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A Volume-of-Fluid method with interface reconstruction for ice growth in supercooled water

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ABSTRACT

A new method is presented to simulate ice growth in supercooled water with the Volume-of-Fluid based multiphase code Free Surface 3D. The method relies on the knowledge of the reconstructed interface in each interfacial cell. The time integration is implicit in order to circumvent severe time step restrictions. It includes heat conduction and the release of latent heat during phase change as well as mass flux across the interface. The method is described in detail including the specific treatment related to the piecewise linear interface reconstruction. The morphology of ice crystals proves to converge on fine grids. Furthermore, the growth velocity of dendrites is independent of the orientation with respect to the used Cartesian grid.

1. Introduction

Weather prediction is of great interest to meteorologists, industry and society as a whole. It is a matter of current research and yet many processes are far from being understood. Processes in the atmosphere and especially in clouds are characterised by large differences in scale. The macrophysical motion of clouds in the atmosphere determines the temperature and pressure in a cloud. This motion is induced by air streams or convection as a result of temperature differences. Nucleation of ice germs within the fluid water phase may either be homogeneous or heterogeneous. Homogeneous nucleation requires temperatures as low as $-40\,°C$. Heterogeneous nucleation induced by aerosol particles, for instance, starts nucleation at considerably smaller supercooling, see Vali [1]. The size of these nuclei is in the nanometre range. However, the freezing of water drops releases a large amount of latent heat that has a significant influence on the temperature and pressure [2]. Similar statements hold for evaporation in clouds. However, the microphysical processes in the atmosphere are not described comprehensively. This is particularly true for the initiation of ice growth in clouds [1,3], although ice particles play a major role at the incurrence of precipitation in temperate climate zones.

Our in-house code Free Surface 3D (FS3D) uses a Volume-of-Fluid (VOF) method with Piecewise Linear Interface Calculation (PLIC) for the Direct Numerical Simulation (DNS) of incompressible multiphase flow. DNS of supercooled water droplets will help to understand the freezing process of these droplets by allowing a detailed and time resolved view on the ice phase spreading within the droplet. For instance, one objective will be to determine numerically the duration to freeze a spherical water droplet when the ice nucleus is initiated at distinct positions on the radius. By comparing this to the freezing duration of droplets from experiments, the preferable positions of nuclei within the droplet can be determined. Apart

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from water droplets, hail formation and shedding phenomena shall be investigated with FS3D in the future. The present work lays the groundwork for the intended investigations.

The four major prerequisites for simulations of the freezing of supercooled water droplets are a nucleation model, rigid body motion of the solid ice particles, a second VOF variable to account for the three phases, air, liquid water and ice, and implementation of the phase change process. The second prerequisite (rigid body motion) is presented in another paper [4]. The phase change method was previously compared to a method that is implemented in OpenFOAM and uses a Level-Set approach. These results, comprising a 1D and 2D test case, were presented in Rauschenberger et al. [5]. The focus of the current paper lies on the numerical method and the peculiarities arising when using a VOF-PLIC approach for the application. It is shown that the method converges on fine grids and that growing dendrites are independent of orientation with respect to the Cartesian grid used for the computations.

Different kinds of ice can be distinguished. The most common kind in nature is ice Ih, i.e. ice one hexagonal. In the temperature range $T > 233.15$ K, other kinds of ice appear only for pressures of approximately $p > 2000$ bar. In this work, the temperature range under consideration is above 233.15 K at atmospheric pressure.

Two regimes are distinguished in the freezing of supercooled water. In the first regime, the released latent heat reduces the supercooling of the fluid surrounding the developing ice phase. This regime is called the fast regime because the transition of metastable supercooled water to ice is very fast. In the second regime, ice growth is slower because the environment is at temperatures only slightly below the local phase change temperature. Hence, the velocity of the phase change is governed by the ability to transport away heat from the interface by diffusion. The mathematical description of the physical process at the interface is the same and both regimes can be captured with the method presented here. However, the inner structure of the ice phase leading to opaqueness, by way of example, cannot be captured yet.

