A HEAT AND MASS TRANSFER MODEL FOR BREAD BAKING: AN INVESTIGATION USING NUMERICAL SCHEMES

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To My Dear Friend ...

who is my inspiration and support...

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Summary

The final step in bread making is the actual baking process in which the raw dough, under the influence of heat, is transferred into a light, porous, readily digestible and flavored product. This transformation involves various reactions which change the structural nature of dough and are highly complex due to a vast series of physical, chemical and biochemical interactions.

The production of superior quality bread requires close monitoring of the supplied heat, rate of application of heat, duration of baking etc. Though many facts of the chemical and physical changes during baking are already known, there are still processes remaining to be understood. To study the physical changes during baking such as heat and mass transfer, a good mathematical model is very helpful. Though lots of researches are going on in this area, there are only a few good, complete models. A good model helps to reduce the number of practical experiments and to set up correct parameters so as to produce the desired result which in case, is the bread of good quality.

Baking can be considered as a simultaneous heat and mass transfer problem where heat is transmitted to the dough piece in different ways namely radiation, convection and conduction and mass is transmitted by diffusion in the form of liquid water and water vapor. In the present study, a one dimensional model proposed by Thorvaldsson and Janestad [Thorvaldsson et.al, 1999] is studied and the validity of the model is verified through different numerical approaches such as finite difference and finite element schemes. It is noteworthy that although the suggested scheme is very much sensitive to the size of time interval, for a range of time intervals, the results obtained through simulation well explains the heat and mass transfer during baking. When the time interval is decreased to a smaller value, the schemes become inconsistent and the result seems to be divergent. This may be due to the adoption of algebraic inequalities to correct the water and vapor levels after diffusion and evaporation, which makes some sudden fluctuations in the water and vapor levels for small time intervals. The adoption of algebraic inequalities to deal with the phase change makes this change more instantly. The study is then extended to a two dimensional model which is a new approach and the corresponding numerical model is simulated. The two dimensional study revealed the similarity of one and two dimensional models which will help to further investigate the two dimensional model since it is easier to implement the one dimensional model. Then an improved procedure is suggested in order to reduce the sensitivity of the scheme on the length of the time interval and thus to increase the convergence range of the model.

Chapter One discusses one and two dimensional mathematical models and the theory behind them. Chapter Two explains how to implement the model using finite element scheme and finite difference scheme and the algebraic inequalities and equations which control the balance between the liquid water and the vapor content

according to the saturated vapor content which varies as temperature increases. Computational results for one and two dimensional models and the stability of the schemes are discussed and compared in Chapter Three. Since the numerical model is not convergent in certain ranges of the time interval, an improved methodology is suggested in Chapter Four, to simulate the model for small time intervals and its results are also presented.

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Everyone is kneaded out of the same dough but not baked in the same oven ...

Anonymous

Introduction

Food is an inevitable part of our daily life. Food supplies the necessary energy to our body to carry out metabolic activities and other needs. Food industry is under pressure both to provide food that is more natural and less processed and which has a higher level of safety. Production of food, that meets environmental and economic factors with minimum expenditure of energy is a key factor in food industry.

One of the ways in which these challenges can be met is by developing a highly capable computer simulation of the process which can be used to control and design the actual process. The simulation can be used as a powerful tool to understand the quality of product with available resources. It also reduces the number of experiments that need to be performed and optimizes the baking process which will, in turn, eliminate the unnecessary wastage of resources, time and money.

A lot of the foods are well baked or heat treated ones. During baking or heat treatment, a large number of changes are taking place inside the food. This includes chemical, rheological and structural changes like volume expansion, crust

formation, enzymatic activities etc.

The common method of baking is by using an oven at a controlled temperature. Baking is a simultaneous heat and mass transfer problem which transforms a rough dough in to a light, digestive and flavored bread. In this process heat is transferred through the dough with the help of basic heat transfer mechanisms- conduction across the medium, convection between a surface and a moving fluid and radiation through electromagnetic radiation between two surfaces at two different temperatures.

Together with the heat and mass transfer the entire process of baking is a complex procedure where the increase in temperature plays a vital role in mass transfer in the form of liquid water and water vapor. The complexity increases since the whole system need to be controlled so as to produce the final product which has all the qualities of an eatable food.

The need of a good numerical model to simulate, control and monitor the baking process paves the path for a lot of research in baking practice. Till now many models have been proposed by the researchers like Hirsekorn [Hirsekorn, 1971], Hayakawa *et al.* [Hayakawa and Hwang, 1981], Zanoni [Zanoni and Peri, 1993] and many others. The models proposed are based on individual assumptions and though they succeeded in modelling the processes based on their own assumptions, a general approach was not always considered [Wang and Sun., 2003].

In most of the models for bread baking or drying, the liquid water and water vapor diffusion are treated together in which the decreasing water content at the surface produces the concentration gradient. But in 1988 De Varies *et al.*

[De Varies U., Sluimer and Blocksma, 1988] described a evaporation - condensation model for baking process and according to that the diffusion of vapor towards the center of the dough also contributes to the concentration gradient. Water evaporates at the warmer sides of the dough when the temperature of the dough is increased and the water vapor concentration is lower than the vapor saturation concentration at a temperature. Then, this vapor diffuses in the gas phase and during its transition from a hotter region to a cooler region it condenses back and becomes water. The evaporation of water takes place when it crosses the boiling point which is pressure dependent or when it has enough latent heat, as long as the total vapor pressure is less than the corresponding saturation pressure which is temperature dependent. In short, when temperature inside the dough increases as the time increases, water content evaporates to water vapor and when this vapor exceeds saturated vapor content, it condense back to water. In addition to this evaporation condensation process, vapor and water undergo diffusion also.

The current model which is the subject of interest is a one dimensional model proposed by Thorvaldsson and Janestad [Thorvaldsson et.al, 1999] . The model is analyzed using various numerical schemes and a two dimensional model is proposed based on this current one dimensional model. Then both these models are simulated with the help of MATLAB and the obtained results are discussed in detail. Since the simulated results of both, one and two dimensional models shows a sensitiveness towards the length of time interval, an improved methodology to implement the model is also proposed in the present study after analyzing the possible reasons for this time sensitiveness.

Chapter 1

The Mathematical Model and The Theory

1.1 Introduction

A good model is one that will enable us to computationally reproduce the experimental results through some numerical methods. The present study is based on a one dimensional model, described by Thorvaldsson and Janestad [Thorvaldsson et.al, 1999] that is based on the following three processes:

1. The heat transfer during baking.
2. The diffusion of liquid water.
3. The diffusion of water vapor.

1.2 One Dimensional Model

The one dimensional model proposed by Thorvaldsson and Janestad is as follows [Thorvaldsson et.al, 1999],

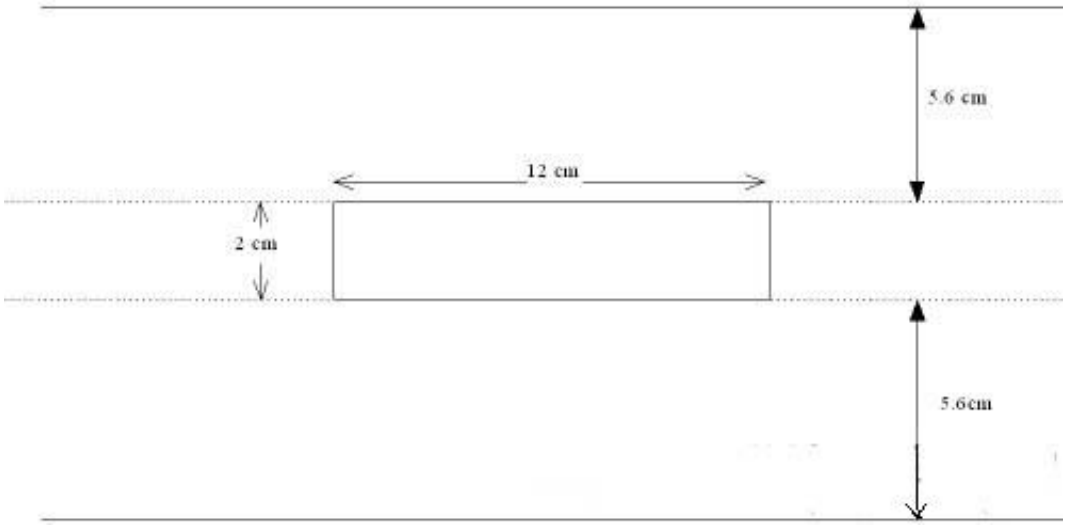

Figure 1.1: Diagram for one dimensional Model in an Oven

The bread sample of dimension $12cm \times 12cm \times 2cm$ is taken. The dough is placed inside the oven which is maintained at a temperature of 210^oC. If it is assumed that the physical properties are not changing in any two directions (here, sides with lengths 12cm are with homogeneous properties), an one dimensional heat and mass transfer can be considered to investigate the heat transfer in one direction (here, side with length 2cm). In this model, the surfaces that are exposed to oven heat undergo heat transfer due to convection and radiation and in the inner part of the dough, the heat is transferred through conduction. The model is governed by a set of three differential equations. One for heat transfer, one for water vapor diffusion and the last one for liquid water diffusion. The three equations in the system are connected each other with a set of algebraic conditions which updates liquid water and water vapor with the help of tabled values for saturated vapor pressure content.

The equation for heat transfer can be derived from the energy conservation equation by including a term which accounts for the latent heat in water evaporation. The temperature $T(x,t)$ at the point x and in time t can be described as follows [Thorvaldsson et.al, 1999], [Holman, 1968],

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c_p}\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\lambda}{c_p}\frac{\partial W}{\partial t} + \frac{\lambda W}{c_p \rho}\frac{\partial \rho}{\partial t}, \qquad 0 < x < x_{L/2}, \qquad t > 0. \tag{1.1}$$

with boundary and initial conditions [Holman, 1968], [Balaban and Pigott, 1988],

$$-k\left(\frac{\partial T}{\partial x}\right)_{x=0} = h_r(T_r - T_s) + h_c(T_{air} - T_s) - \lambda \rho D_W \left(\frac{\partial W}{\partial x}\right)_{x=0}, \tag{1.2}$$

$$\left(\frac{\partial T}{\partial x}\right)_{x=x_{L/2}} = 0, \qquad t > 0,$$

$$T(x,0) = T_0(x), \qquad 0 \leqslant x \leqslant x_{L/2}.$$

where $T(x,t)$ is the temperature in K, x is the space co-ordinate in m, ρ is the density in kg/m^3 which depends on the water content, c_p is the specific heat in J/kgK, k is thermal conductivity in W/mK, λ is the latent heat of evaporation of water in J/kg and $W(x,t)$ is the liquid water content in Kg water/ Kg product. T_{air}, T_s, T_r are the temperatures in K in the surrounding air, at the surface of the bread and at the radiation source respectively. T_0 is the initial temperature, D_W is liquid water diffusivity in m^2/s and ρ is the density of the water. The heat transfer coefficient h in W/m^2K is divided into two parts h_r and h_c, where h_r is given by,

$$h_r = \frac{\sigma(T_r^2 - T_s^2)(T_r - T_s)}{1/\epsilon_p + 1/\epsilon_r - 2 + 1/F_{i,j}} \tag{1.3}$$

where σ is the Stefan-Boltzmann constant and ϵ_p and ϵ_r are the emissivity of bread and radiation source respectively. $F_{i,j}$ is a shape factor which can be calculated from the dimensions of the bread and the oven [De Witt, 1990]. Shape factor $F_{i,j}$

can be defined as the fraction of radiation leaving the surface i that is intercepted by the surface j. In this case $F_{i,j}$ is the shape factor between the radiator and surface of the bread which can be viewed as the aligned parallel rectangles.

$$F_{i,j} = \frac{2}{\pi ab}\Bigg[\ln\sqrt{\frac{a_1 b_1}{1+a^2+b^2}} + a\sqrt{b_1}\arctan\frac{a}{\sqrt{b_1}} + b\sqrt{a_1}\arctan\frac{b}{\sqrt{a_1}} - a\arctan a - b\arctan b\Bigg]. \tag{1.4}$$

where

$$a = \frac{a_{sp}}{L}, \qquad a = \frac{b_{sp}}{L},$$
$$a_1 = 1 + a^2, \qquad b_1 = 1 + b^2.$$

where, a_{sp} and b_{sp} are the length and width of the sample and L is the distance between radiator source and sample source. Other parameters and the formulas can be found in the paper by Thorvaldsson *et al.* [Thorvaldsson et.al, 1999].

