CHAPTER 3

MATHEMATICAL FORMULATION

3.1 MATHEMATICAL MODELS

Mathematical models are proposed and the solution procedure for the air-precooling, heat-cool model, freeze-drying of spherical perishable product model are evaluated to obtain time-temperature histories for specific boundary conditions. The model developed with the present boundary condition will help us to obtain thermal property data from the time-temperature histories. The details of the solution procedure for i) Air cooling of slab, sphere, and cylinder, ii) Heat-Cool model, iii) Freeze-drying of spherical perishable product are presented in depth and the solution procedure are evaluated mostly using the finite difference technique.

3.1.1 Formulation

The starting point for all the three problems is the Fourier heat conduction equation. The equation of conservation of thermal energy for the case of a stationary solid is written as [116].

\[ \nabla \cdot (K \nabla T) + q_{\text{int}} = \rho c \frac{dT}{dt} \quad (3.1) \]

The assumption made in the present analyses are

i. The dimensions of the product are such that one dimensional analysis is applicable

ii. The transport properties are independent of temperature

iii. The internal heat generation is negligible \( (q_{\text{int}} = 0) \)

iv. The thermophysical properties of the perishable products are independent of direction.

In the light of above assumption equation (3.1) can be rewritten as,

\[ \frac{1}{r^n} \frac{\partial}{\partial r} \left( r^n \frac{\partial T}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) = \frac{\partial T}{\partial t} \quad (3.2) \]
where $r =$ space co-ordinate
$\alpha =$ thermal diffusivity
and $n=0$ for slabs, $n=1$ for cylinder, $n=2$ for sphere.

3.1.2 **Air-precooling**

In this case, the product to be precooled is exposed to a flow of refrigerated air at temperature $t_0$ and relative humidity $\phi$. The following additional assumptions are made in the present analysis. 1) The product is freely exposed to the flow of the cooling medium and the heat flux over the entire product surface is uniform. 2) At the beginning of the process, the temperature distribution is uniform throughout the product. To complete the statement of the problem, based on the assumptions listed earlier, the following initial and boundary conditions are written as,

$$t = t_i \text{ for } 0 \leq r \leq r_0 \text{ at } \theta = 0 \quad (3.3)$$

The specific boundary condition is cooling at the surface only (for all the three geometries namely a finite slab, a cylinder and sphere). The physical models and coordinate systems in cartesian, cylindrical and spherical coordinate systems for the pre-cooling case is shown in Fig.3.1 and in cartesian coordinates for heat-cool model in Fig 3.2. A uniform, thin and constantly evaporating moisture film exists at the product surface for both the cases throughout the cooling period.

3.2 **PRE-COOLING MODEL**

The formulation of the problem will be complete when the boundary conditions are specified for all the cases. The conditions of the symmetry yields the following condition at $r = 0$, for all the three geometries. ie, about the 1) Mid-plane of the slab, 2) the centre of the sphere, 3) axis of the cylinder yields,

$$\frac{\partial t}{\partial r} = 0 \text{ at } r = 0 \text{ and } \theta > 0 \quad (3.4)$$

3.3 **HEAT-COOL MODEL**

In this case, one end of the product is exposed to the ambient at a dry bulb temperature $t_{db}$ and a wet bulb temperature $t_{wb}$, while the other end
FIGURE 3-1 PHYSICAL MODEL AND COORDINATE SYSTEM FOR AIR-PRECOOLING PROBLEM.
FIGURE 3.2 PHYSICAL MODEL AND COORDINATE SYSTEM FOR HEAT-COOL METHOD.

CONSTANT HEAT FLUX $q_c$

AMBIENT DRY BULB TEMPERATURE $= t_{db}$

AMBIENT WET BULB TEMPERATURE $= t_{wb}$
is subjected to a uniform heat flux. The above type of boundary condition is simulated using plane electric heaters. The constant heat flux imposed at one end of the slab can be represented mathematically as,

$$\frac{\partial T}{\partial r} = -\frac{q_c}{k} \text{ at } r = 0 \text{ and } \theta > 0$$  \hspace{1em} (3.5)

It is seen that equation [3.4] is a particular case of equation [3.5] when $q_c = 0$. The boundary condition at the surface ($r = r_0$) is the one that actually differentiates the cooling of perishable products (or for that matter any moist body) from the cooling of solid dry products.

3.4 STATEMENT OF THE PROBLEM

The heat conducted at the product surface may be written as

$$k \frac{\partial T}{\partial r} = q_s \text{ at } r = r_0 \text{ and } \theta > 0$$  \hspace{1em} (3.6)

where $q_s = \text{Total quantity of energy transferred at the surface.}$

Stoecker [1] has derived a simple expression for the heat transferred at a wetted surface in terms of the enthalpy potential as,

$$q_s = \frac{h}{c_p + Wc_p \mu c} \left( H_{db} - H_s \right)$$  \hspace{1em} (3.7)

combining (3.7) and (3.6) we get,

$$\frac{\partial T}{\partial r} = \frac{h}{k(c_p + Wc_p \mu c)} \left( H_{db} - H_s \right) \text{ at } r = r_0 \text{ and } \theta > 0$$  \hspace{1em} (3.8)

The set of equation (3.2), (3.3), (3.4) and (3.7) complete the statement of problem. However it may be observed that in equation (3.8) enthalpy of moist air appears as an additional unknown quantity. It needs to be expressed in terms of temperature. The enthalpy of saturated air can be expressed as a quadratic function of its drybulb temperature to a high degree of accuracy.

Thus,

$$H_{db} = a + b \ t_{db} + c \ t_{db}^2$$  \hspace{1em} (3.9)

In order to express the enthalpy of the unsaturated air in terms of temperature, it is assumed that the fractional relative humidity is given by the ratio of specific humidities under unsaturated and saturated conditions.

