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MESOSCOPIC MODELING OF FREEZING OF SUPERCOOLED WATER

Edin Berberović
University of Zenica, Polytechnic Faculty
Fakultetska 1, 72000 Zenica
Bosnia and Herzegovina

ABSTRACT
The computational model for the simulation of freezing of supercooled water is presented. The model is based on the mesoscopic scale approach combining the analytical solution for the dendrite growth at small scales with the numerical solution for the temperature at larger scales. It utilizes the interface capturing methodology based on phase-field which is implemented in the open-source software OpenFOAM®. The capability of the model is verified by computing cases of freezing of supercooled water at different initial supercoolings.
Keywords: mesoscopic modeling, freezing, supercooled water

1. INTRODUCTION
In order to simulate dendritic ice growth morphology in water freezing, a problem of a large difference in length scales must be approached. The ice growing into the supercooled water consists of the primary dendrites on which secondary dendritic tips evolve on a microscopic scale. During the ice growth in the melt a mushy zone is developed on a macroscopic scale. Due to the large length-scale discrepancy computing of all the details of the solidification on the microscopic scale would require a computational effort that is beyond the widely available computer power. To overcome this problem a model was presented in [1] based on defining an intermediate mesoscopic scale in the mushy region. Such a model enables to determine the propagation of the grain front formed by virtually connecting the tips of the evolving dendrites without resolving the structures within the grain. The main idea is to combine the numerical solution of the heat diffusion equation on this mesoscopic scale, with a local analytical solution for growth of a dendrite tip at the small length scale. The analytical solution is matched with the computationally obtained temperature field outside the grain at a small distance from the grain surface, called the stagnant-film thickness [1].

2. COMPUTATIONAL MODEL
The basics of the mesoscopic modeling was used in [1, 2] for the solidification of a pure supercooled liquid and a binary alloy. The analytical solution for the tip velocity is integrated into the model by using the value for the supercooling obtained from the numerical solution for the temperature on the larger mesoscopic scale. The grain iso-surface connects the tips of the dendrites and is a mixture consisting of the ice dendrites and water. The iso-surface is at the temperature of freezing and the grain grows into the supercooled water due to release of the latent heat of freezing. The analytical solution for the tip velocity, the so-called stagnant film solution, is coupled to the selection criterion for the radius of the dendrite tip to enable the calculation of both, the tip velocity and its radius, depending on the supercooling ΔT. The supercooling obtained from the numerical solution for the heat diffusion at a small thickness δ_f around the grain is supplied into the analytical solution

$$\Delta T = \left(L / c_p\right) \mathrm{Pe}\, e^{\mathrm{Pe}} \left\{ E_1\left(\mathrm{Pe}\right) - E_1\left[\mathrm{Pe}\left(1 + 2\left(\delta_f / R_{tip}\right)\right)\right]\right\}, \qquad \ldots (1)$$

where E_1 is the exponential integral function. The dendrite tip radius is expressed from the selection criterion as a function of Pe number and eliminated from the analytical solution to obtain an expression of the form $\Delta T=f(\mathrm{Pe})$ that is numerically solved to calculate the dendrite tip velocity corresponding to the supercooling at the distance δ_f from the grain. The grain front is numerically propagated with the normal velocity by using the phase-field approach [3]. The interface between the ice grain and the surrounding water is replaced by a thin transitional region over which the indicator variable ϕ smoothly changes from 1 to 0. The evolution of the grain is obtained from the equation

$$\frac{\partial \phi}{\partial t} + \mathbf{v}_n \cdot \nabla \phi = b\left[\nabla^2 \phi - \frac{\phi(1-\phi)(1-2\phi)}{w^2} - |\nabla \phi| \nabla \cdot \left(-\frac{\nabla \phi}{|\nabla \phi|} \right) \right], \qquad \text{... (2)}$$

where $\mathbf{v}_n$ is the dendrite tip velocity. The supercooling ΔT is obtained from the values for the temperature evaluated at the points at the confocal envelope, determined from the numerical solution of the energy diffusion equation around the grain

$$\rho c_p \frac{\partial T}{\partial t} = \nabla (k \nabla T). \qquad \text{...(3)}$$