Equations for the diffusion of liquid water and vapor water can be derived from Fick's Law and the equations are [Bird, Stweart and Lightfot, 1960], [Hines, 1985],

$$\frac{\partial V}{\partial t} = \frac{\partial}{\partial x}\left(D_V \frac{\partial V}{\partial x}\right), \qquad 0 < x < x_{L/2}, \qquad t > 0 \tag{1.5}$$

with boundary and initial conditions,

$$\left(\frac{\partial V}{\partial x}\right)_{x=0} = h_V(V(0,t) - V_{air}), \tag{1.6}$$
$$\left(\frac{\partial V}{\partial x}\right)_{x=x_{L/2}} = 0, \qquad t > 0,$$
$$V(x,0) = V_0(x), \qquad 0 \leqslant x \leqslant x_{L/2}.$$

and

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial x}\left(D_W \frac{\partial W}{\partial x}\right), \qquad 0 < x < x_{L/2}, \qquad t > 0 \quad (1.7)$$

with boundary and initial conditions,

$$\left(\frac{\partial W}{\partial x}\right)_{x=0} = h_W(W(0,t) - W_{air}), \quad (1.8)$$

$$\left(\frac{\partial W}{\partial x}\right)_{x=x_{L/2}} = 0, \qquad t > 0,$$

$$W(x,0) = W_0(x), \qquad 0 \leqslant x \leqslant x_{L/2}.$$

where $V(x,t)$ and $W(x,t)$ are water vapor and liquid water content and h_V and h_W are mass transfer coefficients of vapor and water at the surface. h_V depends on the temperature content and h_W depends on water as well as temperature content. D_W is the diffusion coefficient for water which is a constant and D_V is diffusion coefficient for vapor which depends on the temperature content. V_{air} and W_{air} are vapor content and water content of the oven air respectively. V_0 and W_0 are initial content of vapor and water respectively.

The above two equations describe the diffusion of water and vapor in the dough during baking and the phase change is carried out with the help of a set of algebraic inequalities which are explained in section 1.4. Therefore V and W in these two equations are "adjusted" water and vapor. rather than the actual water and vapor content at a time.

1.3 Two Dimensional Model

A two dimensional mathematical model can be obtained by extending the one dimensional model. The bread sample of the dimensions $12cm \times 2cm \times 2cm$ is taken

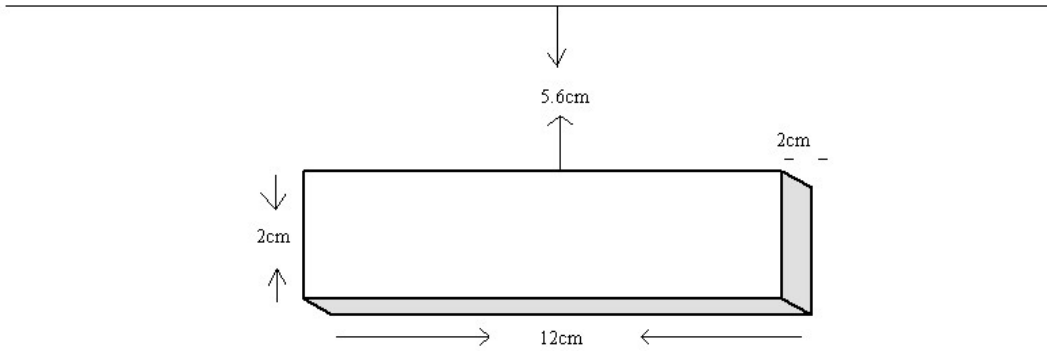

Figure 1.2: Diagram for two dimensional model in an Oven

for modeling. Like in the one dimensional case, the model is considered as a two dimensional model if it is assumed that the physical properties of the third side (side with length 12cm) remains the same. The two dimensional mathematical model is as follows,

Temperature distribution in the model is calculated from the equations,

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c_p}\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)^T k\left(\frac{\partial T}{\partial x}, \frac{\partial T}{\partial y}\right) + \frac{\lambda}{c_p}\frac{\partial W}{\partial t} + \frac{\lambda W}{c_p \rho}\frac{\partial \rho}{\partial t}, \qquad 0 < x, y < L/2, \qquad t > 0. \tag{1.9}$$

with boundary and initial conditions,

$$\begin{aligned} -k\left(\frac{\partial T}{\partial x}\right)_{x=0} &= h_r(x)(T_r - T_s(0,y)) + h_c(T_{air} - T_s(0,y)) - \lambda \rho D_W \left(\frac{\partial W}{\partial x}\right)_{x=0}, \\ -k\left(\frac{\partial T}{\partial y}\right)_{y=0} &= h_r(y)(T_r - T_s(x,0)) + h_c(T_{air} - T_s(x,0)) - \lambda \rho D_W \left(\frac{\partial W}{\partial y}\right)_{y=0}, \end{aligned} \tag{1.10}$$

$$\left(\frac{\partial T}{\partial x}\right)_{x=x_{L/2}} = 0, \qquad t > 0,$$
$$\left(\frac{\partial T}{\partial y}\right)_{y=y_{L/2}} = 0, \qquad t > 0,$$
$$T(x, y, 0) = T_0(x, y), \qquad 0 \leqslant x, y \leqslant L/2.$$

where $T(x, y, t)$ is the temperature in K, x and y are the space co-ordinates in m.

The diffusion equations for liquid water and water vapor in the two dimensional model are as follows,

$$\frac{\partial V}{\partial t} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)^T D_V \left(\frac{\partial V}{\partial x}, \frac{\partial V}{\partial y}\right), \qquad 0 < x, y < L/2, \qquad t > 0 \quad (1.11)$$

with boundary and initial conditions,

$$\left(\frac{\partial V}{\partial x}\right)_{x=0} = h_V(x)(V(0, y, t) - V_{air}),$$
$$\left(\frac{\partial V}{\partial y}\right)_{y=0} = h_V(y)(V(x, 0, t) - V_{air}),$$
$$\left(\frac{\partial V}{\partial x}\right)_{x=x_{L/2}} = 0, \qquad t > 0,$$
$$\left(\frac{\partial V}{\partial y}\right)_{y=y_{L/2}} = 0, \qquad t > 0,$$
$$V(x, y, 0) = V_0(x, y), \qquad 0 \leqslant x, y \leqslant L/2. \quad (1.12)$$

and

$$\frac{\partial W}{\partial t} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)^T D_W \left(\frac{\partial W}{\partial x}, \frac{\partial W}{\partial y}\right), \qquad 0 < x, y < L/2, \qquad t > 0 \quad (1.13)$$

with boundary and initial conditions,

$$\begin{aligned}
&\left(\frac{\partial W}{\partial x}\right)_{x=0} = h_W(x)(W(0,y,t) - W_{air}),\\
&\left(\frac{\partial W}{\partial y}\right)_{y=0} = h_W(y)(W(x,0,t) - W_{air}),\\
&\left(\frac{\partial W}{\partial x}\right)_{x=x_{L/2}} = 0, \qquad\qquad t > 0,\\
&\left(\frac{\partial W}{\partial y}\right)_{y=y_{L/2}} = 0, \qquad\qquad t > 0,\\
&W(x,y,0) = W_0(x,y), \qquad\qquad 0 \leqslant x, y \leqslant L/2.
\end{aligned} \tag{1.14}$$

where $V(x,y,t)$ and $W(x,y,t)$ are water vapor and liquid water content in time t at the point (x,y). The remaining parameters are the same as those in the case of the one dimensional problem and the phase change is carried out using the same set of algebraic inequalities (Section 1.4) which are used in one dimensional case.

1.4 Conditions for Vapor and Water Update

To deal with the phase change or to correct vapor and water contents according to the increasing temperatures, a set of algebraic conditions are used, as discussed below. When temperature increases, water becomes water vapor and starts to diffuse more easily through the dough. This diffusion also helps to transfer the temperature more rapidly. So when the temperature increases there is a change in the composition of liquid water and water vapor content. The amount of the vapor which can be presented at a particular temperature is calculated from the saturated vapor pressure. This saturated vapor pressure is obtained from the standard vapor pressure tables [Nordling and Österman, 1996]. The vapor content is calculated

from the vapor pressure using the ideal gas equation,

$$P\tilde{V} = nRT \tag{1.15}$$

where

$$\begin{aligned} P &= Pressure\ \ of\ \ the\ \ gas \\ \tilde{V} &= Volume\ \ of\ \ gas \\ n &= No.\ \ of\ \ moles\ \ of\ \ gas \\ R &= Universal\ \ gas\ \ constant\ \ in\ \ J.mol^{-1}.K^{-1} \end{aligned}$$

From the above ideal gas equation, the water vapor density can be estimated as,

$$\rho_v = \frac{PM}{RT} \tag{1.16}$$

where

$$M = Molar\ \ mass\ \ of\ \ the\ \ gas\ \ in\ \ Kg/mol$$

Since the vapor concentrations is much smaller than 1, and if ρ_d is the pure dough/ bread density and ρ_m is the density of dough/ vapor mixture, the vapor concentration can be calculated as,

$$V \approx \frac{\rho_v}{\rho_m} - \frac{\rho_v}{\rho_d} \tag{1.17}$$

In this model, due to the difficulty to model the bubble growth inside the bread during baking, a fix ratio between the pure dough and the mixture is assumed (although it is not true in practice, it is a common assumption).

Now using equation (1.16), the equation (1.17) be written as,

$$V = \frac{PM}{RT\rho_d} C \tag{1.18}$$

where C is a constant (about 0.75) which is offset by assuming the evaporation is higher than the saturation condition proportionally.

Vapor and water contents of the dough are then updated using this saturated vapor with the help of following algebraic inequalities and equations.

$$\begin{aligned} if \quad & (Water \;\; content + Vapor \;\; Content) < Saturated \;\; Vapor \;\; Content \\ & Updated \;\; Vapor = (Water \;\; content + Vapor \;\; Content) \\ & Updated \;\; Water = 0 \end{aligned} \tag{1.19}$$

and,

$$\begin{aligned} if \quad & (Water \;\; content + Vapor \;\; Content) \geq Saturated \;\; Vapor \;\; Content \\ & Updated \;\; Vapor = Saturated \;\; Vapor \\ & Updated \;\; Water = (Water \;\; content + Vapor \;\; Content) \\ & \qquad\qquad -Saturated \;\; Vapor \end{aligned} \tag{1.20}$$

Using the updated values of water and vapor contents the diffusion equation is solved.