Thus,

$$\phi = \frac{w'}{w}$$  \hspace{1em} (3.10)
Using the enthalpy of moist air definition we have,

\[ H = C_p t + WH_w \]  

(3.11)

Where \( H_w \) = enthalpy of saturated water vapour.

Equation (3.10) together with equation (3.11) yields an expression for the enthalpy of unsaturated air and it is easily deduced to be,

\[ H_{db} = \frac{\phi H_d + C_p t_{db}}{1-\phi} \]  

(3.12)

The above equation yields an expression for the enthalpy of unsaturated air in terms of temperature, saturated enthalpy and humidity. Introduction of equation (3.12) into equation (3.8) gives on rearrangement,

\[ \frac{\partial t}{\partial r} = -\frac{1}{k(C_p + WC_{pw})} \left( H_s - H_{db} \right) + \left(1-\phi\right) \left(H_{db} - C_p t_{db}\right) \]

at \( r = r_0 \) and \( \Theta > 0 \) (3.13)

3.4.1 Non-dimensional quantities

It can be seen from the above equation, the number of dimensional variables and physical parameters are quite large. For simplification of mathematical procedure, the variables and parameters are expressed in non-dimensional form. The right hand side of above equation is a function of temperature only when the enthalpy of saturated air is expressed as defined in equation (3.9). Now the solution for the problem is sought in a general form so that it is applicable to a wide variety of products at various processing conditions. Whenever a moist material is exposed to an unsaturated airflow, the minimum temperature of the product surface obtainable is the wetbulb temperature of the cooling air. With this objective, the following dimensionless quantities are introduced.

\[ Bi = \frac{h r_0}{k} \; ; \; Ki = \frac{q_c r_0}{k(t_i - t_{wb})} \; ; \; \Theta^* = \frac{a \Theta}{r_0^2} \; ; \; t^* = t - t_{wb} \]  

(3.14)

From the above definition it is found that \( Bi, Ki, \Theta^*, t^* \) and \( R \) are respectively Biot number, Kirpichev number Fourier number, Temperature(dimensionless) and dimensionless radius. Introduction of these quantities into equation (3.2, 3.3, 3.4) and (3.13) yields respectively,

\[ \frac{1}{R^n} \frac{\partial}{\partial r} \left( R^n \frac{\partial t^*}{\partial R} \right) = \frac{\partial \Theta^*}{\partial \Theta} \]  

(3.15)

\[ t^* = 1 \text{ for } 0 < R \leq 1 \text{ at } \Theta^* = 0 \]  

(3.16)

\[ \frac{\partial t^*}{\partial R} = 0 \text{ at } \Theta = 0 \text{ and } \Theta^* = 0 \text{ (air - precooling)} \]  

(3.17)
\[
\frac{3t'}{3R} = -\text{Bi} \quad \text{at } R = 0 \quad \text{and } \theta^* > 0 \quad \text{(Heat-Cool)} \quad (3.18)
\]

\[
\frac{3t'}{3R} = \frac{-\text{Bi}}{(c_p + \omega C_p \rho w)} \left( \frac{H_s - H_{db}}{t'_{ib}} + (1 - \Phi) \left( H_{db} - C_p t_{db} \right) \right) \quad \text{at } R = 1 \quad \text{and } \theta^* > 0 \quad (3.19)
\]

Right hand side of equation (3.19) can further be simplified and written in terms of dimensionless form. The saturation enthalpy \( H_s \) is to be expressed in terms of the dimensionless surface temperature \( t' \) using equation (3.9). The enthalpy difference \( (H_s - H_{db}) \) in terms of dimensionless temperature \( t' \) can be written as below

\[
(H_s - H_{db}) = (b + 2c t_{wb}) (t_i - t_{wb}) + c t_s^2 (t_i - t_{wb})^2 - c t_{db}^2 (t_i - t_{wb})^2 \quad (3.20)
\]

The above equation (3.20) is introduced into equation (3.19) which yields on rearrangement,

\[
\frac{3t'}{3R} = -\text{Bi} (c_1 t_s^2 + c_2 t_{ib} + c_3) \quad \text{at } R = 1 \quad \theta^* > 0 \quad (3.21)
\]

Where \( c_1, c_2 \) and \( c_3 \) are constants which are defined later. The equation (3.21) holds good for all the three geometries, (slab shaped, spherical, and cylindrical) considered for air-precooling and Heat-cool models. The constants \( c_1, c_2 \) and \( c_3 \) are listed for both air cooling and heat-cool models.

In the case of pre-cooling, cooling takes place by forced convection. The heat transfer coefficient in this case can easily be evaluated for different flow conditions knowing the Reynold number.

In the case of heat-cool model, where a constant heat flux at \( R = 0 \) is applied and cooling by ambient takes place at \( R = 1 \) is due to the free convection effects. The heat transfer in such case is a function of the product of Grashof and Prandtl numbers of the fluid. The dimensionless heat transfer coefficient or the Nusselt number \( (Nu) \) for the free convection condition is given as [118]

\[
Nu = \frac{h_f c_L}{K_f} = c(Gr Pr)^5 \quad (3.22)
\]

where \( Gr \), the Grashof number, is based on the temperature difference between
the product surface and ambient temperature and \( L \) is the width for a square plate [119].

### 3.4.2 Modified Grashof number

In the present case, the surface temperature is an unknown quantity varying with time. Therefore the heat transfer coefficient at the surface will also be varying with time. To take care of this a modified Grashof number \( \text{Gr}_i \) is introduced in the present analysis.