The change of ϕ from 1 to 0 near the grain front is defined as the hyperbolic tangent profile. The characteristic width w is calculated as $w \geq \sqrt{2}|d|$, where d is the spacing between two adjacent cell centers in the numerical mesh. The iso-surface of the grain envelope is defined as ϕ_{env} = 0.95. The solution of the model starts by calculating the position $\mathbf{x}_{ce}$ of the confocal envelope around the grain. Then, the supercooling is determined from the value for the temperature at the confocal envelope T_{ce}. The propagation velocity of the grain front is obtained by solving the analytical stagnant film model, Eq. (1), and the new position of the grain front is calculated explicitly from Eq. (2). Finally, the temperature field around the grain is obtained from the numerical solution of Eq. (3) by using the finite-volume solution, from which the temperature at the confocal envelope T_{ce} is determined. The model is implemented in the open-source software OpenFOAM® [4]. The stabilization factor b in Eq.(2) affects the accuracy of the phase-field interface capturing and can be set up to the stability limit depending on the time step size and the mesh resolution [2]. The time step size is self-adjusted during the simulation and the parametar b is set as a fraction of the limiting value [3]. The propagation velocity of the grain front $\mathbf{v}_\mathrm{n}$ is determined in all the mesh-cells within the transition region $0.01<\phi<0.99$. The mesh-cells are generally not aligned with different normal directions and the velocities $\mathbf{v}_\mathrm{n}$ must be determined at every cell-center within the transitional band. To apply the proper supercooling from the confocal envelope to each cell within the band, the exact locations of the points $\mathbf{x}_{ce}$ at the confocal envelope are determined by using the interface reconstruction procedure [3]. Once $\mathbf{x}_{ce}$ is found, the cell $\mathrm{P_{ce}}$ is found within which each point $\mathbf{x}_{ce}$ is located. The temperature at the confocal envelope is then explicitly calculated by using the temperature gradient obtained from the numerical solution as $T_{ce} = T_{Pce} + (\mathbf{x}_{ce} - \mathbf{x}_{Pce}) \cdot \nabla T_{Pce}$. Finally, the values for the local supercooling are determined as $\Delta T=T_m-T_{ce}$. For the calculation of the exponential integral function $E_1(x)$, the expression provided in [5] is used. For the numerical solution of Eq. (3), the icing temperature T_m is explicitly set in the cells within the grain, as well as at the immersed points which are used to add the contribution to the source term and the diagonal coefficients in the finite-volume solution matrix.

3. RESULTS

For the verification of the model, freezing is computed for two initial supercoolings: ΔT=3 and 5 K. The two-dimensional computational domain shown in Fig. 1 has dimensions of 1×1 mm discretized by 100×100 cells. At the initial time the spherical ice nucleus has a radius $R>6w$ to ensure smooth enough initial transition of the phase-field. Uniform temperature corresponding to the initial supercooling is set everywhere with zero-gradient boundary condition for the heat diffusion, reflecting adiabatic boundaries. Uniform properties of the supercooled water are listed in Table 1.

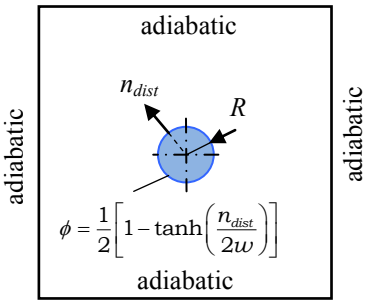

Table 1. Thermophysical properties for water.

density ρ, kg/m^3	998.84
heat conductivity k, W/(m·K)	0.562
specific heat c_p, J/(kg·K)	4219
latent heat of freezing L, J/kg	333000
surface tension σ_{sl}, N/m	0.028
thermal diffusivity α, m^2/s	$1.33228 \cdot 10^{-7}$

Figure 1. Sketch of the computational domain.