Chapter 2

Implementation of the Mathematical Model

2.1 Introduction

The mathematical model of any physical or chemical process can be a good and complete model, when it is implemented successfully, through proper schemes and the results obtained are satisfactory.

Here the mathematical model for baking, is implemented through different numerical schemes. The implementation of the model is carried out through the following procedure [Thorvaldsson et.al, 1999],

1. Temperature is calculated from the heat transfer equation (1.1), with the help of conditions in (1.2).

2. The saturated water vapor is estimated using a steam table for new temperature with the help of equation (1.18) and using this saturated vapor, water vapor and liquid water contents are updated using the inequalities (1.19) and

(1.20).

3. Vapor content is calculated from the diffusion equation (1.5), with the help of the conditions (1.6).

4. After this diffusion, the amounts of vapor and water are again updated using the same procedure which is described in step 2.

5. Then water content is calculated from the diffusion equation (1.7) with (1.8).

6. This entire procedure is repeated for each time step.

2.2 One Dimensional Model

The one dimensional model which is explained in the previous chapter is validated through Finite Difference Scheme and Finite Element Scheme. The implementation is explained below;

2.2.1 Finite Difference Scheme

Implementation of one dimensional model through finite difference scheme is carried out as below. Firstly the computational domain is discretized into a finite number of points say N in space direction and M in time direction where the solutions for unknown values are approximated. Then the differential equations are approximated using corresponding difference equations.

In the present study, the time derivative is approximated using a backward difference scheme and the space derivative is approximated using a general "θ" method from which the explicit, implicit and the Crank-Nicholson difference schemes can be derived. The difference approximations for time and space derivatives are as

follows,

$$\frac{\partial U(x_i, t_{j+1})}{\partial t} = \frac{U_{i,j+1} - U_{i,j}}{\Delta t}$$

$$\frac{\partial^2 U(x_i, t_{j+1})}{\partial x^2} = (1-\theta)\left(\frac{U_{i-1,j+1} - 2U_{i,j+1} + U_{i+1,j+1}}{(\Delta x)^2}\right) + (\theta)\left(\frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{(\Delta x)^2}\right)$$

Here Δt is the time increment and Δx is the spatial increment. When $\theta = 0$ the method is an implicit difference scheme where as $\theta = 1$ gives an explicit scheme. The Crank-Nicholson difference scheme is obtained by taking $\theta = 0.5$. The Robin type boundary conditions are discretized using a central difference,

$$\frac{\partial U}{\partial x} \approx \frac{U_{i+1,j} - U_{i-1,j}}{2\Delta x}$$

Discretization of Governing Equations

Equations for heat transfer and diffusion of liquid water and water vapor are approximated in the discretized computational domain.

Heat Transfer Equation

Equation for heat transfer is discretized as follows,

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c_p}\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\lambda}{c_p}\frac{\partial W}{\partial t} + \frac{\lambda W}{c_p \rho}\frac{\partial \rho}{\partial t},$$

Since

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial x}\left(D_W \frac{\partial W}{\partial x}\right)$$

For simplicity, this heat transfer equation can be rewritten by ignoring the last term since it doesn't make a significant contribution to the total heat transfer (which

is verified using simulations) and thus the governing equation for heat transfer becomes [Thorvaldsson et.al, 1999],

$$\frac{\partial T}{\partial t} = \frac{1}{\rho c_p}\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\lambda}{c_p}\frac{\partial}{\partial x}\left(D_W\frac{\partial W}{\partial x}\right). \tag{2.1}$$

Taking k and D_W outside the derivative since they are constants (by using the chain rule) and then discretizing,

$$\frac{T_{i,j+1}-T_{i,j}}{\Delta t} = \frac{k}{\rho c_p}\left((1-\theta)\left(\frac{T_{i-1,j+1}-2T_{i,j+1}+T_{i+1,j+1}}{(\Delta x)^2}\right) + (\theta)\left(\frac{T_{i-1,j}-2T_{i,j}+T_{i+1,j}}{(\Delta x)^2}\right)\right) + \frac{\lambda D_W}{c_p}\left(\frac{W_{i-1,j}-2W_{i,j}+W_{i+1,j}}{(\Delta x)^2}\right)$$

Equivalently,

$$\begin{aligned} -\alpha_1 T_{i-1,j+1} + (1+2\alpha_1)T_{i,j+1} - \alpha_1 T_{i+1,j+1} \\ = \alpha_2 T_{i-1,j} + (1-2\alpha_2)T_{i,j} + \alpha_2 T_{i+1,j} + \alpha_3(W_{i-1,j} - 2W_{i,j} + W_{i+1,j}) \\ i = 0,1,2,3....N. \end{aligned} \tag{2.2}$$

where

$$\alpha_1 = \frac{k\Delta t}{\rho c_p(\Delta x)^2}(1-\theta) \qquad \alpha_2 = \frac{k\Delta t}{\rho c_p(\Delta x)^2}(\theta) \qquad \alpha_3 = \frac{\lambda D_W \Delta t}{c_p(\Delta x)^2}$$

and the boundary conditions at $i = 0$ and $i = N$ are (using equation(1.2)),

$$\begin{aligned} -k\left(\frac{T_{1,j}-T_{-1,j}}{2\Delta x}\right) &= h_r(T_r - T_{0,j}) + h_c(T_{air} - T_{0,j}) - \lambda\rho D_W h_W(W_{0,j} - W_{air}) \\ \frac{T_{N+1,j}-T_{N-1,j}}{2\Delta x} &= 0 \end{aligned} \tag{2.3}$$

the boundary conditions for water diffusion are,

$$\begin{aligned} \frac{W_{1,j}-W_{-1,j}}{2\Delta x} &= h_W(W_{0,j} - W_{air}) \\ \frac{W_{N+1,j}-W_{N-1,j}}{2\Delta x} &= 0 \\ j &= 1,2,...M \end{aligned} \tag{2.4}$$

or it can be written as,

$$T_{-1,j} = T_{1,j} - \left(\frac{2\Delta x(h_r + h_c)}{k}\right) T_{0,j} + \frac{2\Delta x h_r}{k} T_r + \frac{h_c}{k} T_{air} - 2\Delta x \lambda \rho D_W h_W (W_{0,j} - W_{air})$$

$$T_{N+1,j} = T_{N-1,j}$$

$$W_{-1,j} = W_{1,j} - 2\Delta x h_W (W_{0,j} - W_{air})$$

$$W_{N+1,j} = W_{N-1,j} \tag{2.5}$$

Clearly from equation (2.1) it can be seen that for calculating the T at $(j+1)^{th}$ time level it requires other two $(j+1)^{th}$ level unknown values of T and known values at $(j)^{th}$ level. That is, even though initial data $T_{i,0}$ i=0,1,2....M are known, it is not possible to get the values of the unknown at the $(j+1)^{th}$ level with a single explicit step (using the equation (2.1) only once) but by using the equation for i=0,1,2....N and solving linear system thus formed for the unknowns with the help of boundary conditions of heat transfer equation and diffusion equation. At boundary, equation (2.1) becomes,

$$\begin{aligned} &-\alpha_1 T_{-1,j+1} + (1+2\alpha_1) T_{0,j+1} - \alpha_1 T_{1,j+1} \\ &\qquad = \alpha_2 T_{-1,j} + (1-2\alpha_2) T_{0,j} + \alpha_2 T_{1,j} + \alpha_3 (W_{-1,j} - 2W_{0,j} + W_{1,j}) \end{aligned} \tag{2.6}$$

$$\begin{aligned} &-\alpha_1 T_{N-1,j+1} + (1+2\alpha_1) T_{N,j+1} - \alpha_1 T_{N+1,j+1} \\ &\qquad = \alpha_2 T_{N-1,j} + (1-2\alpha_2) T_{N,j} + \alpha_2 T_{N+1,j} + \alpha_3 (W_{N-1,j} - 2W_{N,j} + W_{N+1,j}) \end{aligned}$$

here the ghost points $T_{-1,j}$, $T_{-1,j+1}$, $T_{N+1,j}$, $T_{N+1,j+1}$, $W_{-1,j}$ and $W_{N+1,j}$ are replaced using the equation (2.5) and thus the following linear system is obtained,

$$AX = B \tag{2.7}$$

where

$$A = \begin{pmatrix} 1+2\alpha_1\left(1+\frac{2\Delta x(h_r+h_c)}{k}\right) & -2\alpha_1 & 0 & - & - & 0 & 0 & 0 \\ -\alpha_1 & 1+2\alpha_1 & -\alpha_1 & - & - & 0 & 0 & 0 \\ - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & - & - & -\alpha_1 & 1+2\alpha_1 & -\alpha_1 \\ 0 & 0 & 0 & - & - & 0 & -2\alpha_1 & 1+2\alpha_1 \end{pmatrix}, \tag{2.8}$$

$$B = \begin{pmatrix} \alpha_2 T_{-1,j} + (1-2\alpha_2)T_{0,j} + \alpha_2 T_{1,j} + \alpha_3(W_{-1,j} - 2W_{0,j} + W_{1,j}) + C \\ \alpha_2 T_{0,j} + (1-2\alpha_2)T_{1,j} + \alpha_2 T_{2,j} + \alpha_3(W_{0,j} - 2W_{1,j} + W_{2,j}) \\ .... \\ \alpha_2 T_{N-2,j} + (1-2\alpha_2)T_{N-1,j} + \alpha_2 T_{N,j} + \alpha_3(W_{N-2,j} - 2W_{N-1,j} + W_{N,j}) \\ \alpha_2 T_{N-1,j} + (1-2\alpha_2)T_{N,j} + \alpha_2 T_{N-1,j} + \alpha_3(W_{N-1,j} - 2W_{N,j} + W_{N-1,j}) \end{pmatrix}, \tag{2.9}$$

$$X = \begin{pmatrix} T_{0,j+1} \\ T_{1,j+1} \\ .... \\ T_{N-1,j+1} \\ T_{N,j+1} \end{pmatrix}$$

and

$$C = \alpha_1 \left(\frac{2\Delta x h_r}{k} T_r + \frac{2\Delta x h_c}{k} T_{air} - 2\Delta x \lambda \rho D_W h_W (W_{0,j} - W_{air}) \right). \tag{2.10}$$

The unknown values of temperature at discrete points are obtained by solving this linear system. This is repeated for each time interval till it reaches the final time.