Equation (3.22) can be written as,

\[
\text{Nu} = c (t_s^* - t_{db}^*) (\text{Gr}_i \text{Pr})^s
\]

(3.23)

The constant values \( c \) and \( s \) are available for different values of the product \( (\text{Gr}_i \text{Pr}) \) in [118]. Nusselt number can be written in terms of Biot number as,

\[
\text{Nu} = \frac{k}{\text{Bi} L}
\]

(3.24)

Combining equation (3.24) and (3.23) we get,

\[
\text{Bi} = \frac{k}{K} \frac{r_0}{L} c[(\text{Gr}_i \text{Pr})(t_s^* - t_{db}^*)]^s
\]

(3.25)

Defining modified biot number \( \text{Bi}_i \) as

\[
\text{Bi}_i = \frac{k}{K} \frac{r_0}{L} c(\text{Gr}_i \text{Pr})^s
\]

(3.26)

substituting the equation (3.26) in (3.21) the boundary condition at \( r_0 = r \) for the heat-cool model is written as,

\[
\frac{dT}{dR} = -\text{Bi}_i(t_s^* - t_{db}^*)^s(c_1 t_s^* + c_2 t_{db}^* + c_3) \text{ at } R = 1, \Theta^* > 0
\]

(3.27)

### 3.5 EVALUATION OF CONSTANTS

In equation (3.37) and (3.21) the value of the constants \( C_1, C_2 \) and \( C_3 \) are as follows

\[
\begin{align*}
C_1 &= -\text{Bi} \frac{c(t_i - t_{wb})}{(c_p + WC_{pw})} \quad C_2 = -\text{Bi} \frac{(b + 2c t_{wb})}{(c_p + WC_{pw})} \\
C_3 &= -\text{Bi} \frac{(H_{db} - c_p t_{db})(1 - \phi)}{(t_i - t_{wb})(c_p + WC_{pw}) - C_2 t_{db} - C_1 t_{db}^2}
\end{align*}
\]

(3.28)
In the above expression, the temperature $t_1$, $t_{db}$ and $t_{wb}$ appear explicitly. These temperatures can be non-dimensionalized by defining another dimensionless temperature $t^*$ as,

$$ t^* = \frac{ct}{(c_p + WC_{pw})} \quad (3.29) $$

It is expressed in dimensionless form so that they are useful in any system in which the temperatures are expressed. Introduction of equation (3.29) into equation (3.28) yields on rearrangement,

$$ C_1 = -Bi(t_i^* - t_{wb}^*) \\
C_2 = -Bi\left(\frac{b}{c_p + WC_{pw}} + 2t_{wb}^*\right) \\
C_3 = -Bi\left[\frac{ac}{(c_p + WC_{pw})^2} + \frac{(b - c_p)t_{db}^*}{(c_p + WC_{pw})} + t_{db}^*\right] \frac{(1 - \varphi)}{(t_i^* - t_{wb}^*)} - C_{2t_{db}^*} - C_{1t_{db}^*2} \quad (3.30) $$

By introducing numerical values of various quantities the above equation (3.30) can further be simplified. The Isobaric specific heat of air $C_p$ is taken to be constant at 0.24 K cal/kg°C, and the value of $WC_{pw}$ is close to 0.005 k Cal/kg °C [11/]. In the case of air-cooling the quadratic relation between enthalpy of saturated air and its temperature defined in equation (3.9) is written as,

$$ H = 3.951 + 0.0736 t + 0.0189 t^2 \quad (3.31) $$
in K Cal/kg of dry air when 't' is in °C. This expression is applicable in the temperature range of 4 °C to 40 °C the range encountered in the pre-cooling practice.

After introduction of the numerical values and simplification, equation (3.29) and (3.30) yield respectively,

$$ t^* = 0.0708 t \quad (3.32) $$

$$ C_1 = -Bi(t_i^* - t_{wb}^*) \quad (3.33) $$

$$ C_2 = -Bi(0.3724 + 2t_{wb}^*) $$

$$ C_3 = -Bi(1.307 - 0.5981 t_{db}^* + t_{db}^* - (1 - \varphi)) \frac{1 + (-t_{wb}^*)}{(t_i^* - t_{wb}^*)} $$
The set of equation (3.15 to 3.17) and (3.21) define the problem of air-cooling of perishable products in dimensionless form. The governing parameter are the Biot number Bi, the relative humidity $\phi$, the initial product temperature $t_i$, the ambient dry bulb temperature $t_{db}$ and ambient wet bulb temperature $t_{wb}$.

3.6 HEAT-COOL MODEL

Values of the constants $a, b,$ and $c$ in equation (3.9) are as shown below:

\[
\begin{align*}
    a &= 46.9821 \\
    b &= -2.496 \\
    c &= 0.0673
\end{align*}
\]

These values are obtained for the temperature range of 25 °C to 60 °C. After introduction of the numerical values and simplification equation 3.29 and 3.30 yield respectively.

\[
t^+ = 0.2241 \, t
\]

\[
C_1 = (t^+_i - t^+_{wb})
\]

\[
C_2 = 2t^+_{wb} - 10.4096
\]

\[
C_3 = 45.9917 - 11.3909 \, t^+_db + t^+_db \left( \frac{1-\phi}{t^+_i - t^+_{wb}} \right) - C_2 t^+_db - C_1 t^+_db
\]

It is easily seen that in case of air-precooling, the governing parameters are the biot number $Bi$, the ambient dry bulb temperature $t^+_{db}$, the ambient wet bulb temperature $t^+_{wb}$ and the initial product temperature $t^+_i$.

