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A numerical analysis of ice crystal growth on cold surfaces

A.Z. Şahin

Department of Mechanical Engineering,
King Fahd University of Petroleum & Minerals,
Dhahran, 31261, Saudi Arabia

ABSTRACT

A numerical study of ice crystal growth is presented. The ice crystal is assumed to grow in either cylindrical or spherical shape. The models permit a continuous determination of the phase change interface and the temperature distribution. A finite difference approach is used to solve the model equations. Numerical results are compared with available theoretical and experimental data. The effect of the velocity, ice crystal base temperature and biot number are considered for the determination of the growth rate of the ice crystal.

INTRODUCTION

It is well known that when humid air is exposed to a solid surface which is colder that the dew-point temperature of the air, condensation will take place as the air is cooled, and that the water vapor leaving the air will pass directly from gaseous to solid state of frost if the surface temperature is below 0 ^{o}C.

Although there has been a number of attempts to make analytical simulations and experimental observations of crystal structure during the early stage of frost formation, it is apparent that very little is known about the fundamental nature of ice crystal growth. Yonko and Sepsy [1] investigated frost growth experimentally. Jones and Parker [2] developed a theoretical model of frost growth based on molecular diffusion of water vapor at the frost surface using energy and mass balances. In addition to the mass and heat balances, equation of state was incorporated by Sami and Duong [3] who compare their frost growth results with those of Yonko and Sepsy

[1] and Jones and Parker [2]. Sahin [4] studied the density of frost layer during the crystal growth period making use of the sublimation density of ice crystals obtained experimentally. It is apparent that, still there is a need for a fundamental understanding of the nature of frost formation including the vapor-condensation process to assist in predicting the rate of ice crystal growth.

MATHEMATICAL MODEL OF ICE CRYSTAL GROWTH

In this study, two simple analytical models are selected to investigate the growth of an ice crystal in which the ice crystal is assumed to grow in either cylindrical or spherical shape. The following assumptions are made for the models:

a) ice crystal is assumed to grow in eitler cylindrical or spherical shape,
b) the humidity ratio around the ice crystal remains uniform,
c) the surface temperature of the ice crystal is constant, 0 °C,
d) the physical properties remain uniform throughout the ice crystal,
e) the ice-gas interface is smooth and
f) the ice crystal grows on an initial nucleus of dimensions r_o and z_o for cylindrical case and of dimension r_o for spherical case.

Cylindrical Model of ice crystal growth

With the assumptions made above, the conservation of energy in the cylindrical coordinate system for a two dimensional transient conduction case is given by,

$$\frac{1}{\alpha}\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) \tag{1}$$

where $\alpha = k/(\rho C_P)$ is the thermal diffusivity of the solid ice crystal.

Introducing the nondimensional parameters,

$$R = \frac{r}{r_o}, \quad Z = \frac{z}{z_o}, \quad \theta = \frac{T - T_b}{T_s - T_b}, \quad \tau = \frac{\alpha t}{z_o^2} \quad \text{and} \quad \Gamma_o = \frac{z_o}{r_o}$$

where T_b and T_s are the temperature of the base and that of the outer surface of the ice crystal respectively, the conservation of energy, equation 1, becomes,

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial Z^2} + \frac{\Gamma_o^2}{R}\frac{\partial}{\partial R}\left(R\frac{\partial \theta}{\partial R}\right). \tag{2}$$

Noting that ice crystal growth is a moving boundary problem, the interface

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equation is given [5] as

$$\rho L \frac{\partial s}{\partial t} = \left[1 + \left(\frac{\partial s}{\partial r}\right)^2\right] \left[k \frac{\partial T}{\partial z} + h(T_s - T_v)\right] \tag{3}$$

where T_v is the temperature of the vapor surrounding the crystal and L is the latent heat. 's' in equation 3 is the location of the crystal surface that is the location of the interface between the ice crystal and the vapor around it; $s(r,t) = Y_r$ or Y_z.