Diffusion Equation for Water Vapor

The diffusion equation for vapor is discretized in the following way,

$$\begin{aligned}\frac{V_{i,j+1}-V_{i,j}}{\Delta t} &= \frac{\left(D_V\frac{\partial V}{\partial x}\right)_{i+1,j}-\left(D_V\frac{\partial V}{\partial x}\right)_{i,j}}{\Delta x} \\ &= \frac{(D_V)_{i+1,j}V_{i+1,j}-\left((D_V)_{i+1,j}+(D_V)_{i,j}\right)V_{i,j}+(D_V)_{i,j}V_{i-1,j}}{(\Delta x)^2}\end{aligned} \tag{2.11}$$

If we use θ method it can be written as,

$$\begin{aligned}&\frac{V_{i,j+1}-V_{i,j}}{\Delta t} = (\theta)\left(\frac{(D_V)_{i+1,j}V_{i+1,j}-((D_V)_{i+1,j}+(D_V)_{i,j})V_{i,j}+(D_V)_{i,j}V_{i-1,j}}{(\Delta x)^2}\right) \\ &+(1-\theta)\left(\frac{(D_V)_{i+1,j+1}V_{i+1,j+1}-((D_V)_{i+1,j+1}+(D_V)_{i,j+1})V_{i,j+1}+(D_V)_{i,j+1}V_{i-1,j+1}}{(\Delta x)^2}\right)\end{aligned} \tag{2.12}$$

or it can be written as,

$$\begin{aligned}&-\alpha_1(D_V)_{i,j+1}V_{i-1,j+1}+(1+\alpha_1((D_V)_{i+1,j+1}+(D_V)_{i,j+1}))V_{i,j+1}-\alpha_1(D_V)_{i+1,j+1}V_{i+1,j+1} \\ &\quad=\alpha_2(D_V)_{i,j}V_{i-1,j}+(1-\alpha_2((D_V)_{i+1,j}+(D_V)_{i,j}))V_{i,j}+\alpha_2(D_V)_{i+1,j}V_{i+1,j}\end{aligned} \tag{2.13}$$

$$i = 0, 1, 2, 3....N.$$

Where

$$\alpha_1 = \frac{\Delta t}{(\Delta x)^2}(1-\theta) \qquad and \qquad \alpha_2 = \frac{\Delta t}{(\Delta x)^2}(\theta).$$

The boundary conditions are

$$\begin{aligned}&\frac{V_{1,j}-V_{-1,j}}{2\Delta x} = h_V(V_{0,j}-V_{air}) \\ &\frac{V_{N+1,j}-V_{N-1,j}}{2\Delta x} = 0\end{aligned} \tag{2.14}$$

$$j = 1, 2, ...M.$$

Then at each time interval a linear system $AX = B$ is formulated by varying $i = 0, 1, 2, ...N$ and with the help of the boundary conditions like it is mentioned in the case of heat transfer equation. This is solved for the unknown value of the vapor at each time interval. Here,

$$A = \begin{pmatrix} (1+\alpha_1\beta) & -\alpha_1\xi_0 & 0 & - & - & 0 & 0 & 0 \\ -\alpha_1\beta_1 & (1+\alpha_1\xi_1) & -\alpha_1\beta_2 & - & - & 0 & 0 & 0 \\ - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & - & - & -\alpha_{N-1} & (1+\alpha_1\xi_{N-1}) & -\alpha_1\beta_N \\ 0 & 0 & 0 & - & - & 0 & -\alpha_1\xi_N & (1+\alpha_1\xi_N) \end{pmatrix}, \tag{2.15}$$

where

$$\beta = ((D_V)_{1,j+1} + (D_V)_{0,j+1}(1 + 2\Delta x h_V)) \tag{2.16}$$
$$\beta_i = (D_V)_{i,j+1}$$
$$\xi_i = ((D_V)_{i,j+1} + (D_V)_{i+1,j+1}).$$

$$B = \begin{pmatrix} \alpha_2(D_V)_{0,j}V_{-1,j} + (1-\alpha_2\eta_0)V_{0,j} + \alpha_2(D_V)_{1,j}V_{1,j} + 2\alpha_1(D_V)_{0,j+1}\Delta x h_V V_{air} \\ \alpha_2(D_V)_{1,j}V_{0,j} + (1-\alpha_2\eta_1)V_{1,j} + \alpha_2(D_V)_{2,j}V_{2,j} \\ .... \\ \alpha_2(D_V)_{N-1,j}V_{N-2,j} + (1-\alpha_2\eta_{N-1})V_{N-1,j} + \alpha_2(D_V)_{N,j}V_{N,j} \\ \alpha_2(D_V)_{N,j}V_{N-1,j} + (1-\alpha_2\eta_N)V_{N,j} + \alpha_2(D_V)_{N,j}V_{N-1,j} \end{pmatrix}, \tag{2.17}$$

where

$$\eta_i = ((D_V)_{i,j} + (D_V)_{i+1,j})$$

and

$$X = \begin{pmatrix} V_{0,j+1} \\ V_{1,j+1} \\ .... \\ V_{N-1,j+1} \\ V_{N,j+1} \end{pmatrix}.$$

Diffusion equation for Liquid Water

The liquid water diffusion equation is discretized as follows (Since D_W is a constant, it is pulled outside the derivative by using the chain rule),

$$\frac{W_{i,j+1} - W_{i,j}}{\Delta t} = D_W \Bigg((1-\theta) \left(\frac{W_{i-1,j+1} - 2W_{i,j+1} + W_{i+1,j+1}}{(\Delta x)^2} \right) + \theta \left(\frac{W_{i-1,j} - 2W_{i,j} + W_{i+1,j}}{(\Delta x)^2} \right) \Bigg) \tag{2.18}$$

or

$$-\alpha_1 W_{i-1,j+1} + (1+2\alpha_1) W_{i,j+1} - \alpha_1 W_{i+1,j+1} = \alpha_2 W_{i-1,j} + (1-2\alpha_2) W_{i,j} + \alpha_2 W_{i+1,j} \tag{2.19}$$

$$i = 0, 1, 2, 3....N$$

where

$$\alpha_1 = \frac{D_W \Delta t}{(\Delta x)^2}(1-\theta) \qquad and \qquad \alpha_2 = \frac{D_W \Delta t}{(\Delta x)^2}(\theta).$$

The boundary conditions are

$$\begin{aligned} \frac{W_{1,j} - W_{-1,j}}{2\Delta x} &= h_W (W_{0,j} - W_{air}) \\ \frac{W_{N+1,j} - W_{N-1,j}}{2\Delta x} &= 0 \end{aligned} \tag{2.20}$$

$$j = 1, 2, ...M.$$

The corresponding linear system is $AX = B$, where,

$$A = \begin{pmatrix} (1+\alpha_1(2+2\Delta x h_W)) & -2\alpha_1 & 0 & - & - & 0 & 0 & 0 \\ -\alpha_1 & (1+2\alpha_1) & -\alpha_1 & - & - & 0 & 0 & 0 \\ - & - & - & - & - & - & - & - \\ 0 & 0 & 0 & - & - & -\alpha_1 & (1+2\alpha_1) & -\alpha_1 \\ 0 & 0 & 0 & - & - & 0 & -2\alpha_1 & (1+2\alpha_1) \end{pmatrix}, \tag{2.21}$$

$$B = \begin{pmatrix} \alpha_2 W_{-1,j} + (1-2\alpha_2) W_{0,j} + \alpha_2 W_{1,j} + 2\alpha_1 \Delta x h_W W_{air} \\ \alpha W_{0,j} + (1-2\alpha_2) V_{1,j} + \alpha_2 W_{2,j} \\ .... \\ \alpha_2 W_{N-2,j} + (1-2\alpha_2) W_{N-1,j} + \alpha_2 W_{N,j} \\ \alpha_2 W_{N-1,j} + (1-2\alpha_2) W_{N,j} + \alpha_2 W_{N-1,j} \end{pmatrix}, \tag{2.22}$$

$$X = \begin{pmatrix} W_{0,j+1} \\ W_{1,j+1} \\ .... \\ W_{N-1,j+1} \\ W_{N,j+1} \end{pmatrix}$$

and

$$W_{-1,j} = W_{1,j} - 2\Delta x h_W (W_{0,j} - W_{air}). \tag{2.23}$$

The linear system is solved for each time interval for the liquid water.

The above three linear systems are solved according to the algorithm or using the procedure given in the beginning of this chapter to validate the model for one dimensional bread baking.

2.2.2 Finite Element Scheme

The finite element scheme is implemented as follows,

System of Equations

The governing equations can be written as a system of equations as follows,

$$\frac{\partial}{\partial t}\begin{pmatrix} T \\ V \\ W \end{pmatrix} = \frac{\partial}{\partial x}\left(\begin{pmatrix} \frac{k}{\rho c_p} & 0 & \frac{\lambda D_W}{c_p} \\ 0 & D_V & 0 \\ 0 & 0 & D_W \end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix} T \\ V \\ W \end{pmatrix}\right) \tag{2.24}$$

or

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(A\frac{\partial U}{\partial x}\right) \tag{2.25}$$

where

$$U = \begin{pmatrix} T \\ V \\ W \end{pmatrix} \qquad and \qquad A = \begin{pmatrix} \frac{k}{\rho c_p} & 0 & \frac{\lambda D_W}{c_p} \\ 0 & D_V & 0 \\ 0 & 0 & D_W \end{pmatrix}. \tag{2.26}$$

After approximating $\frac{\partial}{\partial t}$ using the backward difference finite difference formula and integrating after multiplying the test function $P \in (H^1 \times H^1 \times H^1)$, the following expression is obtained:

$$\int_\Omega \frac{U^j - U^{j-1}}{\Delta t} P dx = \int_\Omega \frac{\partial}{\partial x}\left(A\frac{\partial U^j}{\partial x}\right) P dx \tag{2.27}$$

Variational Formulation

The variational formulation of each equation of the system (2.24) can be formulated from (2.27) using integration by parts.

Heat Transfer Equation:

The variational formulation of the heat transfer equation is as follows,

$$\int_\Omega \frac{T^j - T^{j-1}}{\Delta t} P dx = \int_\Omega \left(\frac{1}{\rho c_p} \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\lambda}{c_p} \frac{\partial}{\partial x} \left(D_W \frac{\partial W}{\partial x} \right) \right) P dx \qquad (2.28)$$
$$= \int_\Omega \left(c_1 \frac{\partial^2 T}{\partial x^2} + c_2 \frac{\partial^2 W}{\partial x^2} \right) P dx$$

where $c_1 = \frac{k}{\rho c_p}$ and $c_2 = \frac{\lambda D_W}{c_p}$ (k and D_W are pulled out since they are constants). ie,

$$\int_\Omega T^j P dx - \int_\Omega T^{j-1} P dx = c_1 \Delta t \int_\Omega \frac{\partial^2 T}{\partial x^2} P dx + c_2 \Delta t \int_\Omega \frac{\partial^2 W}{\partial x^2} P dx \qquad (2.29)$$

$$= c_1 \Delta t \left[P(x_{L/2}) \left(\frac{\partial T}{\partial x} \right)_{x=x_{L/2}} - P(0) \left(\frac{\partial T}{\partial x} \right)_{x=0} \right] - c_1 \Delta t \int_0^{x_{L/2}} \frac{\partial T}{\partial x} \frac{\partial P}{\partial x} dx$$
$$+ c_2 \Delta t \left[P(x_{L/2}) \left(\frac{\partial W}{\partial x} \right)_{x=x_{L/2}} - P(0) \left(\frac{\partial W}{\partial x} \right)_{x=0} \right] - c_2 \Delta t \int_0^{x_{L/2}} \frac{\partial W}{\partial x} \frac{\partial P}{\partial x} dx$$

$$= \frac{c_1 \Delta t}{k} P(0) \left[h_r (T_r - T(0,t)) + h_c (T_{air} - T(0,t)) - \lambda \rho D_W \left(\frac{\partial W}{\partial x} \right)_{x=0} \right]$$
$$- c_1 \Delta t \int_0^{x_{L/2}} \frac{\partial T}{\partial x} \frac{\partial P}{\partial x} dx - c_2 \Delta t P(0) \left[h_W (W(0,t) - W_{air}) \right] - c_2 \Delta t \int_0^{x_{L/2}} \frac{\partial W}{\partial x} \frac{\partial P}{\partial x} dx.$$

After performing necessary substitutions and then rearranging the terms in such a way that one side of the equation contains unknown terms at the j^{th} level and the other side contains terms at the $(j-1)^{th}$ time level, the following equation is obtained,

$$\int_0^{x_{L/2}} \left(c_1 \Delta t \frac{\partial T^j}{\partial x} \frac{\partial P}{\partial x} + T^j P \right) dx + \frac{c_1 \Delta t}{k} (h_r + h_c) T(0,t) P(0) \qquad (2.30)$$

$$= \int_0^{x_{L/2}} T^{j-1} P dx - c_2 \Delta t \int_0^{x_{L/2}} \frac{\partial W^{j-1}}{\partial x} \frac{\partial P}{\partial x} dx + \frac{c_1(0) \Delta t}{k} (h_r T_r + h_c T_{air}) P(0,t)$$
$$- \frac{\lambda \rho D_W h_W}{k} c_1(0) \Delta t (W^{(j-1)}(0,t) - W_{air}) P(0) - c_2 \Delta t h_W (W^{j-1}(0,t) - W_{air}) P(0)$$

which is the variational form for the heat transfer equation.