While in the case of heat-cool, the parameters are modified Biot number, $Bi_j$, the three temperature $t^+_db$, $t^+_wb$, $t^+_i$ and nondimensional heat flux parameter $K_i$, called the kirpichev number. It can be observed from the above equations for pre-cooling and heat-cool model cases that the governing equation is linear for both the cases whereas the boundary condition as given by equation (3.21) and (3.27) are non-linear.
3.7 FREEZE-DRYING

A mathematical model for freeze-drying of perishable products in the form of spheres is presented here. This model is highly useful for predicting the dehydration characteristics of granulated and pelletized products in particle beds or fluidized beds. Also, since a generalised surface heat flux function is considered, the analysis is capable of taking into account the gas conduction and convection effects if suitable correlations are available. The Fourier heat conduction equation is the starting point of the analysis. The following assumptions are made.

1. The heat flux over the product surface is uniform
2. The drying process is heat transfer limited.
3. The drying front is distinct and a clearcut boundary exists between the dry shell and the frozen core.

The physical model and coordinate system for freeze-drying problem is studied where in a spherical perishable particle of radius \( r_0 \), frozen to an initial uniform temperature \( t_f \), is exposed to a uniform surface heat flux defined by an arbitrary function \( G_1 \), and is represented in Figure 3.3.

3.7.1 Freeze-drying mathematical formulation

For the dry shell, the heat conduction equation (3.2) is rewritten as,

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial t}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\partial t}{\partial r} \right) \text{ for } \delta_d \leq r \leq r_0
\]

(3.37)

Based on the physical model and the assumptions mentioned earlier, the initial and boundary conditions are formulated as follows.

\[
t = t_f \text{ for } 0 \leq r \leq r_0 \text{ at } \theta = 0
\]

(3.38)

\[
d = 0 \text{ at } \theta = 0
\]

(3.39)

\[
k \frac{\partial t}{\partial r} = G_1(t_s) \text{ at } r = r_0, \theta > 0
\]

(3.40)

\[
k \frac{\partial t}{\partial r} = -\delta_{\text{ice}} \lambda \delta G \left( \frac{\partial t}{\partial \theta} \right) \text{ at } r = \delta \text{ and } \theta = 0
\]

(3.41)

The condition given in equation (3.41) is written with the assumption that there is no heat transfer to the ice core and equation (3.41) represents the
FIGURE 3.3 COORDINATE SYSTEM FOR FREEZE-DRYING PROBLEM.

a) PHYSICAL MODEL OR SPHERE

b) EQUIVALENT SLAB (Goodman's method)
heat conducted through the drying front which is equal to the heat dissipated as latent heat of sublimation. Based on the assumption, the following condition can also be written.

\[ t = t_f \text{ at } r = \delta_d \text{ and } \theta > 0 \]  
\[ \frac{dt}{dr} = 0 \text{ at } r = \delta_d \text{ and } \theta > 0 \]  

As in the case of air-cooling discussed earlier, the following dimensionless quantities are defined to facilitate in obtaining a generalized solution.

\[ R = \frac{r}{r_0}, \quad t' = \frac{t - t_f}{t_{sc} - t_f}, \quad \theta^* = \frac{\alpha \theta}{r_0^2} \]  

With the introduction of these quantities, equation (3.37 to 3.43) can be rephrased in the following form.

\[ \frac{1}{R} \frac{\partial}{\partial R} \left( R t' \right) = \frac{\partial t'}{\partial \theta^*} \text{ for } \delta_d \leq R < 1 \]  
\[ t' = 0 \text{ for } 0 \leq R \leq 1 \text{ at } \theta^* = 0 \]  
\[ \delta_1^* = 1 \text{ at } \theta^* = 0 \]  
\[ \frac{\partial t'}{\partial R} = G_1(t'_1) \text{ at } R = 1, \theta^* > 0 \]  
\[ \frac{\partial \delta^*}{\partial R} = \rho_{ice} \frac{h_{sc}}{r_0} \alpha /K(t_{sc} - t_f) \cdot \frac{d\delta^*}{d\theta^*} \]  
\[ t' = 0 \text{ at } R = \delta_d \text{ and } \theta^* > 0 \]  
\[ \frac{\partial t'}{\partial R} = 0 \text{ at } R = \delta_d \text{ and } \theta^* > 0 \]  

The problem of freeze-drying of spherical particle is completely defined in dimensionless form by the set of equations (3.45 to 3.51).

**3.8 SOLUTION PROCEDURES**

A number of techniques are available to solve the partial differential heat conduction equations. A few of them are useful in solving many complicated problems such as

1. Classical method (separation of variables)
2. Integral method (Laplace transform, Fourier transform)
3. Use of Green's function
4. Approximate integral methods (heat balance integral method)
5. Analog method
6. Numerical methods (Finite difference method, finite element method)
3.9 FINITE DIFFERENCE TECHNIQUE

For all the three geometries considered, the finite difference technique is adopted for the solution.

3.9.1 Air-precooling, Slab shaped product

The grid system for finite difference formulation is shown in fig. 3.4a. In this grid, the thickness of the slab is divided into 'm' meshes, each with a thickness ΔR and with nodes placed on each boundary. Similarly, the reference frame for time is also divided into number of time steps each equal to Δθ*. Thus the two boundary surfaces are designated by the nodal points i = 0 and i = m and the intermediate points are designated by the subscript n and n = 1 corresponds to the time Δθ* = 0. Thus t_i,n indicates the temperature at a location iΔR and time (n - 1)Δθ*. In the present investigation, an implicit scheme known as Crank-Nicolson scheme is used. This scheme does not place any restriction on the mesh size for stability. For this scheme, all the finite differences are written about the point R_i, θ_n+½. (Marked + in figure 3.4a and 3.4b). The finite difference scheme for various nodal points are written as follows:

For 1 ≤ i ≤ (m-1) equation (3.15) yields,

\[ t_{i-1,n+1} - 2t_{i,n+1} + t_{i+1,n+1} = \frac{2}{2(ΔR)^2} t_{i,n} \] (3.52)

