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Comparative assessment of Volume-of-Fluid and Level-Set methods by relevance to dendritic ice growth in supercooled water

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ABSTRACT

Two relevant computational models, one relying on a Level-Set approach, the other one on a Volume-of-Fluid tracking procedure with piecewise linear interface reconstruction, are comparatively assessed in terms of their capability to simulate crystallization of supercooled water. The models are preliminary validated by computing a one-dimensional freezing front propagation for which an analytic solution exists. Afterwards, the tip velocity of two-dimensional dendrites growing in supercooled water is determined and compared with corresponding experimental results and theoretical predictions in the range of supercooling between 1 K and 30 K. Present modeling results following closely both the underlying theory and experimental findings show very good mutual agreement.

1. Introduction

Droplet dynamics problems under extreme boundary conditions play an important role in a number of technical and natural processes. In the framework of the collaborative research center SFB-TRR 75 (Droplet Dynamics under Extreme Ambient Conditions) relevant problems are studied in detail (see e.g. a project overview of Weigand and Tropea [1]). One of the most frequently encountered freezing processes involving droplets is certainly the formation of an ice-layer on an aircraft wing during its collision with supercooled droplets. This and the process of the ice-crystal growth in clouds are studied in different sub-projects of the SFB-TRR 75. For these two fundamentally different applications two different numerical codes have been used, both based on the finite volume method. For the computational study of crystal growth processes in clouds, the in-house code FS3D (Free Surface 3D) was chosen, utilizing advantage of an orthogonal Cartesian mesh. The formation of an ice-layer by drop impact onto an aircraft wing occurs in a more complex geometrical environment. For such an application the open source software OpenFOAM® was selected. The two codes use different front tracking methods. In conjunction with the OpenFOAM® code an appropriate Level-Set approach has been proposed and implemented, whereas the FS3D code benefits from a Volume-of-Fluid (VOF) method with Piecewise Linear Interface Calculation (PLIC).

Accordingly, the objective of the present work is a comparative validation of both tools on the basis of some generic configurations. Two cases of particular interest are the 1-D ice-layer growth for which an analytic solution was derived [2] and a 2-D case, where the tip velocity of parabolic-shaped dendrites is validated along with the experimental data of [3–11]. Furthermore, the predictive performances of the two front capturing methods are mutually compared. The numerical simulations have been performed under conditions where pure water may retain its liquid state at temperatures as low as approximately −35 °C before homogeneous nucleation starts. Correspondingly the water is in a metastable state. In the case of heterogeneous nucleation, the critical temperature is respectively higher. With the FS3D code the intention is to perform direct numerical simulations of the entire relevant scale span characterizing the droplet freezing process. At the microscale, a nucleation model initiates the ice seed in a potentially deformed liquid droplet; afterwards the phase growth starts within the droplet on a mesoscale. On the macroscale, the config-

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urations including droplet–droplet and droplet-ice interactions will be studied. The droplet-wall interaction, ice-wall interaction and ice growth at walls as encountered during wing icing will be studied using the OpenFOAM® software. Here the correct capturing of the hydrodynamics of the supercooled liquid particle approaching the wall and its spreading on the wall is of decisive importance. The OpenFOAM® code enables handling of arbitrarily complex wall geometries.

A complexity arising from the process of ice seed growing in liquid water that is cooled down to temperatures below its equilibrium solidification temperature is closely connected to an unstable freezing surface. In this process supercooling acts as the driving force towards the phase growth; the interface is instable [12–14] and small perturbations at the ice surface lead to a bump-like expansion of ice propagating into the liquid which experiences a steeper temperature gradient. This enhances locally the ice growth and the formation of dendrites. As described in detail in Section 2, this effect is attenuated by the product of surface tension and the local curvature. For that, an exact representation of the interface morphology is indispensable. Accordingly, the direct numerical solution of such a process corresponding to the time-dependent Stefan problem represents a great challenge. An appropriate front tracking method accounting for the moving solid–liquid interface is required. Over the last decades various computational models have been applied for the simulation of dendritic growth.