Vapor Diffusion Equation:

The variation form of vapor diffusion equation is derived as follows,

$$\int_\Omega \frac{V^j - V^{j-1}}{\Delta t} P dx = \int_\Omega \frac{\partial}{\partial x}\left(D_V \frac{\partial V}{\partial x}\right) P dx \tag{2.31}$$

Or

$$\begin{aligned}
&\int_\Omega V^j P dx - \int_\Omega V^{j-1} P dx = \Delta t \int_\Omega \frac{\partial}{\partial x}\left(D_V \frac{\partial V}{\partial x}\right) P dx \\
&= \Delta t \left[P(x_{L/2}) \left(D_V \frac{\partial V}{\partial x}\right)_{x=x_{L/2}} - P(0) \left(D_V \frac{\partial V}{\partial x}\right)_{x=0} \right] - \Delta t \int_0^{x_{L/2}} D_V \frac{\partial V}{\partial x}\frac{\partial P}{\partial x} dx \\
&= -(D_V)_0 \Delta t P(0) \left[h_V (V(0,t) - V_{air})\right] - \Delta t \int_0^{x_{L/2}} D_V \frac{\partial V}{\partial x}\frac{\partial P}{\partial x} dx.
\end{aligned} \tag{2.32}$$

After rearranging the terms,

$$\begin{aligned}
\int_0^{x_{L/2}} \left(\Delta t D_V \frac{\partial V^j}{\partial x}\frac{\partial P}{\partial x} + V^j P\right) dx + \Delta t (D_V)_0 h_V V(0,t) P(0) \\
= \int_0^{x_{L/2}} V^{j-1} P dx + \Delta t (D_V)_0 h_V V_{air} P(0),
\end{aligned} \tag{2.33}$$

which is the variational formulation for vapor diffusion equation.

Liquid Water Diffusion Equation:

Derivation of the variational of diffusion equation for liquid water is in a way similar to derivation of the variational form of vapor diffusion, since both the equations are same except for the vapor and water terms. So we can write the variational

form of liquid water diffusion as below,

$$\int_0^{x_{L/2}} \left(\Delta t D_W \frac{\partial W^j}{\partial x} \frac{\partial P}{\partial x} + W^j P \right) dx + \Delta t D_W h_W W(0,t) P(0) = \int_0^{x_{L/2}} W^{j-1} P dx + \Delta t D_W h_W W_{air} P(0) \tag{2.34}$$

Triangulation

After the variational formulation, next step of finite element scheme is to generate a triangulation or the discretization of region into several smaller regions. Here since the problem is one - dimensional a uniform cartesian grid $x_i = ih$, $i = 0, 1, 2, ...N$, $h = 1/N$ is used and those smaller regions are $[x_{i-1}, x_i]$.

Basis Function

Basis function is the function with which the unknown function in a given region is approximated. In this simulation a piecewise linear basis function is used based on the triangulation.

$$\phi_i(x) = \begin{cases} \frac{x - x_{i-1}}{h} & (x_{i-1} \leq x \leq x_i) \\ \frac{x_{i+1} - x}{h} & (x_i \leq x \leq x_{i+1}) \\ 0 & (otherwise) \end{cases} \tag{2.35}$$

They are also known as hat functions.

Approximate Solution and Reformulation of Weak Form

Now the approximate solution can be expressed as the linear combination of basis functions as follows,

$$T = \sum_{i=0}^{N} T_i \phi_i \tag{2.36}$$
$$V = \sum_{i=0}^{N} V_i \phi_i$$
$$W = \sum_{i=0}^{N} W_i \phi_i$$

Then substituting in the equations (2.30), (2.33) and (2.34) and reformulating we get the following equations;

Heat Transfer Equation:

$$c_1 \Delta t \sum_{i=0}^{N} T_i \left(\int_0^{x_{L/2}} \frac{\partial \phi_i}{\partial x} \frac{\partial P}{\partial x} dx \right) + \sum_{i=0}^{N} T_i \left(\int_0^{x_{L/2}} \phi_i P dx \right) + \frac{c_1 \Delta t}{k} (h_r + h_c) T_0 P(0) \tag{2.37}$$
$$= \sum_{i=0}^{N} T_i \left(\int_0^{x_{L/2}} \phi_i P dx \right) - c_2 \Delta t \sum_{i=0}^{N} W_i \left(\int_0^{x_{L/2}} \frac{\partial \phi_i}{\partial x} \frac{\partial P}{\partial x} dx \right) + \frac{c_1(0) \Delta t}{k} (h_r T_r + h_c T_{air}) P(0)$$
$$- \frac{\lambda \rho D_W h_W}{k} c_1(0) \Delta t (W_0 - W_{air}) P(0) - c_2 \Delta t h_W (W_0 - W_{air}) P(0)$$

Now $P(x)$ is chosen as $\phi_1, \phi_2, ..., \phi_N$ respectively to get the stiffness matrix A. For element $e_i = (x_i, x_{i+1})$, $i = 0, 1...N$, the local stiffness matrix is given by,

$$K_i^e = \begin{pmatrix} \int_{x_i}^{x_{i+1}} c_1 \Delta t \phi_i'^2 dx & \int_{x_i}^{x_{i+1}} c_1 \Delta t \phi_i' \phi_{i+1}' dx \\ \int_{x_i}^{x_{i+1}} c_1 \Delta t \phi_{i+1}' \phi_i' dx & \int_{x_i}^{x_{i+1}} c_1 \Delta t \phi_{i+1}'^2 dx \end{pmatrix}$$
$$+ \begin{pmatrix} \int_{x_i}^{x_{i+1}} \phi_i^2 dx & \int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \\ \int_{x_i}^{x_{i+1}} \phi_{i+1} \phi_i dx & \int_{x_i}^{x_{i+1}} \phi_{i+1}^2 dx \end{pmatrix} \tag{2.38}$$

and the local load vector is

$$F_i^e = \begin{pmatrix} L(\phi_i) \\ L(\phi_{i+1}) \end{pmatrix} \tag{2.39}$$

where

$$\begin{aligned} L(\phi_i) = T_i \left(\int_{x_i}^{x_{i+1}} \phi_i \phi_i dx \right) + T_{i+1} \left(\int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \right) \\ -\Delta t W_i \left(\int_{x_i}^{x_{i+1}} c_2 \phi_i' \phi_i' dx \right) - c_2 \Delta t W_{i+1} \left(\int_{x_i}^{x_{i+1}} \phi_i' \phi_{i+1}' dx \right). \end{aligned} \tag{2.40}$$

Due to the Robin boundary condition at the boundary $x = 0$ the 1st elementary matrix has an extra term, as follows,

$$K_0^e = K_0^e + \frac{c_1 \Delta t}{k}(h_r + h_c) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{2.41}$$

and

$$\begin{aligned} F_0^e = F_0^e + [\frac{c_1(0)\Delta t}{k}(h_r T_r + h_c T_{air}) - \frac{\lambda \rho D_W h_W}{k} c_1(0) \Delta t (W_0 - W_{air}) \\ -c_2 \Delta t h_W (W_0 - W_{air})] \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \end{aligned} \tag{2.42}$$

To get stiffness matrix, the local stiffness matrices are added together in such a way that the second row of the i^{th} element matrix is added with the first row of $(i+1)^{th}$ elementary matrix.

Vapor Diffusion Equation:

$$\begin{aligned} &\Delta t \sum_{i=0}^{N} (D_V)_i V_i \left(\int_0^{x_{L/2}} \frac{\partial \phi_i}{\partial x} \frac{\partial P}{\partial x} dx \right) + \sum_{i=0}^{N} V_i \left(\int_0^{x_{L/2}} \phi_i P dx \right) + (D_V)_0 \Delta t h_V V_0 P(0) \\ &= \sum_{i=0}^{N} V_i \left(\int_0^{x_{L/2}} \phi_i P dx \right) + (D_V)_0 \Delta t h_V V_{air} P(0) \end{aligned} \tag{2.43}$$

Similarly we will get the following local stiffness matrix,

$$K_i^e = ((D_V)_i \Delta t) \begin{pmatrix} \int_{x_i}^{x_{i+1}} \phi_i'^2 dx & \int_{x_i}^{x_{i+1}} \phi_i' \phi_{i+1}' dx \\ \int_{x_i}^{x_{i+1}} \phi_{i+1}' \phi_i' dx & \int_{x_i}^{x_{i+1}} \phi_{i+1}'^2 dx \end{pmatrix}$$
$$+ \begin{pmatrix} \int_{x_i}^{x_{i+1}} \phi_i^2 dx & \int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \\ \int_{x_i}^{x_{i+1}} \phi_{i+1} \phi_i dx & \int_{x_i}^{x_{i+1}} \phi_{i+1}^2 dx \end{pmatrix} \tag{2.44}$$

and the local load vector is

$$F_i^e = \begin{pmatrix} L(\phi_i) \\ L(\phi_{i+1}) \end{pmatrix} \tag{2.45}$$

where

$$L(\phi_i) = V_i \left(\int_{x_i}^{x_{i+1}} \phi_i \phi_i dx \right) + V_{i+1} \left(\int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \right) \tag{2.46}$$

and on the boundary,

$$K_0^e = K_0^e + (D_V)_0 \Delta t h_V \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{2.47}$$

and

$$F_0^e = F_0^e + (D_V)_0 \Delta t h_V V_{air} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{2.48}$$

Liquid Water Diffusion Equation:

$$\Delta t \sum_{i=0}^{N} D_W W_i \left(\int_0^{x_{L/2}} \frac{\partial \phi_i}{\partial x} \frac{\partial P}{\partial x} dx \right) + \sum_{i=0}^{N} W_i \left(\int_0^{x_{L/2}} \phi_i P dx \right) + D_W \Delta t h_W W_0 P(0)$$
$$= \sum_{i=0}^{N} W_i \left(\int_0^{x_{L/2}} \phi_i P dx \right) + D_W \Delta t h_W W_{air} P(0) \tag{2.49}$$