At the surface i = 0, we have from equation 3.17

\[ t_{i,1} = t_{i,0} \text{ for all the values of } n \] (3.53)

The initial condition equation (3.16) can be written as

\[ t_{i,1} = 1 \text{ for all } i \] (3.54)

Equation 3.21 is recalled as

\[ \frac{∂t}{∂R} = -Bi(C_1t_{S}^2 + C_2t_{S} + C_3) \text{ at } R = 1, \quad θ = 0 \] (3.21)

The finite difference equation for equation (3.21) is written as

\[ \frac{t_{m+1,n+1} - t_{m-1,n+1}}{2(ΔR)} = -Bi(C_1t_{m,n+1}^2 + C_2t_{m,n+1} + C_3) \] (3.55)
FIGURE 3.4 THE FINITE DIFFERENCE GRID SYSTEMS.
Equation (3.52) to (3.55) complete the statement of the problem in finite difference formulation. The final set of algebraic equations can be obtained from these equations as follows. Combining equation (3.53) and (3.52) yields,

\[
\begin{bmatrix}
-2L & 2L & 2L & -2L & 2L & 2L & -2L & 2L & 2L & \\
2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
\end{bmatrix}
\begin{bmatrix}
L_o, n+1 \\
L_1, n+1 \\
L_2, n+1 \\
L_3, n+1 \\
L_4, n+1 \\
L_5, n+1 \\
L_6, n+1 \\
L_7, n+1 \\
L_8, n+1 \\
L_9, n+1 \\
\end{bmatrix} = \begin{bmatrix}
2L & 2L & 2L & -2L & 2L & 2L & -2L & 2L & 2L & \\
2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
2L & 2L & -4L & 2L & -4L & 2L & -4L & 2L & -4L & \\
\end{bmatrix}
\begin{bmatrix}
L_o, n \\
L_1, n \\
L_2, n \\
L_3, n \\
L_4, n \\
L_5, n \\
L_6, n \\
L_7, n \\
L_8, n \\
L_9, n \\
\end{bmatrix}
\quad \text{for } i = 0
\]  (3.56)

Equation (3.56) and (3.52) form the first half of the tridiagonal system of equations to be solved. However, problem arises at the other boundary \( i = m \), where \( t_{m,n+1} \) values are not known. As already pointed out equation (3.21), and equation (3.55) are non-linear. In situations where nonlinearity occurs at the boundary, it is recommended to use backward difference scheme to avoid oscillations [120]. The backward difference analog to the equation (3.15) which does not have a restriction on the size of \( \Delta \theta^* \) for stability is,

\[
t_{n+1} - 2 \frac{(AR)^2}{\Delta \theta} t_{n+1} - 2 \frac{(AR)^2}{\Delta \theta} t_{m,n+1} = \frac{(AR)^2}{\Delta \theta} t_{m,n}
\]  (3.57)

Applying equation (3.57) to the surface \( i = m \) we get,

\[
t_{m-1,n+1} - 2 \frac{(AR)^2}{\Delta \theta} t_{m,n+1} - 2 \frac{(AR)^2}{\Delta \theta} t_{m+1,n+1} = \frac{(AR)^2}{\Delta \theta} t_{m,n}
\]  (3.58)

In the above equation, \( t_{n+1} \) is the temperature at a fictitious point located one increment beyond the boundary. Combining equations (3.55) and (3.58), we get

\[
2t_{m-1,n+1} - 2 \frac{(AR)^2}{\Delta \theta} t_{m,n+1} = 2BiAR \left( L_1 \frac{t_{m,n+1} + t_{m+1,n+1}}{2} + C_2 \frac{t_{m,n+1} - t_{m-1,n+1}}{2} \right) + \frac{(AR)^2}{\Delta \theta} t_{m,n}
\]  (3.59)

Equation (3.52), (3.56), and (3.59) form the tridiagonal system of equations to be solved. An efficient method has been developed by Thomas [120] to solve the tridiagonal system of equations. The Thomas algorithm is given in Appendix A. The first half of the tridiagonal system comprising of equation (3.52) and (3.56) are solved easily. Since equation (3.59) is non-linear in \( t_{m,n+1} \) which is an unknown, it is first solved by the well known Newton-Raphson technique. Once the value of \( t_{m,n+1} \) is determined the other half of the tridiagonal scheme can be solved. For a given set of parameter, \( B_1 \), \( t_{db}^+ \), \( t_{wb}^+ \), and \( t_i \) the method of computation is as follows.

i. An initial time increment \( \Delta \theta \) (equal to 0.0001 in this case) is given.
ii. The nonlinear equation (3.59) is solved for \( t_{m,n+1} \) using the Newton-Raphson technique and the tridiagonal system of equations (3.52), (3.56) and (3.59) are solved using the Thomas algorithm.

iii. Since the Crank-Nicolson method is stable at every time stage, \( \Delta \theta^* \) is set equal to 0.0001 and the above step is repeated till an asymptotic value of \( t_{i,n}^* \) is achieved.

iv. The initial temperature distribution is set as given by equation (3.54) as

\[
t_{i,1} = 1 \quad \text{for } i = 0,1,2,3, \ldots, m
\]

### 3.9.2 Air-precooling, cylindrical shaped product

The solution procedure for this case is similar to that given for the case of a slab, except at the centre where a singularity occurs. The governing equation (3.15) and the boundary conditions given in equations (3.16), (3.17) and (3.21) are rewritten in the following form.

\[
\frac{\partial^2 t'}{\partial R^2} + \frac{1}{R} \frac{\partial t'}{\partial R} = \frac{\partial^2 t'}{\partial \theta^*^2} 
\]

(3.60)

\[
t' = 1 \quad \text{for } 0 < R < 1 \text{ at } \theta^* = 0 
\]