Equation 3 can be nondimensionalized by introducing the following parameters in addition to those defined above:

$$Y_R = \frac{Y_r}{r_o}, \quad Y_Z = \frac{Y_z}{z_o}, \quad G = \frac{L}{C_P(T_s - T_b)},$$

$$Bi = \frac{hz_o}{k} \quad \text{and} \quad Bi_r = \frac{hr_o}{k} = \frac{Bi}{\Gamma_o}.$$

Then, the interface boundary equations for the top and side surface of the cylindrical ice crystal become,

$$G \frac{\partial Y_Z}{\partial \tau} = \left[1 + \Gamma_o^2 \left(\frac{\partial Y_Z}{\partial R}\right)^2\right] \left[\frac{\partial \theta}{\partial Z} + Bi(1 - \theta_v)\right] \tag{4}$$

and

$$\frac{G}{\Gamma_o^2} \frac{\partial Y_R}{\partial \tau} = \left[1 + \frac{1}{\Gamma_o^2} \left(\frac{\partial Y_R}{\partial Z}\right)^2\right] \left[\frac{\partial \theta}{\partial R} + Bi_r(1 - \theta_v)\right] \tag{5}$$

respectively.

Initial temperature condition is taken as uniform and equal to the surface temperature ($\theta = 0$) and the relevant boundary conditions are:

$$\theta = 0 \quad \text{at} \quad Z = 0,$$

$$\theta = 1 \quad \text{at} \quad Z = Y_Z,$$

$$\frac{\partial \theta}{\partial R} = 0 \quad \text{at} \quad R = 0 \quad \text{and}$$

$$\theta = 1 \quad \text{at} \quad R = Y_R.$$

Spherical Model of ice crystal growth

The conservation of energy in the spherical coordinate system for a two dimensional transient conduction case is given by,

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial R^2} + \frac{2}{R}\frac{\partial \theta}{\partial R} + \frac{1}{R^2 \sin \phi}\frac{\partial}{\partial \phi}\left(\sin \phi \frac{\partial \theta}{\partial \phi}\right) \tag{6}$$

where $\tau = \alpha t / r_o^2$ in this case.

Equation 6 will have singularity when solved for $R = 0$, $\phi = 0$ and $\phi = \pi$. The singularities at $\phi = 0$ and π can be removed by the following transformation:

$$X = \frac{1 - \cos \phi}{2}$$

where $0 \le \phi \le \pi$. Then, the energy equation, equation 6, becomes

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial R^2} + \frac{2}{R}\frac{\partial \theta}{\partial R} + \frac{1}{R^2}\frac{\partial}{\partial X}\left[(X - X^2)\frac{\partial \theta}{\partial X}\right]. \tag{7}$$

The singularity at $R = 0$ is already avoided by assuming an initial nucleus of small finite dimension.

The interface equation in spherical case is given [5] as

$$\rho L \frac{\partial s}{\partial t} = \left[1 + \frac{1}{s^2}\left(\frac{\partial s}{\partial \phi}\right)^2\right]\left[k\frac{\partial T}{\partial r} + h(T_s - T_v)\right]. \tag{8}$$

's' in equation 8 is the location of the crystal surface that is the location of the interface between the ice crystal and the vapor around it; $s(r,t) = Y_r$.

Equation 8 can be nondimensionalized by utilizing the parameters which are defined above. Then, the interface boundary equation surface of the spherical ice crystal becomes,

$$G\frac{\partial Y_R}{\partial \tau} = \left[1 + \frac{1}{Y_R^2}\left(\frac{\partial Y_R}{\partial \phi}\right)^2\right]\left[\frac{\partial \theta}{\partial R} + Bi_r(1 - \theta_v)\right]. \tag{9}$$

Equation 9 can be simplified by neglecting the effect of curvature and assuming that $\partial Y_R / \partial \phi = 0$ so Y_R increases uniformly with ϕ. Then equation 9 becomes:

$$G\frac{\partial Y_R}{\partial \tau} = \left[\frac{\partial \theta}{\partial R} + Bi_r(1 - \theta_v)\right]. \tag{10}$$

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Initial temperature condition is taken as uniform and equal to the surface temperature ($\theta = 0$) and the relevant boundary conditions are:

$$\theta = 0 \quad \text{at} \quad X = 0,$$

$$\theta = 0 \quad \text{at} \quad X = 1.0,$$

$$\theta = 1 \quad \text{at} \quad R = Y_R \quad \text{and}$$

$$\frac{\partial \theta}{\partial R} = 0 \quad \text{at} \quad R = 0.$$

NUMERICAL SOLUTION FOR CRYSTAL GROWTH

Analytical solutions for the above models are extremely difficult. Therefore a finite difference technique is used to obtain solutions within a desired accuracy.