Special care is given to the choice of the stagnant-film thickness δ_f as the input parameter, which is related to the value of the tip radius R_{tip}. Since the tip radius itself is a part of the analytical solution, it is difficult to choose the correct value in advance. The film thickness is scaled with the diffusion length scale l_{diff} in [2], where it was shown that the grain tip velocity approaches the theoretical value if δ_f is approximately of the same order of magnitude as l_{diff}. When δ_f is set sufficiently small, the local supercooling at the confocal envelope is not uniform and the grain tip velocities are varying and produce the characteristic grain shape. The best results for the grain shape are obtained by using $\delta_f/l_{diff} \approx 0.5$. In the case of freezing, the thermal diffusion length is estimated as $l_t=\alpha/v_{tip}$, where v_{tip} is the velocity of the primary dendrite tip. Thus, the physical meaning of the stagnant film thickness is the thickness of the diffusion boundary layer around the grain surface. For the estimation of l_t the experimental values for icing front velocities from [6] are used, and the obtained l_t is equal to $9.87224 \cdot 10^{-5}$ m at 3 K and $3.38157 \cdot 10^{-5}$ m at 5 K. The results for the grain evolution at various time instants for the two initial supercoolings are shown in Fig. 2.

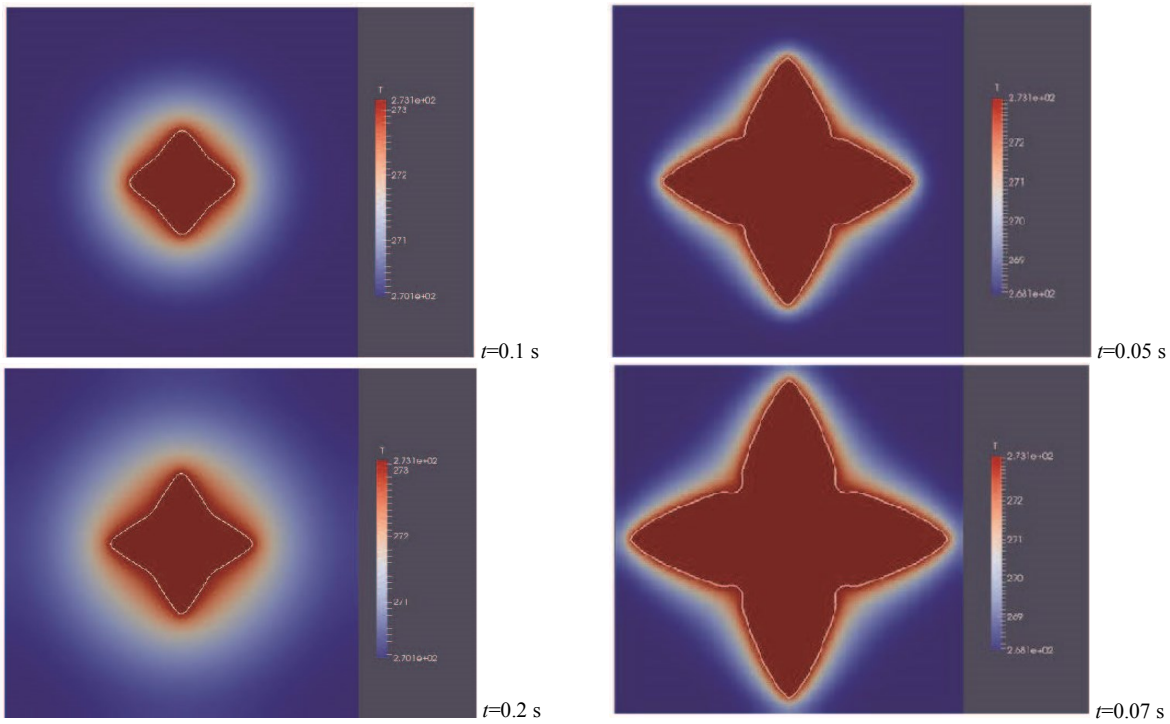

Figure 2. The computed grain evolution and the temperature distribution for $\Delta T=3$ K, $\delta_f/l_t=0.5$ (left) and for $\Delta T=5$ K, $\delta_f/l_t=1.3$ (right).