(3.61)

\[
\frac{\partial t'}{\partial R} = 0 \quad \text{at } R = 1, \theta^* > 0 
\]

(3.62)

\[
\frac{\partial t'}{\partial \theta^*} = -B_i \left( C_1 t_{s}^2 + C_2 t_{s} + C_3 \right) \text{ at } R = 1, \theta^* > 0 
\]

(3.63)

The finite difference grid system for writing the Crank-Nicolson algorithm [120] is shown in the Fig.3.5. The space range of 0 to 1 is divided into 100 equal spacings (each grid position being represented by subscript \( m \)) thus giving a space interval of \( \Delta R = 0.01 \). The grid locations are shifted by half spacing, to avoid the singularity at the axis. The time grids are denoted by the subscript \( n \). The finite difference scheme for various space grid location are written as follows. For \( 2 < m < 99 \) equation 3.60 gives,

\[
\begin{align*}
\left[ \frac{2m - 2}{2m - 1} t_{m-1,n+1}^* + \left( -2 - \frac{2(\Delta R)^2}{(\Delta \theta^*)^2} \right) t_{m,n+1}^* + \left( \frac{2m}{2m-1} \right) t_{m+1,n+1}^* \right] & = \left( \frac{2m-2}{2m-1} \right) t_{m-1,n}^* \\
\left[ \frac{2m}{2m-1} t_{m+1,n+1}^* + \left( 2 - \frac{2(\Delta R)}{(\Delta \theta^*)^2} \right) t_{m,n}^* \right] & = \left( \frac{2m}{2m-1} \right) t_{m,n}^*
\end{align*}
\]

(3.64)
FIGURE 3.5 NON-DIMENSIONAL CO-ORDINATES FOR AIR-COOLING.
For \( m = 1 \), equation (3.62) yields,
\[
\frac{3 t'}{\Delta R} = \frac{t'_i - t'_o}{\Delta R} = 0
\]
(3.65)
which gives on rearrangement as below
\[
t'_i, n = t'_o, n \quad \text{and} \quad t'_i, n+1 = t'_o, n+1
\]
Hence from equation (3.64) we get,
\[
\begin{bmatrix}
-2 - \frac{2(\Delta R)^2}{(\Delta \theta^*)} \\
\frac{2(\Delta R)^2}{(\Delta \theta^*)}
\end{bmatrix}
t'_i, n+1 + 2t'_2, n+1 = \begin{bmatrix}
2 - \frac{2(\Delta R)^2}{(\Delta \theta^*)} \\
\frac{2(\Delta R)^2}{(\Delta \theta^*)}
\end{bmatrix} t'_i, n - 2t'_2, n
\]
(3.66)
For \( m = 100 \), equation (3.63) yields on introduction of equation (3.29)
\[
C_1 t^{100, n+1} + C_2 t^{100, n+1} + C_3 \frac{t^{100, n+1} - t^{100, n+1}}{\Delta R} = 0
\]
(3.67)
which yields on rearrangement,
\[
t^{101, n+1} = t^{100, n+1} + R \left( C_1 t^{100, n+1} + C_2 t^{100, n+1} + C_3 \right)
\]
(3.68)
While non-linearity occurs at the boundary, it is recommended to use the backward difference scheme to avoid oscillations. Hence at the surface, the backward difference analogue is written as,
\[
t_{99, n+1} + \frac{\Delta R}{2} t_{100, n+1} + \Delta R t_{100, n+1} = \begin{bmatrix}
-1 - \frac{(\Delta R)^2}{(\Delta \theta^*)} \\
\frac{(\Delta R)^2}{(\Delta \theta^*)}
\end{bmatrix} t^{100, n} - C_1 \frac{(\Delta R)}{\Delta \theta^*}
\]
(3.69)
The expression for the surface temperature can be written as,
\[
t'_s = t'_i + \frac{t_{101} - t_{100}}{2}
\]
(3.70)
This relation together with equation (3.53) results in the expression,
\[
t'_s = t_{100} + \frac{\Delta R}{2} \left( C_1 t_{100}^2 + C_2 t_{100}^2 + C_3 \right)
\]
(3.71)
For a given set of parameter \( B_i, \Phi, t_0, \) and \( t_i \), the following computational procedure is adopted.

i. The initial temperature distribution is set as given by equation (3.61) Thus \( t_{m,0} = 1 \) \((m = 1, 100)\)

ii. An initial time increment \( \Delta \theta^* \) (equal to 0.0001 in the present case) is given.

iii. The 'tridiagonal' system of equations (3.64), (3.66), and (3.69) is solved by applying Thomas Algorithm.
iv. This method being very stable and insensitive to the changes in the magnitude of the quantity, \( \frac{\partial^2 t}{\partial R^2} + \frac{2}{R} \frac{\partial t}{\partial t} = \frac{\partial^2 t}{\partial t^2} \) for 0 < r < 1, \( \frac{\partial t}{\partial t} > 0 \) (3.72)

A complication namely the singularity at R = 0 as in the cylinder problem arises in this case also. By changing the dependent variable \( t' = \frac{Q}{R} \) the governing equation reduces to the form,

\[
\frac{\partial^2 Q}{\partial R^2} = \frac{\partial Q}{\partial t} \quad (3.73)
\]

Equation (3.73) can be recognised equivalent to heat conduction equation in cartesian coordinates. The spherical problem can thus be converted to one of an equivalent slab. The finite difference equation for the grid system of Fig 3.4a is used in this case. The modified governing equation after applying the 'L HOSPITAL'S' rule to equation (3.72) is written as,

\[
\frac{3 \frac{\partial^2 t'}{\partial R^2}}{\partial t} = \frac{\partial t'}{\partial t} \quad (3.74)
\]

Only the finite difference equations is given here as the evaluation procedure is very much similar to the cases described earlier.