After discretization equation 2, the following explicit form of finite difference formulation is obtained for the cylindrical model

$$\theta_{i,j}^{n+1} = \theta_{i,j}^{n} + \Gamma_o^2 \Delta\tau \left[\frac{1}{\Gamma_o^2} \frac{\theta_{i,j-1}^n - 2\theta_{i,j}^n + \theta_{i,j+1}^n}{(\Delta Z)^2} + \frac{\theta_{i-1,j}^n - 2\theta_{i,j}^n + \theta_{i+1,j}^n}{(\Delta R)^2} + \frac{\theta_{i+1,j}^n - \theta_{i-1,j}^n}{2i(\Delta R)^2} \right]. \tag{11}$$

The explicit form of finite difference approximation given by the equation 11 provides a relatively straight forward expression for the determination of the unknown $\theta_{i,j}^{n+1}$ at a new time step from the knowledge of $\theta_{i,j}^n$ at the previous time step.

The interface equations, equations 4 and 5, can be written in discretized form as follows:

$$Y_{Z(i,j)}^{n+1} = Y_{Z(i,j)}^{n} + \frac{\Delta\tau}{G} \left\{ 1 + \Gamma_o^2 \left[\frac{Y_{Z(i+1,j)}^n - Y_{Z(i-1,j)}^n}{2\Delta R} \right]^2 \right\} \times \left[\frac{\theta_{i,j}^n - \theta_{i,j-1}^n}{\Delta Z} + Bi(1 - \theta_v) \right] \tag{12}$$

and

$$Y_{R(i,j)}^{n+1} = Y_{R(i,j)}^{n} + \Gamma_o^2 \frac{\Delta\tau}{G} \left\{ 1 + \frac{1}{\Gamma_o^2} \left[\frac{Y_{R(i,j+1)}^n - Y_{R(i,j-1)}^n}{2\Delta Z} \right]^2 \right\} \times \left[\frac{\theta_{i,j}^n - \theta_{i-1,j}^n}{\Delta R} + Bi_r(1 - \theta_v) \right] \tag{13}$$

An empirical correlation for the Biot number used in this study for cylindrical shaped ice crystals is given as [6]:

$$Bi = \frac{k}{k_v}\left(0.315 + 0.87 Pr^{1/3} Re^{1/2}\right)$$

where k_v is the thermal conductivity of the vapor around the crystals.

Equation 11 is used to evaluate the temperature distribution on the ice crystal and then the interface is advanced both in r and z directions using equations 12 and 13.

After discretization equation 7, the following explicit form of finite difference formulation is obtained for the spherical model

$$\begin{aligned}\theta_{i,j}^{n+1} = \theta_{i,j}^{n} + \Delta\tau \Bigg\{ & \frac{i+1}{i(\Delta R)^2}\theta_{i+1,j}^{n} - \frac{2}{(\Delta R)^2}\theta_{i,j}^{n} + \frac{i-1}{i(\Delta R)^2}\theta_{i-1,j}^{n} \\ & + \frac{1}{(i\Delta R)^2}\Bigg[\left(j\Delta X - (j\Delta X)^2\right)\left(\frac{\theta_{i,j+1}^{n} - 2\theta_{i,j}^{n} + \theta_{i,j-1}^{n}}{(\Delta X)^2}\right) \\ & + (1-2j\Delta X)\left(\frac{\theta_{i,j+1}^{n} - \theta_{i,j-1}^{n}}{2\Delta X}\right)\Bigg]\Bigg\}. \end{aligned} \tag{14}$$

The interface equation, equation 10, can be written in discretized form as:

$$Y_{R(i,j)}^{n+1} = Y_{R(i,j)}^{n} + \frac{\Delta\tau}{G}\left[\frac{\theta_{i,j}^{n} - \theta_{i-1,j}^{n}}{\Delta R} + Bi_r(1-\theta_v)\right] \tag{15}$$

The empirical correlation for the Biot number used for spherical shaped ice crystals is given as [6]:

$$Bi = \frac{k}{k_v}\left(2.0 + 0.216 Pr^{1/3} Re^{1/2}\right).$$

RESULTS AND DISCUSSION

Development of the temperature profile along the axial direction of a cylindrical ice crystal is given in figure 1. The dimensional growth of the ice crystal with time is given in figure 2. The axial growth is found to be faster, as concluded and observed previously [4]. The length of the ice crystal's