Ice growth is governed by two conditions on the interface between water and ice: the temperature at which a phase change takes place (the interface temperature T_γ) and the Stefan condition [6] which states that the latent heat released at the interface during the phase change amounts to the sum of heat conducted away from the interface. Hence, the Stefan condition allows to determine the velocity of the interface in consequence of the phase change. For a flat interface $T_\gamma = T_m = 273.15$ K and $p = 1$ bar. On curved interfaces, the pressure rise leads to a reduction of the interface temperature. The relative change $(T_m - T_\gamma)/T_m$ is determined by the dimensionless surface energy $\Sigma = \sigma\kappa/(\rho L)$ (Gibbs–Thomson effect, see Eq. (3)). If curvature is negative, the Gibbs–Thomson equation will imply a rise of the interface temperature. However, the phase diagram of water shows that ice does not exist above the temperature at the triple point $T_T = 273.16$ K. Hence, the maximum interface temperature is limited by T_T for negative curvature. In general, the temperature distribution within the ice is more homogeneous because its heat conductivity is about four times the value of water. Hence, the velocity of the interface essentially depends on the heat conduction and convection within the liquid phase.

One difficulty in describing the growth of an ice nucleus in supercooled water is the instability of the interface in between water and ice. This instability was examined theoretically by Mullins and Sekerka [7] for a spherical particle and for a plane interface [8]. They expanded an infinitesimal deviation from sphericity into spherical harmonics for their theoretical investigation. According to this analysis, the interface of a spherical nucleus grows instable as soon as the radius of the nucleus exceeds

$$r_{inst} = \frac{1}{2}\left[(l+1)(l+2) + 2 + l(l+2)\frac{k_s}{k_l}\right] r_{nuc}, \qquad (1)$$

where k denotes the heat conductivity and r_{nuc} the nucleation radius. $l = 1$ means a translation of the nucleus. The minimum growth radius of the second harmonic ($l = 2$, an ellipsoid) must exceed $7r_{nuc}$. However, the radius must be considerably larger than predicted by Eq. (1) in order to develop a marked instability [7]. Harmonics of higher order grow at respectively higher radii.

The development of a bump on the interface between ice and water is shown in Fig. 1(a). The bump locally rises the curvature and at the same time, the interface extends across the warmer thermal boundary layer into supercooled water. Two contrary effects occur: On the one hand, the dimensionless surface energy Σ rises and lowers T_γ which leads to a smaller temperature gradient, see Fig. 1(b) curve A. Hence, the growth of the bump is retarded. On the other hand, the temperature gradient rises because of the higher supercooling outside the boundary layer, see curve B. If the bump keeps on growing, a dendrite develops. Dendritic growth is essentially governed by these two effects. If both are equal in magnitude, the dendrite grows with constant velocity.

The product of surface energy and curvature stabilises the growth. The term $\sigma/(\rho L)$ has the dimension of a length and determines the dimension of the growth patterns. Fig. 2 shows an ice crystal with dendrites that grew on a film of water–tenside mixture. The reason for the hexagonal structure lies in the molecular structure of the crystal lattice [9]. A basic cell of the lattice is a prism with a hexagonal base and this molecular structure is reflected in the anisotropy of the surface energy. A model for this effect is described in Section 3.3.

The numerical simulation of the Stefan problem requires very precise interface capturing. Small structures can only be resolved if the grid allows it. This means that in particular the curvature and normal vector must be computed precisely. In the past decades, different methods were developed that are discussed briefly hereafter.

A front-tracking method was introduced by Juric and Tryggvason [10] on a fixed Cartesian grid. They showed simulations of dendritic solidification in two dimensions using the Immersed-Boundary Method (IBM) [11] for the information exchange between the Eulerian and Lagrangian points on the interface and finite differences for the heat conduction equation. The