At R = 0,

\[
-2 \left[ -\frac{2}{3} \left( \frac{\Delta R}{\partial t^*} \right) \right] t_{0,n+1} + 2t_{1,n+1} = -2t_{1,n} + \left[ 2 - \frac{2}{3} \left( \frac{\Delta R}{\partial t^*} \right) \right] t_{0,n} \quad (3.75)
\]

For the point, 1 < i < (m-1),

\[
\left[ \frac{1}{2} \left( \Delta R \right) \right] t_{i-1,n} + \left[ \frac{1}{2} \left( \Delta R \right) \right] t_{i+1,n} + \left[ 2 - \frac{2}{3} \left( \frac{\Delta R}{\partial t^*} \right) \right] t_{i,n} \quad (3.76)
\]

For the point, i = m,

\[
\left[ -\frac{\Delta R}{\partial t^*} \right] t_{m,n+1} + 2t_{m-1,n} = 2m \left( \frac{\Delta R}{\partial t^*} \right) t_{m,n} \quad (3.77)
\]

Equation (3.75), (3.76), and (3.77) complete the set of finite difference equations to describe the air-precooling of moist material in the shape of sphere. The computation procedure for the above equation is given as below.

For a given set of parameters, Bi, \( \phi \), \( t_o \) and \( t_i \), the following computational procedure is adopted.

3.9.3 Air-precooling spherical shaped product

The governing equation (3.15) for \( n = 2 \) is written as below.

\[
\frac{\partial^2 t}{\partial R^2} + \frac{2}{R} \frac{\partial t}{\partial R} = \frac{\partial^2 t}{\partial t^2} \quad (3.15)
\]

For a given set of parameters, Bi, \( \phi \), \( t_o \), and \( t_i \), the following computational procedure is adopted.
i. The initial temperature distribution is set as given by equation (3.16) thus, \( t'_{m,0} = 1 \) for \((m=1,i)\).

ii. An initial time increment \( \Delta \theta^* \) (equal to 0.0001) is given.

iii. The non-linear equation (3.77) is solved for \( t'_{m,n+1} \) and the tridiagonal system of equations (3.75), (3.76) and (3.77) are solved using the Thomas Algorithm.

iv. Since the Crank-Nicolson method is stable at every time stage, \( \Delta \theta^* \) is increased (by 10% of previous value in the present case) and step (iii) is repeated.

### 3.10 SOLUTION PROCEDURE, HEAT-COOL MODEL

The solution procedure for this case is similar to that of the slab described earlier. The grid shown before is used in this case. The final equations alone are given here.

The finite difference equations for various nodes are as follows:

For \( 1 \leq i \leq (m-1) \) Equation 3.52 can be recalled as

\[
t_{i-1,n+1} = -2\left(\frac{2(\Delta R)}{(\Delta \theta^*)}\right) t_{i-1,n} + t_{i+1,n+1} = -2\left(\frac{2(\Delta R)}{(\Delta \theta^*)}\right) t_{i,n} + 2\left(\frac{2(\Delta R)}{(\Delta \theta^*)}\right) t_{i+1,n+1} (3.52)
\]

The boundary condition at \( R = 0 \) is obtained from equation (3.18) as

\[
\begin{align*}
&t_{i,n+1} - t_{i-1,n+1} = -K_i \Delta R \\
&t_{i,n} - t_{i-1,n} = -K_i \Delta R
\end{align*}
\]

(3.78)

Substituting equations (3.78) in (3.52), the finite difference equation for the point \( i = 0 \) is obtained as

\[
\begin{bmatrix}
-1-2 \left(\frac{\Delta R}{(\Delta \theta^*)}\right) t_{0,n+1} + t_{1,n+1} = t_{0,n} + 2\left(\frac{2(\Delta R)}{(\Delta \theta^*)}\right) t_{1,n+1} - 2K_i \Delta R
\end{bmatrix}
\]

(3.79)

The backward difference analog for the point \( i = m \) obtained by equations (3.27) and (3.57) is written as,

\[
2t_{m-1,n+1} = -2\left(\frac{\Delta R}{(\Delta \theta^*)}\right) t_{m,n+1} + 2\left(\frac{\Delta R}{(\Delta \theta^*)}\right) t_{m,n+1} + 2K_i \Delta R (t_{m,n} - t_{m,n+1})^S
\]

(3.80)
Equation (3.55) is non-linear in \( f \), which is an unknown to be determined. Newton-Raphson technique is used to solve this non-linear equation. Thus equations, (3.79), (3.80), and (3.52) form the tridiagonal system of equations for the case of heat-cool model. The computational procedure is similar to the one explained for the case of slab system.

The numerical algorithms for the solution of finite difference equations have been derived and they yield numerical solution to the original differential equations. Such solutions are obtained in the present investigation by programming the algorithms on an IBM 360/44 digital computer. The final values of \( \Delta R \) and \( \Delta \theta \) used in the present investigation are 0.01 and 0.0001 respectively. It is found that the computer memory space required for the solution of the differential equation with the non-linear boundary condition is 256k. The numerical methods explained here are used to solve the linear differential equations with non-linear boundary conditions formulated for the case of pre-cooling (for all the three geometries) and heat-cool model (slab). Time-Temperature characteristics are generated for various parameter values of Biot number, product initial temperature, cooling air dry bulb and wet bulb temperatures in the case of pre-cooling and for various values of modified Biot number, Kirpichev number, product initial temperature, dry bulb and wet bulb temperature of the ambient in the case of heat-cool model.