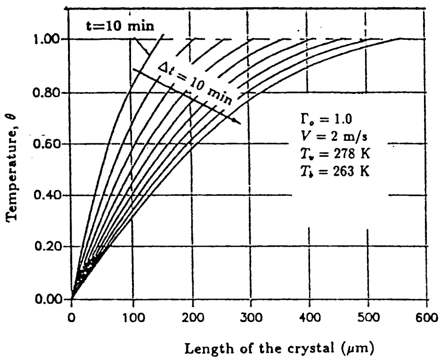

Fig. 1. Axial temperature profiles for the cylindrical model.

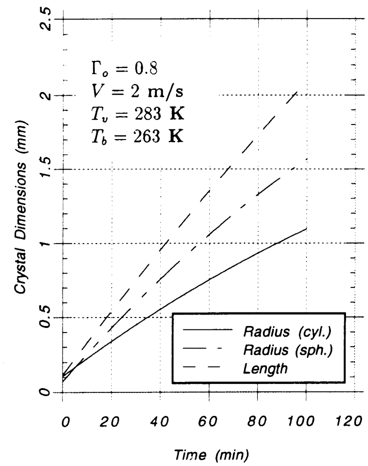

Fig. 2. Dimensions of ice crystal

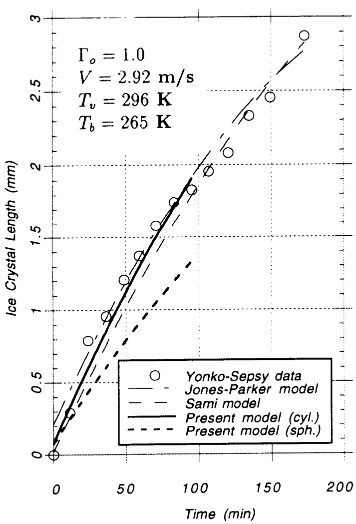

Fig. 3. Comparison of ice crystal size

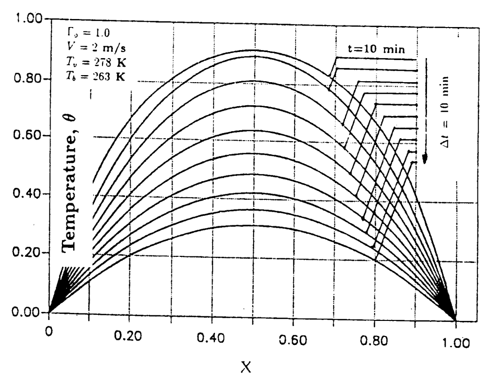

Fig. 4. Temperature profiles for the spherical model.

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variation with time, which is the primary concern in frost formation, is compared with some previous results from the literature [1,2,3] in figure 3 for the validity and accuracy of the model. It is clear that the present model gives quite accurate predictions during the first 100 minutes. It is known that during the later stages of frost formation, development of frost layer can no longer be characterized by crystal growth due to the diffusion that dominates the mass transfer process [4]. Therefore discrepancy of the previous studies with the present model after the initial period of 100 minutes is expected. 100 minutes is set to be a limit for the present study, because the size of most of the practically observed cylindrical ice crystals is less likely greater than that is developed in this period. The shape of older ice crystals are usually in a more complex type rather than being simple cylindrical. The temperature rise in the spherical ice crystal at the mid-radius with respect to parameter X is given in figure 4. The radial growth of spherical ice crystal is included in figure 2 for comparison with the cylindrical model and also is given in figure 3. Spherical model gives a lower estimate of ice crystal growth in general.

CONCLUSIONS

Conclusions derived from the present study are as follows:

1. The numerical model developed eliminates the inherent difficulties in formulation and applying complicated methods to predict ice crystal growth.
2. The proposed cylindrical crystal model gives reasonable accuracy in predicting the size of the ice crystals during the early period of crystal growth.
3. The cylindrical ice crystals grow faster in the axial direction.
4. The spherical crystal model under estimates the crystal size in general.
5. Crystals that grow for long time period attain a complex shape, therefore care should be taken when using the present simple model to simulate them.

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