bubbles contaminated by surfactants (see, e.g., Chesters, 1991; Liao and Lucas, 2010). The surface of clean bubbles is often called to be fully mobile, while the surface of contaminated bubbles is denoted as fully immobile. From a physical point of view, this means that at the corresponding surfaces, slip or no-slip boundary conditions hold and that the process is either inertia or viscous controlled (see below).

Two examples of a film drainage model considering contaminated bubbles with a fully immobile surface are the models proposed by Hartland (1967) and Jeffreys and Davis (1971). In these models the reduction of the film thickness is determined by the laminar outflow of the liquid trapped between the circular contact surface A_{f} of the bubbles. However, in both models the actual size of the contact surface remains unspecified, i.e., for the application of the models some value of A_{f} has to be assumed. The approaches of Hartland (1967) and Jeffreys and Davis (1971) were later extended by Sagert and Quinn (1976) including the effect of the van-der-Waals force on the drainage. Furthermore, it was suggested to consider the size of the contact surface varying with time and to experimentally obtain this variation by fitting a power series to the results of high-speed movies of the coalescence processes. However, the actual form of the power series was not given by Sagert and Quinn (1976). Additionally, the applicability to arbitrary flows is difficult, since the variation of the contact surface varies with the flow and bubble properties, c.f., Jeelani and Hartland (1991) and Section 2.1. Furthermore, for certain flow configurations the coalescence process may be very fast, i.e., the experimental determination of the variation of the contact surface may be highly challenging.

The second group of film drainage models tackles the coalescence of clean bubbles. Kirkpatrick and Lockett (1974) proposed a drainage model estimating the reduction of the film thickness by the inertial outflow (described by the Bernoulli equation) of the liquid trapped between the constant contact surfaces of the