3.11 FREEZE - DRYING OF SPHERICAL PERISHABLE PRODUCT

The set of equations (3.45) to (3.51) defining the freeze-drying problem for spherical particles is recalled as,

\[
\frac{1}{R} \frac{\partial}{\partial R} (R t^*) = \frac{\partial \delta^*}{\partial \theta^*} \quad \text{for} \quad \delta_d^* < R < 1
\]  

(3.45)

\[
t^* = 0 \quad \text{for} \quad R \leq 1 \quad \text{at} \quad \theta^* = 0
\]  

(3.46)

\[
\delta^* d = 1 \quad \text{at} \quad \theta^* = 0
\]  

(3.47)

\[
\frac{\partial t^*}{\partial R} = G_1(t^*_c) \quad \text{at} \quad R = 1, \quad \theta^* > 0
\]  

(3.48)

\[
\frac{\partial t^*}{\partial R} = - \rho_{\text{ice}} A h_{sg} \frac{\alpha}{K(t^*_{sc} - t_1)}. \frac{d\delta^*}{d\theta^*}
\]  

(3.49)

\[
t^* = 0 \quad \text{at} \quad R = \delta_d^* \quad \text{and} \quad \theta^* = 0
\]  

(3.50)

\[
\frac{\partial t^*}{\partial R} = 0 \quad \text{at} \quad R = \delta_d^* \quad \text{and} \quad \theta^* > 0
\]  

(3.51)
3.11.1 Solution procedure

For this problem alone, Goodman's integral technique is applied to obtain the solution for the above set of equations. As in the case of air-cooling of spherical perishable product, a new variable is defined as,
\[ Z = R t^* \]  
(3.81)

In terms of this new variable, equation (3.41) reduces to
\[ \frac{\partial^2 Z}{\partial R^2} = \frac{\partial Z}{\partial \Theta^*} \]  
(3.82)

The above equation is similar to that of the heat conduction equation in cartesian coordinate system. The other boundary conditions are also expressed in terms of new variable. Equation (3.46) and (3.50), yield respectively,
\[ Z = 0 \quad \text{for} \quad 0 < R < 1 \quad \text{at} \quad \Theta^* = 0 \]  
(3.83)
and
\[ Z = 0 \quad \text{for} \quad R = \delta^* \quad \text{for} \quad \Theta^* > 0 \]  
(3.84)

At the surface, i.e., at \( R = 1 \) equation (3.81) gives,
\[ Z_s = t_s^* \]  
(3.85)

The boundary conditions involving the derivatives are derived as follows:
Equation (3.81) is differentiated with respect to \( R \) to give,
\[ \frac{\partial Z}{\partial R} = t^* + R \frac{\partial t^*}{\partial R} \]  
(3.86)

Equation (3.51), together with equations (3.50), and (3.86) yields,
\[ \frac{\partial Z}{\partial R} = 0 \quad \text{at} \quad R = \delta^* \quad \text{and} \quad \Theta^* > 0 \]  
(3.87)

Equation (3.48) together with equations (3.85) and (3.86) result in,
\[ \frac{\partial Z}{\partial R} = t_s^* + G_1(t_s^*) = Z_s + G_1(Z_s) = G_1(Z_s) \quad \text{at} \quad R = 1 \quad \text{and} \quad \Theta^* > 0 \]  
(3.88)

Equation (3.49), in conjunction with equation (3.86) yields,
\[ \frac{\partial Z}{\partial R} = -\rho \text{ ice} \frac{d}{d \delta^*} \frac{\delta^*}{d \delta^*} \frac{d}{d \delta^*} \frac{d}{d \delta^*} \]  
(3.89)

The above expression, on substitution from equation (3.50) gives,
\[ \frac{\partial Z}{\partial R} = -\rho \text{ ice} \frac{d}{d \delta^*} \frac{\delta^*}{d \delta^*} \frac{d}{d \delta^*} \frac{d}{d \delta^*} \quad \text{at} \quad R = \delta^* \quad \Theta^* > 0 \]  
(3.89)
Equation (3.82) to (3.84) and (3.87) to (3.89) define the freeze-drying problem for the equivalent slab in terms of the new variable \( Z \). Using Leibnitz's rule, equation (3.82) is integrated between the limits \( \delta_d^* \) to 1 gives
\[
\frac{\partial}{\partial R} R \frac{\partial}{\partial \delta d^*} \int_{\delta d^*}^{1} Z dR = \int_{\delta d^*}^{1} dR \frac{\partial}{\partial \delta d^*} Z dR \quad (3.90)
\]
The conditions given in equations, (3.84), (3.88), and (3.89) are substituted into equation (3.89) to give on simplification.
\[
G = \frac{d}{d \delta^*} \left[ I_d - \rho_{\text{ice}} \lambda h_{sg} K(t_{sc} - t_f) \frac{\delta_d^*}{2} \right] (3.91) \quad I_d = \int_{\delta d^*}^{1} Z dR \quad (3.92)
\]
A parabolic profile for \( Z \) in terms of the space variable is assumed to be of the form,
\[
Z = C_1 + C_2(R - \delta_d^*) + C_3(R - \delta_d^*)^2 \quad (3.93)
\]
Equation (3.83) and (3.87) provide all the conditions for evaluating the coefficients in the above profile. For a given value of the parameter \( \rho_{\text{ice}}, \lambda, h_{sg}, \alpha, K \), and a known heat flux function \( G \_1 \) (Ex: Radiation, gas conduction, convection or any combination of them), the following computational procedure is adopted.

i) The heat flux function \( G_1(t^*_s) \) is transformed into dimensionless form using the definition of \( t^*_s \) and function \( G(Z_s) \) is obtained as given in equation (3.88).

ii) Knowing that the initial value of surface temperature \( t^*_s = Z_s \), equation (3.85) is zero, small increments (0.005 in this case) are given to it and the function \( G(Z_s) \) is evaluated (121).