The local and global stiffness matrix is obtained exactly in the same way as above.

$$K_i^e = (D_W \Delta t) \begin{pmatrix} \int_{x_i}^{x_{i+1}} \phi_i'^2 dx & \int_{x_i}^{x_{i+1}} \phi_i' \phi_{i+1}' dx \\ \int_{x_i}^{x_{i+1}} \phi_{i+1}' \phi_i' dx & \int_{x_i}^{x_{i+1}} \phi_{i+1}'^2 dx \end{pmatrix}$$

$$+ \begin{pmatrix} \int_{x_i}^{x_{i+1}} \phi_i^2 dx & \int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \\ \int_{x_i}^{x_{i+1}} \phi_{i+1} \phi_i dx & \int_{x_i}^{x_{i+1}} \phi_{i+1}^2 dx \end{pmatrix} \tag{2.50}$$

and the local load vector is

$$F_i^e = \begin{pmatrix} L(\phi_i) \\ L(\phi_{i+1}) \end{pmatrix} \tag{2.51}$$

where

$$L(\phi_i) = W_i \left(\int_{x_i}^{x_{i+1}} \phi_i \phi_i dx \right) + W_{i+1} \left(\int_{x_i}^{x_{i+1}} \phi_i \phi_{i+1} dx \right) \tag{2.52}$$

and on the boundary,

$$K_0^e = K_0^e + D_W \Delta t h_W \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{2.53}$$

and

$$F_0^e = F_0^e + D_W \Delta t h_W W_{air} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{2.54}$$

2.3 Two Dimensional Model

The results of one dimensional simulation shows that the model is more sensitive towards time interval than the spatial one and since in finite difference and finite element schemes, the partial derivative with respect to time is approximated using the finite difference scheme, there is not much gain in using the finite element scheme. So the two dimensional model is validated using the finite difference scheme only.

2.3.1 Finite Difference Scheme

The Finite Difference Scheme for the two dimensional model is carried out as below,

Heat Transfer Equation

If the domain is discretized into the discrete points (x_j, y_i) where $i = 0, 1, 2, ...N_1$ and $j = 0, 1, 2, ...N_2$, The two dimensional heat transfer equation can be given as follows,

$$\begin{aligned}\frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t} = \frac{k}{\rho c_p}[(1-\theta_1)\left(\frac{T_{i,j-1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j+1}^{n+1}}{(\Delta x)^2}\right) + (\theta_1)\left(\frac{T_{i,j-1}^{n} - 2T_{i,j}^{n} + T_{i,j+1}^{n}}{(\Delta x)^2}\right) \\ +(1-\theta_2)\left(\frac{T_{i-1,j}^{n+1} - 2T_{i,j}^{n+1} + T_{i+1,j}^{n+1}}{(\Delta y)^2}\right) + (\theta_2)\left(\frac{T_{i-1,j}^{n} - 2T_{i,j}^{n} + T_{i+1,j}^{n}}{(\Delta y)^2}\right)] \\ +\frac{\lambda D_W}{c_p}\left(\frac{W_{i-1,j}^{n} - 2W_{i,j}^{n} + W_{i+1,j}^{n}}{(\Delta y)^2} + \frac{W_{i,j-1}^{n} - 2W_{i,j}^{n} + W_{i,j+1}^{n}}{(\Delta x)^2}\right)\end{aligned}$$

or it can be reduced to,

$$\begin{aligned}-\alpha_1 T_{i-1,j}^{n+1} + (1 + 2\alpha_1 + 2\alpha_2)T_{i,j}^{n+1} - \alpha_1 T_{i+1,j}^{n+1} - \alpha_2 T_{i,j-1}^{n+1} - \alpha_2 T_{i,j+1}^{n+1} \qquad (2.55)\\ = \alpha_3 T_{i-1,j}^{n} + (1 - 2\alpha_3 - 2\alpha_4)T_{i,j}^{n} + \alpha_3 T_{i+1,j}^{n} + \alpha_4 T_{i,j-1}^{n} + \alpha_4 T_{i,j+1}^{n} \\ +\alpha_5(W_{i-1,j}^{n} - 2W_{i,j}^{n} + W_{i+1,j}^{n}) + \alpha_6(W_{i,j-1}^{n} - 2W_{i,j}^{n} + W_{i,j+1}^{n}) \\ i = 0, 1, 2, 3....N_1. \qquad j = 0, 1, 2, 3....N_2.\end{aligned}$$

where

$$\alpha_1 = \frac{k\Delta t}{\rho c_p (\Delta y)^2}(1-\theta_2) \qquad \alpha_3 = \frac{k\Delta t}{\rho c_p (\Delta y)^2}(\theta_2)$$

$$\alpha_2 = \frac{k\Delta t}{\rho c_p (\Delta x)^2}(1-\theta_1) \qquad \alpha_4 = \frac{k\Delta t}{\rho c_p (\Delta x)^2}(\theta_1)$$

$$\alpha_5 = \frac{\lambda D_W \Delta t}{c_p (\Delta y)^2} \qquad \alpha_6 = \frac{\lambda D_W \Delta t}{c_p (\Delta x)^2}$$

If the unknowns at $(n+1)^{th}$ level are taken in a continuous manner, a banded matrix which is of size $(N_1 * N_2) \times (N_1 * N_2)$ is obtained and the distance between

$T^n_{i-1,j}$ and $T^n_{i,j}$ and $T^n_{i+1,j}$ and $T^n_{i,j}$ is N_2. And here the boundary conditions for heat transfer equation at $i = 0, j = 0, i = N_1$, and $j = N_2$ are (using equation(1.10)),

$$-k\left(\frac{T^n_{1,j} - T^n_{-1,j}}{2\Delta y}\right) = h_r(y)(T_r - T^n_{0,j}) + h_c(T_{air} - T^n_{0,j}) - \lambda\rho D_W h_W(W^n_{0,j} - W_{air}) \tag{2.56}$$

$$-k\left(\frac{T^n_{i,1} - T^n_{i,-1}}{2\Delta x}\right) = h_r(x)(T_r - T^n_{i,0}) + h_c(T_{air} - T^n_{i,0}) - \lambda\rho D_W h_W(W^n_{i,0} - W_{air}) \tag{2.57}$$

$$\frac{T^n_{N+1,j} - T^n_{N-1,j}}{2\Delta x} = 0 \tag{2.58}$$

$$\frac{T^n_{i,N+1} - T^n_{i,N-1}}{2\Delta x} = 0 \tag{2.59}$$

The boundary conditions for water diffusion equation are,

$$\frac{W^n_{1,j} - W^n_{-1,j}}{2\Delta y} = h_W(y)(W^n_{0,j} - W_{air}) \tag{2.60}$$

$$\frac{W^n_{i,1} - W^n_{i,-1}}{2\Delta x} = h_W(x)(W^n_{i,0} - W_{air}) \tag{2.61}$$

$$\frac{W^n_{N+1,j} - W^n_{N-1,j}}{2\Delta y} = 0 \tag{2.62}$$

$$\frac{W^n_{i,N+1} - W^n_{i,N-1}}{2\Delta x} = 0 \tag{2.63}$$

In the equation (2.55), on the boundary $i = 0$, when $j = 1, 2....N_2-1$, the boundary conditions (2.56) and (2.60) are used to replace the ghost points $T^n_{-1,j}$ and $W^n_{-1,j}$. When $j = 0$, ghost points $T^n_{-1,0}$, $T^n_{0,-1}$, $W^n_{-1,0}$ and $W^n_{0,-1}$ are replaced using the conditions (2.56), (2.60), (2.57) and (2.61). And when $j = N_2$, with the conditions (2.56), (2.60), (2.59) and (2.63), ghost points T^n_{-1,N_2}, T^n_{0,N_2+1}, W^n_{-1,N_2} and W^n_{0,N_2+1} are replaced.

On the boundary $i = N_1$, when $j = 1, 1, ...N_2 - 1$, the ghost points $T^n_{N_1+1,j}$

and $W^n_{N_1+1,j}$ are replaced using the boundary conditions (2.58) and (2.62), when $j = 0$, $T^n_{N_1,-1}$, $T^n_{N_1+1,0}$, $W^n_{N_1,-1}$ and $W^n_{N_1+1,0}$ are replaced using the conditions (2.57), (2.61), (2.58) and (2.62).

When $j = 0$ and $i = 1, 2....N_1 - 1$, conditions (2.57) and (2.61) are used to replace the ghost points $T^n_{i,-1}$ and $W^n_{i,-1}$ and when $j = N_2$ and $i = 1, 2, ...N_1$, the ghost points T^n_{i,N_2+1} and W^n_{i,N_2+1} is replaced using the equations (2.59) and (2.63).

Thus using the above equations (2.55) and the boundary conditions, (2.56-63), the linear system,

$$AX = B$$

is obtained, where A is a banded matrix with 5 bands. And by solving this linear system the unknown values of temperature are obtained.

Diffusion Equation for Water Vapor

For two dimensional model the equation of water vapor diffusion can be discretized as follows,

$$\begin{aligned}\frac{V^{n+1}_{i,j} - V^n_{i,j}}{\Delta t} &= (1-\theta_1)\left(\frac{(D_V)^{n+1}_{i,j+1}V^{n+1}_{i,j+1} - ((D_V)^{n+1}_{i,j+1} + (D_V)^{n+1}_{i,j})V^{n+1}_{i,j} + (D_V)^{n+1}_{i,j}V^{n+1}_{i,j-1}}{(\Delta x)^2}\right) \\ &+(\theta_1)\left(\frac{(D_V)^{n}_{i,j+1}V^{n}_{i,j+1} - ((D_V)^{n}_{i,j+1} + (D_V)^{n}_{i,j})V^{n}_{i,j} + (D_V)^{n}_{i,j}V^{n}_{i,j-1}}{(\Delta x)^2}\right) \\ &+(1-\theta_2)\left(\frac{(D_V)^{n+1}_{i+1,j}V^{n+1}_{i+1,j} - ((D_V)^{n+1}_{i+1,j} + (D_V)^{n+1}_{i,j})V^{n+1}_{i,j} + (D_V)^{n+1}_{i,j}V^{n+1}_{i-1,j}}{(\Delta y)^2}\right) \\ &+(\theta_2)\left(\frac{(D_V)^{n}_{i+1,j}V^{n}_{i+1,j} - ((D_V)^{n}_{i+1,j} + (D_V)^{n}_{i,j})V^{n}_{i,j} + (D_V)^{n}_{i,j}V^{n}_{i-1,j}}{(\Delta y)^2}\right)\end{aligned} \tag{2.64}$$

or after rearranging,

$$\begin{aligned}-\alpha_1(D_V)^{n+1}_{i,j+1}V^{n+1}_{i,j+1} + (1+\alpha_1\eta_1^{n+1}+\alpha_2\eta_2^{n+1})V^{n+1}_{i,j} - \alpha_1(D_V)^{n+1}_{i,j}V^{n+1}_{i,j-1} - \alpha_2(D_V)^{n+1}_{i+1,j}V^{n+1}_{i+1,j}\\ -\alpha_2(D_V)^{n+1}_{i,j}V^{n+1}_{i-1,j} = \alpha_3(D_V)^{n}_{i,j+1}V^{n}_{i,j+1} + (1+\alpha_3\eta_1^{n}+\alpha_4\eta_2^{n})V^{n}_{i,j} - \alpha_3(D_V)^{n}_{i,j}V^{n}_{i,j-1}\\ -\alpha_4(D_V)^{n}_{i+1,j}V^{n}_{i+1,j} - \alpha_4(D_V)^{n}_{i,j}V^{n}_{i-1,j}\end{aligned} \tag{2.65}$$

$$i = 0,1,2,3....N_1. \qquad j = 0,1,2,3....N_2.$$

where,

$$\begin{aligned}\eta_1 &= ((D_V)_{i,j+1} + (D_V)_{i,j}) & \eta_2 &= ((D_V)_{i+1,j} + (D_V)_{i,j})\\ \alpha_1 &= \frac{\Delta t}{(\Delta x)^2}(1-\theta_1) & \alpha_3 &= \frac{\Delta t}{(\Delta x)^2}(\theta_1)\\ \alpha_2 &= \frac{\Delta t}{(\Delta y)^2}(1-\theta_2) & \alpha_3 &= \frac{\Delta t}{(\Delta y)^2}(\theta_2)\end{aligned} \tag{2.66}$$

