Direct numerical simulation of evaporating droplets

Jan Schlottke *, Bernhard Weigand

*Institut für Thermodynamik der Luft- und Raumfahrt (ITLR), Universität Stuttgart, Pfaffenwaldring 31,
70569 Stuttgart, Germany*

Abstract

A model for the three-dimensional direct numerical simulation of evaporating, deforming droplets in incompressible flow is presented. It is based on the volume-of-fluid method and is therefore capable of capturing very strong deformations. The evaporation rate is computed based on the vapour mass fraction and the PLIC reconstruction of the surface. Emphasis is put on the correct calculation of the velocities of the gaseous and liquid phase at the interface which is very important for cases with high mass transfer rates and thus high Stefan flow. It is accomplished by the use of an iterative algorithm that enforces a divergence constraint in cells containing the interface.

Validation comprises a 1D test case for interfacial mass transfer, droplet collisions and oscillations as well as calculation of Sherwood numbers for two different cases of evaporating droplets where low and high mass transfer rates occur. Comparison with data from the literature shows good agreement of the obtained results.

The simulation of a strongly deformed water droplet in a flow at a high Reynolds and Weber number is used to demonstrate the capabilities of the presented method. The emerging flow field in the wake of the droplet is very complex and three-dimensional.
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1. Introduction

Heat and mass transfer across the liquid interface of multiphase flows is of extensive importance to many scientific and technical applications. The growth of raindrops due to condensation is a prominent example of these phenomena taking place in nature, whereas the evaporation of droplets during the combustion of fuel sprays in automotive engines or gas turbines has been subject to a large number of investigations in engineering. Another example is the process of droplets impinging on hot surfaces. It needs to be understood in order to assess the occurrence of thermal stresses in, for instance, lambda probes and serves as a good example of the complex interaction between the surrounding flow field, deformation of the free surface and heat/mass transfer across the liquid interface. In general, the small scales and high velocities hinder experimental access to

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these topics, whereby numerical simulation of the mentioned phenomena has received considerable attention in the past.

Looking at the evaporation of sprays, the breakup-process can lead to strongly 3D deformed droplets with high velocities relative to the surrounding gas. The resulting high Reynolds numbers ($Re_D = D\rho u/\mu$) require a three-dimensional and transient numerical approach due to the complex flow field (the flow around droplets with a Reynolds number $Re_D > 270$ is fully 3D and unsteady) and lead to high computational costs.

The actual process of evaporation can be treated using the analogy of heat and mass transfer for low mass transfer rates only; it is therefore applicable to atmospheric phenomena, for example [16]. However, industrial processes (high-temperature environment) can lead to high mass transfer rates where the mass transfer needs to be considered separated from heat transfer, taking into account the Stefan flow.

The simulation of a multiphase flow with free interfaces still is one of the big challenges in CFD despite decades of work on that topic. Difficulties are, among others, the exact localization of the interface, calculation of surface tension and the high variation of fluid properties which can be three orders of magnitude (e.g. density ratio of water/air). The numerical method should be capable of maintaining a sharp interface without smearing it over a couple of cells due to numerical diffusion. Furthermore, the ability to cover strong topological changes including break-up and coalescence is desired, whereas the conservation of mass should still be guaranteed. Two different classes of methods have been developed in the past to deal with the mentioned tasks: *tracking* and *capturing methods*. *Tracking methods* are the moving mesh, front tracking, boundary integral and particle schemes. They are of Lagrangian type, the interface position is indicated by a Lagrangian marker which could be a particle or a polygon, etc. *Capturing methods* on the other hand are continuum advection, volume tracking, level set and phase field method schemes. Here the interface is captured from a function relating to the phases more than to the interface. A detailed overview of these schemes can be found in [17].

Renksizbulut and others [30,27] have used a *moving mesh method* for the computation of evaporation rates, focusing on droplets. The method is a *mixed method* with moving meshes only in the subset of the grid near the interface whereas the rest of the grid is a fixed Eulerian one. He used the method to determine the influence of variable properties on evaporation [28]. A disadvantage of the model is its limitation to 2D axisymmetric problems and small deformations. Haywood et al. used their model described in [11] to simulate the transient evaporation process of deformed droplets [12]. The model is similar to the one mentioned before and also limited to two-dimensional cases.

Juric and Tryggvason extended the *front tracking method* described in [45] for boiling flows [15].

Son and Dhir developed a model for boiling flow based on the *level set* approach [43,40]. *Level set methods* employ an additional transport variable representing the distance to the phase interface. They are capable of resolving arbitrary changes of the interfaces including break-up and coalescence. One big disadvantage of the original *level set* method is that conservation of liquid mass can not be guaranteed. This issue has been addressed by various authors, amongst others by Enright et al. [3] with their *particle level set* method or by Sussman et al. [42,41] with their coupled level set and volume of fluid method (CLSVOF), improving mass conservation significantly.

A method using the volume-of-fluid (VOF) approach for boiling flow was presented by Welch and Wilson [46]. VOF enables the scientist to detect any changes of topology and is in addition conservative due to its formulation. Welch and Wilson used the heat flux across the interface in order to calculate the mass of the phase changing liquid. They applied their method to a horizontal film-boiling problem in 2D.

Davidson and Rudman presented their VOF-based algorithm for the calculation of transport processes across deforming interfaces, using the analogy between heat and mass transfer [2]. The algorithm is limited to axisymmetric cases and does not consider volume changes due to phase change.

Jung and Sato conducted three-dimensional direct numerical simulations of a high Schmidt number flow over a droplet [14]. They employed a moving, unstructured mesh consisting of prisms at the interface to resolve the viscous boundary layer and tetrahedral cells in the remaining domain. Additional thin layer-cells inside the layer of prism-cells attached to the interface were used for calculation of mass transfer.

Another *level set* based approach to the topic of evaporation was shown by Tanguy et al. [44]. They utilized the Ghost Fluid Method [4] to enable the use of high order discretization schemes at the interface. By developing a model to calculate the interface velocities considering the volume change due to evaporation they were