Juric and Tryggvason [15] have presented a front-tracking method on a fixed Cartesian grid for the simulation of dendritic solidification in two dimensions. The information exchange between the Eulerian and Lagrangian interface points was accomplished by applying the Immersed Boundary Method (IBM) [16]. The heat conduction equation is discretized using finite differences. An iterative scheme for the interface velocity determination serving for the temperature distribution satisfies the Dirichlet boundary condition at the interface. The method was extended to include advection [17] and three-dimensionality [18]. Udaykumar et al. [19] presented an approach similar to that of Juric and Tryggvason [15], however, the interface velocity was determined directly from the Stefan condition imposing temperature at the sharp interface. Beckermann et al. [20] introduced a diffuse interface model accounting for advection within the liquid phase. They conducted 2-D simulations of dendritic growth of an initially round particle with and without melt advection; the study analyzed the tip velocities and radii upstream, downstream and normal to the flow direction. Karagadde et al. [21] presented recently a VOF–IBM–enthalpy approach in conjunction with a 2D simulation of dendritic growth including advection. They applied the enthalpy method utilizing an iterative scheme to update the liquid fraction in a cell due to the enthalpy change. Liquid cells next to the solid ones are seeded with small amounts of solid to initiate growth. They adopted the IBM method to solve the liquid flow including a solid body. The solid phase is advected using the VOF-technique with interface reconstruction. Level-Set methods have been increasingly applied to several problems involving moving boundaries [22,23] and crystallization [24,25] exhibiting good predictive performance in returning qualitative features of the dendrites.

The paper starts with an outline of the underlying physics and the mathematical description of the problem considered. In Section 3, the numerical frameworks pertinent to both codes FS3D and OpenFOAM® is explained. The computational models' validation by means of an analytic solution of a one-dimensional solidification problem as well as the results comparison with respect to the dendrite tip velocities as predicted by the universal law of dendritic growth of Langer and Müller-Krumbhaar [26] are illustrated in Section 4.

2. Physical formulation

For incompressible flow and constant fluid properties, the momentum equations are decoupled from the energy equation. The problem considered is characterized by small Eckert numbers $Ec = \mathbf{u}^2/(c_p\Delta T) \ll 1$ due to low velocity conditions. Here $\mathbf{u}$ denotes the velocity vector, c_p the specific heat capacity and T the temperature. This allows the viscous heating to be neglected with the thermal energy equation governing the temperature field. Since the densities of water ρ_l and ice ρ_s differ only slightly, equal density ρ is used for both phases.

We use the index l for liquid and the index s for solid; $i = (s, l)$ if solid or liquid appear exclusively in an equation valid for both phases. The thermal energy equation governing the dynamics of the temperature field reads [27]

$$\frac{\partial(\rho c_{p,i} T_i)}{\partial t} + \nabla \cdot \left(\rho c_{p,i} T_i \mathbf{u}\right) = \nabla \cdot (k_i \nabla T_i) + \dot{q}_i''', \tag{1}$$

where k denotes the heat conductivity and $\dot{q}'''$ is a volumetric heat source. Eq. (1) is solved in both phases separately. The temperature fields of solid and liquid are connected by the Stefan condition in all interface cells. Assuming local equilibrium, it states that the latent heat released during phase change must be conducted away from the interface in both phases; the corresponding mathematical formulation reads

$$\dot{m}''\left[L - (c_{p,l} - c_{p,s})(T_m - T_\Gamma)\right] = -\lambda_l \nabla T_l \cdot \mathbf{n}_\Gamma + \lambda_s \nabla T_s \cdot \mathbf{n}_\Gamma. \tag{2}$$

Here $\mathbf{n}_\Gamma$ is the interface normal vector, T_Γ the interface temperature and T_m the melting temperature of water. The second term in square brackets accounts for the difference in the heat capacities of water and ice [28]. The mass flux per unit area can also be expressed in terms of the interface velocity: $\dot{m}'' = \rho|\mathbf{V}_\Gamma|$. T_Γ is the fusion temperature of water on curved interfaces. For normal pressure and flat interfaces T_Γ is equal to $T_m = 273.15$ K. In contrast to supercooling, which is the driving force for dendritic growth, the surface tension acts as a counterforce, because it reduces the local supercooling on curved interfaces. These two opposed mechanisms drive other effects like tip splitting and sidebranching and determine consequently the crystal morphology. The relation between surface tension and melting temperature depression can be described by the Gibbs–Thomson relation [28]

$$T_\Gamma = T_m\left(1 - \frac{\gamma\kappa}{\rho L}\right) + \frac{(c_{p,l} - c_{p,s})T_m}{L}\left[T_\Gamma \ln\left(\frac{T_\Gamma}{T_m}\right) + (T_m - T_\Gamma)\right], \tag{3}$$

where the curvature κ of the interface is defined as the sum of the reciprocals of the two main radii of curvature; γ denotes the surface tension. Hence, there are two boundary conditions at the solid–liquid interface. The first one is a Dirichlet boundary condition and determines the interface temperature according to the local curvature. The second one is the Stefan condition, implying the latent heat release being transferred by conduction during phase change into both the solid phase and the liquid phase.

3. Numerical schemes

For phase change problems, in particular water–ice systems, it is of great importance to reproduce the morphology and especially the curvature of the ice particle. This means that the interface between solid and liquid must be well resolved and sharp. Existing methods for the simulation of free surfaces can be classified into two groups [29], namely:

- Interface-tracking methods,
- Interface-capturing methods.