The boundary conditions are

$$\begin{aligned}\frac{V^n_{1,j} - V^n_{-1,j}}{2\Delta y} &= h_V(y)(V^n_{0,j} - V_{air})\\ \frac{V^n_{i,1} - V^n_{i,-1}}{2\Delta x} &= h_V(x)(V^n_{i,0} - V_{air})\\ \frac{V^n_{N+1,j} - V^n_{N-1,j}}{2\Delta y} &= 0\\ \frac{V^n_{i,N+1} - V^n_{i,N-1}}{2\Delta x} &= 0\end{aligned} \tag{2.67}$$

Considering the unknowns continually and by using the equations (2.65) and the boundary conditions (2.67), to replace the ghost points and then varying $i = 0,1,2,3....N_1$ and $j = 0,1,2,3....N_2$ (where N_1 and N_2 are spatial discrete points) a linear system,

$$AX = B$$

is obtained in each time interval and this linear system is solved to obtain the unknown values of the water vapor at discrete points.

Diffusion Equation for Liquid Water Content

The discretization of the liquid water diffusion equation is done similar to that of the vapor diffusion equation. Then the final equations are given as below,

$$-\alpha_1 W_{i,j+1}^{n+1} + (1 + 2\alpha_1 + 2\alpha_2) W_{i,j}^{n+1} - \alpha_1 W_{i,j-1}^{n+1} - \alpha_2 W_{i+1,j}^{n+1} - \alpha_2 W_{i-1,j}^{n+1}$$
$$= \alpha_3 W_{i,j-1}^{n} + (1 - 2\alpha_3 - 2\alpha_4) W_{i,j}^{n} + \alpha_3 W_{i,j+1}^{n} + \alpha_4 W_{i-1,j}^{n} + \alpha_4 W_{i-1,j}^{n} \tag{2.68}$$

$$i = 0, 1, 2, 3....N_1. \qquad j = 0, 1, 2, 3....N_2$$

Where,

$$\alpha_1 = \frac{D_W \Delta t}{(\Delta x)^2}(1 - \theta_1) \qquad \alpha_3 = \frac{D_W \Delta t}{(\Delta x)^2}(\theta_1)$$
$$\alpha_2 = \frac{D_W \Delta t}{(\Delta y)^2}(1 - \theta_2) \qquad \alpha_3 = \frac{D_W \Delta t}{(\Delta y)^2}(\theta_2)$$

the boundary conditions,

$$\begin{aligned}
\frac{W_{1,j}^n - W_{-1,j}^n}{2\Delta y} &= h_W(y)(W_{0,j}^n - W_{air}) \\
\frac{W_{i,1}^n - W_{i,-1}^n}{2\Delta x} &= h_W(x)(W_{i,0}^n - W_{air}) \\
\frac{W_{N+1,j}^n - W_{N-1,j}^n}{2\Delta y} &= 0 \\
\frac{W_{i,N+1}^n - W_{i,N-1}^n}{2\Delta x} &= 0
\end{aligned} \tag{2.69}$$

Thus a linear system for unknowns,

$$AX = B$$

is formulated by using above equation (2.68) and its boundary conditions(2.69). At the boundary the ghost points are replaced by using the boundary conditions as it is mentioned in the case of heat transfer equation. Then this linear system is solved in each time interval to get the water content in each discrete points of the domain.

Chapter 3

Computational Results and Discussions

3.1 Introduction

In previous chapters, the mathematical formulation of the model was discussed with a detailed description of implementation. An efficient code was written in Matlab for each numerical scheme (*Appendix A and Appendix B*) and in this chapter the results of the simulation are analyzed and discussed.

In order to study the behavior of temperature, liquid water and water vapor with respect to the time interval, the profiles are drawn with respect to time. The critical points C1, C2, C3 and C4 are also taken in temperature and liquid water profile in order to study the efficiency and performance of the numerical schemes.

The time when temperature of the bread reaches 100^oC is considered as the first critical point, C1. At this point water dries out and the crust starts forming. C2 is the critical point which gives the time when the water content reaches the peak value. Critical point C3 denote the peak liquid water level. Finally C4 represents the dry out time or the time when the liquid water completely evaporates to

vapor. [Zhou, 2004].

3.2 One Dimensional model

One dimensional model is implemented using finite difference scheme and finite element scheme. The results of the simulation are given below.

3.2.1 Finite Difference Scheme

The simulation in finite difference scheme is carried out using the "θ" method from which the implicit and explicit schemes are obtained by varying "θ". When $\theta = 0$ the scheme is explicit and $\theta = 1$ gives the implicit scheme. It is observed from the results that only when $\theta = 1$, i.e., the implicit scheme gives the correct and converged results. All other θ including $\theta = 0.5$, i.e., the Crank-Nicholson scheme produce wrong divergent results (Fig 3.1). This indicates that implicit scheme may be more reliable for this model.

Another interesting fact is that the implicit scheme gives convergent values only for a particular range of time intervals, say from $\Delta t = 15s$ to $\Delta t = 90s$ (Fig 3.2 and Fig 3.3). Though decreasing time interval is expected to produce a better result, the simulation results do not give such results beyond the mentioned range (Fig 3.4)(The reason for this will be elaborated in Chapter 4). As the time interval increases the rise in water vapor level in the center of bread sample decreases. So the satisfactory results can be seen only in the above mentioned range. The increase or decrease in spatial interval does not have much effect on the result but the profiles are more smooth for lower spatial interval (mesh size)(fig 3.5). The critical points are also plotted for different time intervals (Fig 3.6).

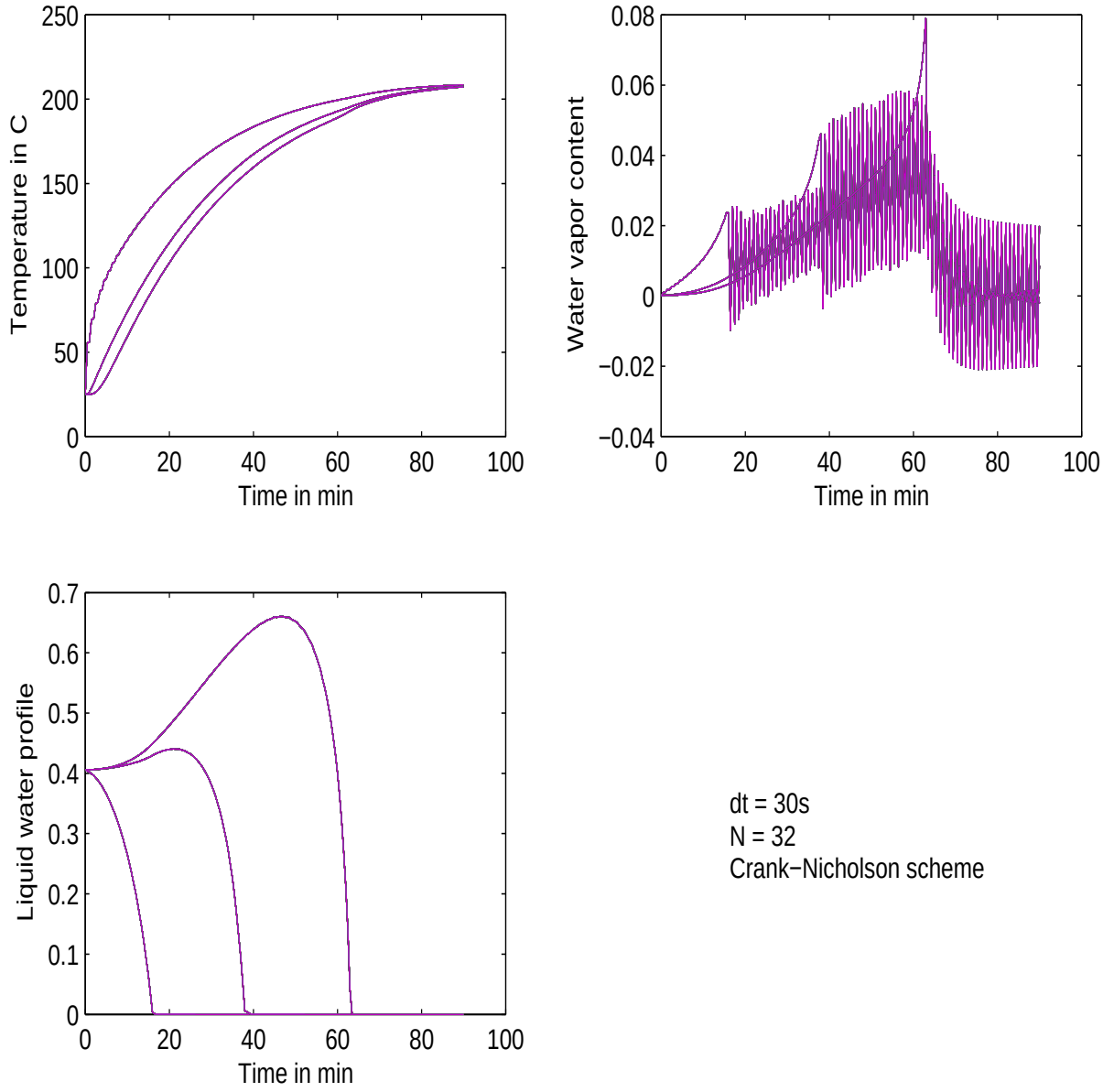

Figure 3.1: Temperature and Moisture profiles for model simulated through Crank-Nicholson Scheme (Surface, halfway to center, center)