As can be seen in the figure, the results are different for different initial supercooling, whereby the grain evolves much faster for higher initial supercooling. It is further observed that the results are different when different values for δ_f/l_t are applied in the same numerical case. As expected, the model is sensitive to the thickness δ_f, which must be properly set for each specific case. The difference in the obtained results is further highlighted in the case with a higher value for $\delta_f/l_t=1.3$. The result showing the distribution of the supercooling at the grain iso-surface is shown in Fig. 3. It is

seen that the supercooling is not constant at the grain surface, being the greatest at the primary grain tips, and the supercooling decreases in time. The model potential is examined quantitatively with respect to the results for the grain width. It was previously found in [1] that the dimensionless grain width scales with the dimensionless distance from the grain tip, revealing a universal power law

$$x / R_{tip} = A\left(y / R_{tip} \right)^{n} \qquad \text{... (4)}$$

where x is the half-width of the grain measured from the axis of symmetry and y is the distance from the grain tip to the center of the grain. The coefficients in Eq. (4) obtained in [1] are A=0.668 and n=0.859. Fig. 3 shows the computed dimensionless grain half-width for ΔT=5 K, δ_f / l_t=1.3 at t = 0.07 s. The computed results scale well with the power scaling law, Eq. (4), with the corresponding coefficients A=4.21 and n=0.63, thereby showing that the model is capable of predicting the power-law shape of the iso-surface of the ice grain.

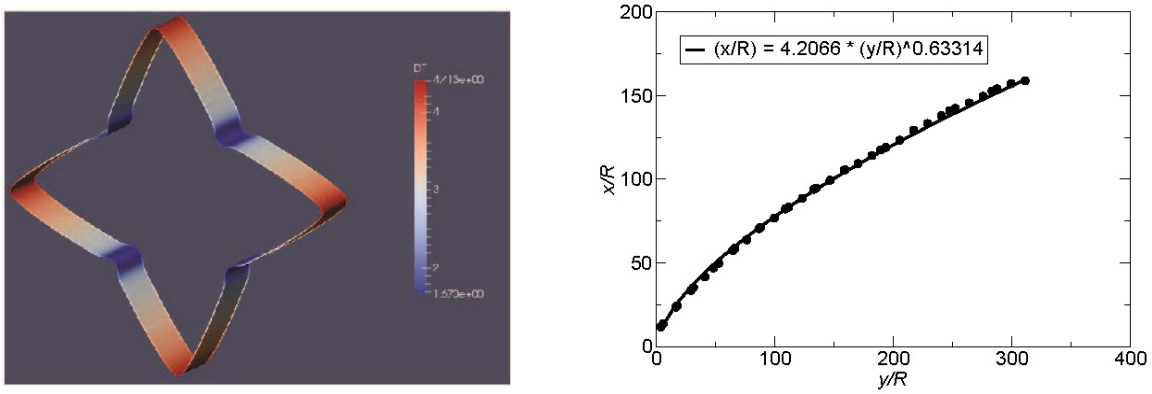

Figure 3. The computed grain evolution and the supercooling for ΔT=5 K, δ_f / l_t=1.3 (left) and the computed dimensionless grain half-width for ΔT=5 K, δ_f / l_t=1.3 at t=0.07 s (right).

4. CONCLUSIONS

The computational model for the computation of solidification of supercooled water is presented. The model utilizes the intermediate mesoscopic scale to avoid high computational costs. It combines the analytical solution for the dendrite growth at smallest scales with the numerical solution for the temperature field at larger scales. It is based on the phase-field interface capturing with imposed boundary conditions in the interface points. The model is tested and verified by computing freezing of supercooled water at different initial values for the supercooling.

5. REFERENCES

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