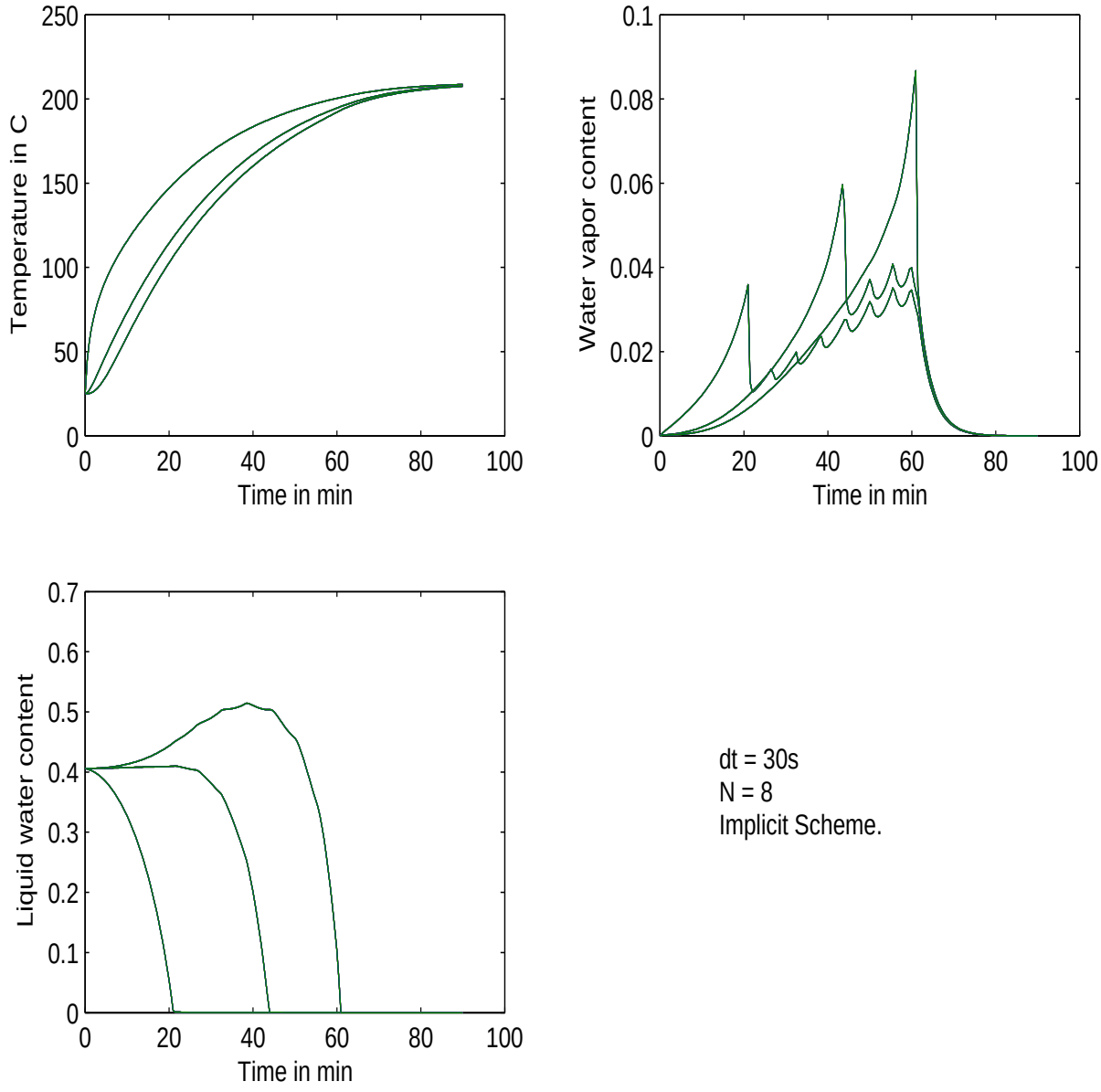

Figure 3.2: Temperature and Moisture profiles for model simulated through Implicit Scheme (Surface, halfway to center, center)

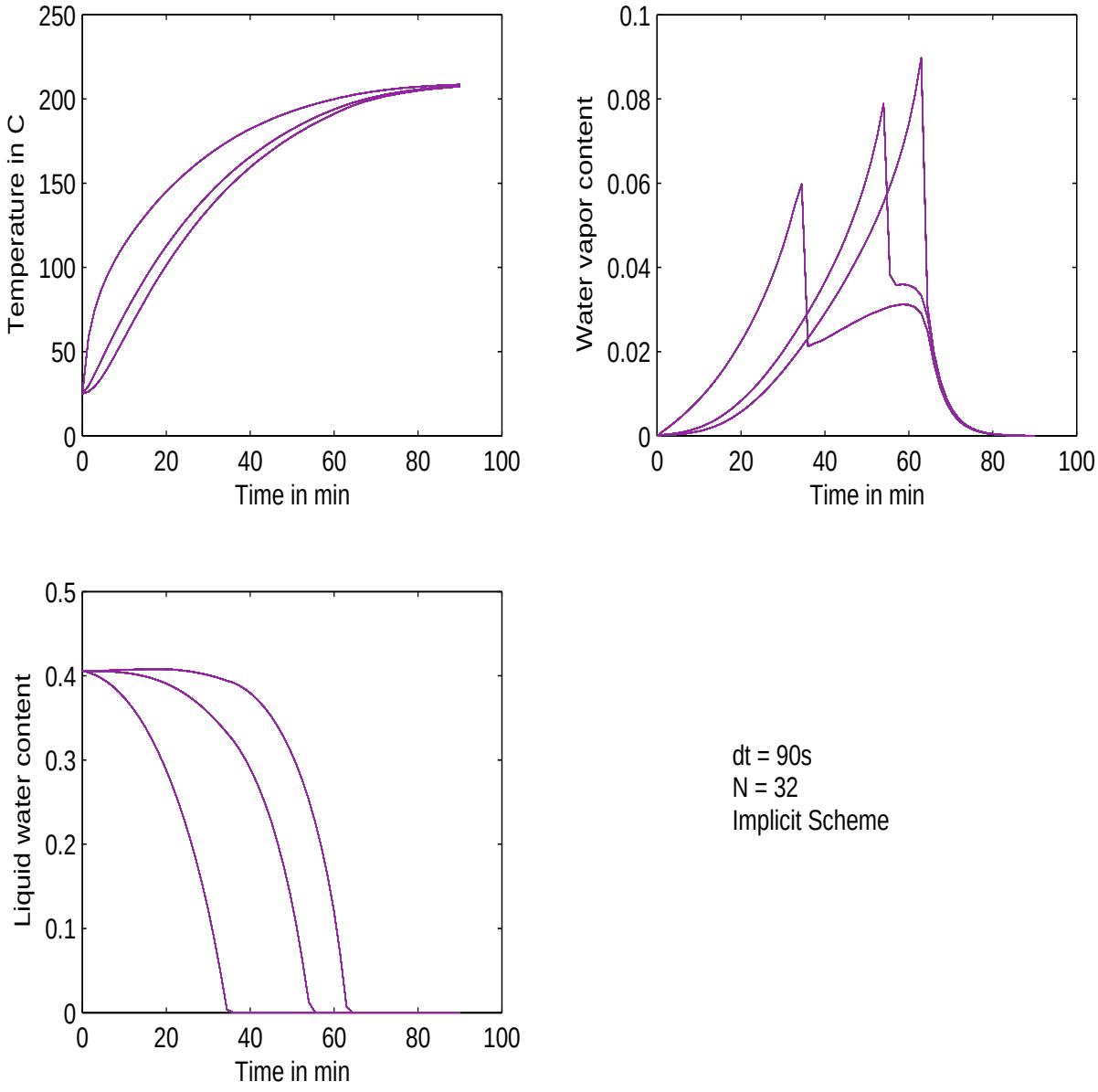

Figure 3.3: Temperature and Moisture profiles for model simulated through Implicit Scheme (Surface, halfway to center, center)

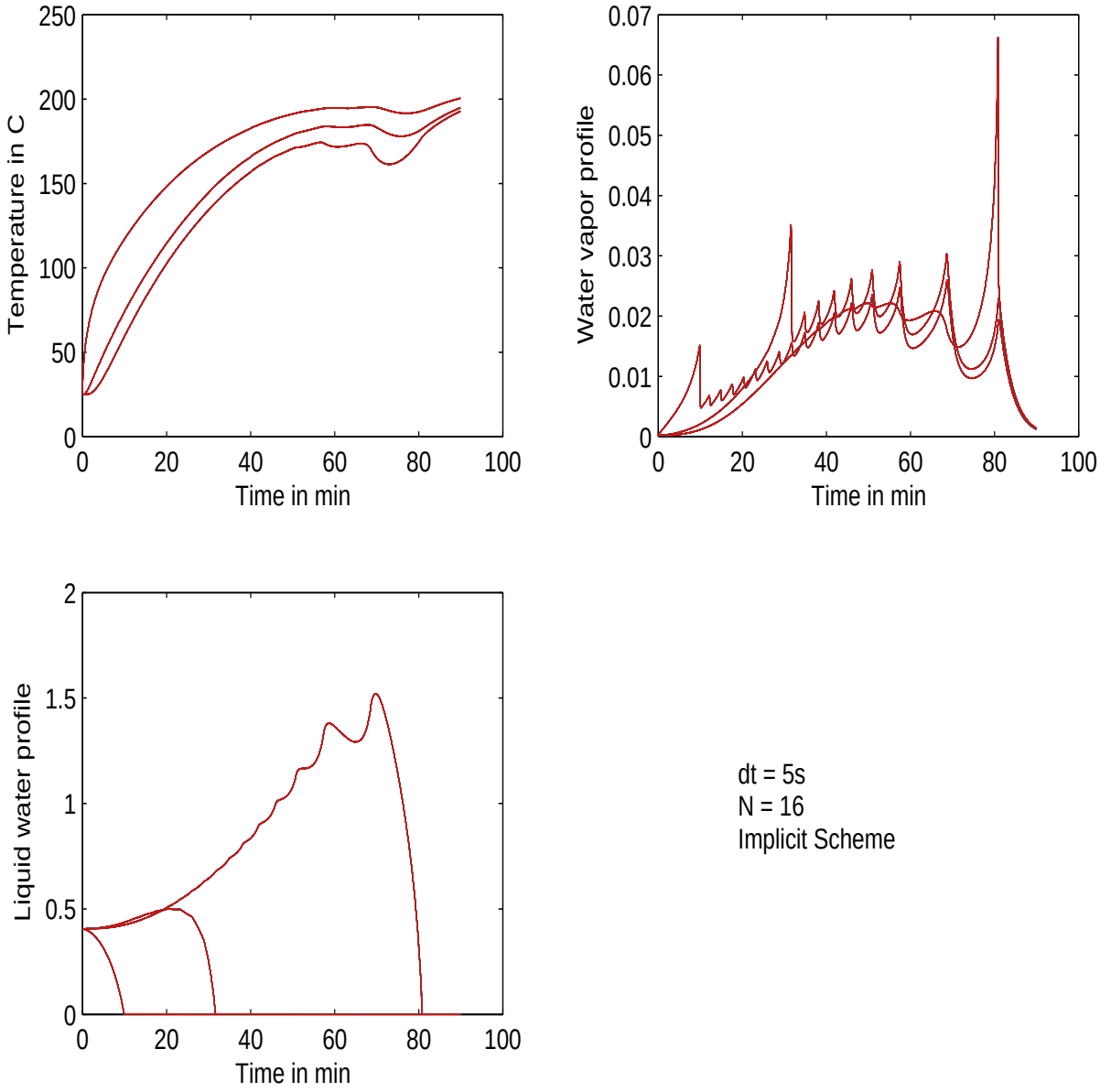

Figure 3.4: Temperature and Moisture profiles for model simulated through Implicit Scheme - Diverged solutions when Δt=5s (Surface, halfway to center, center)

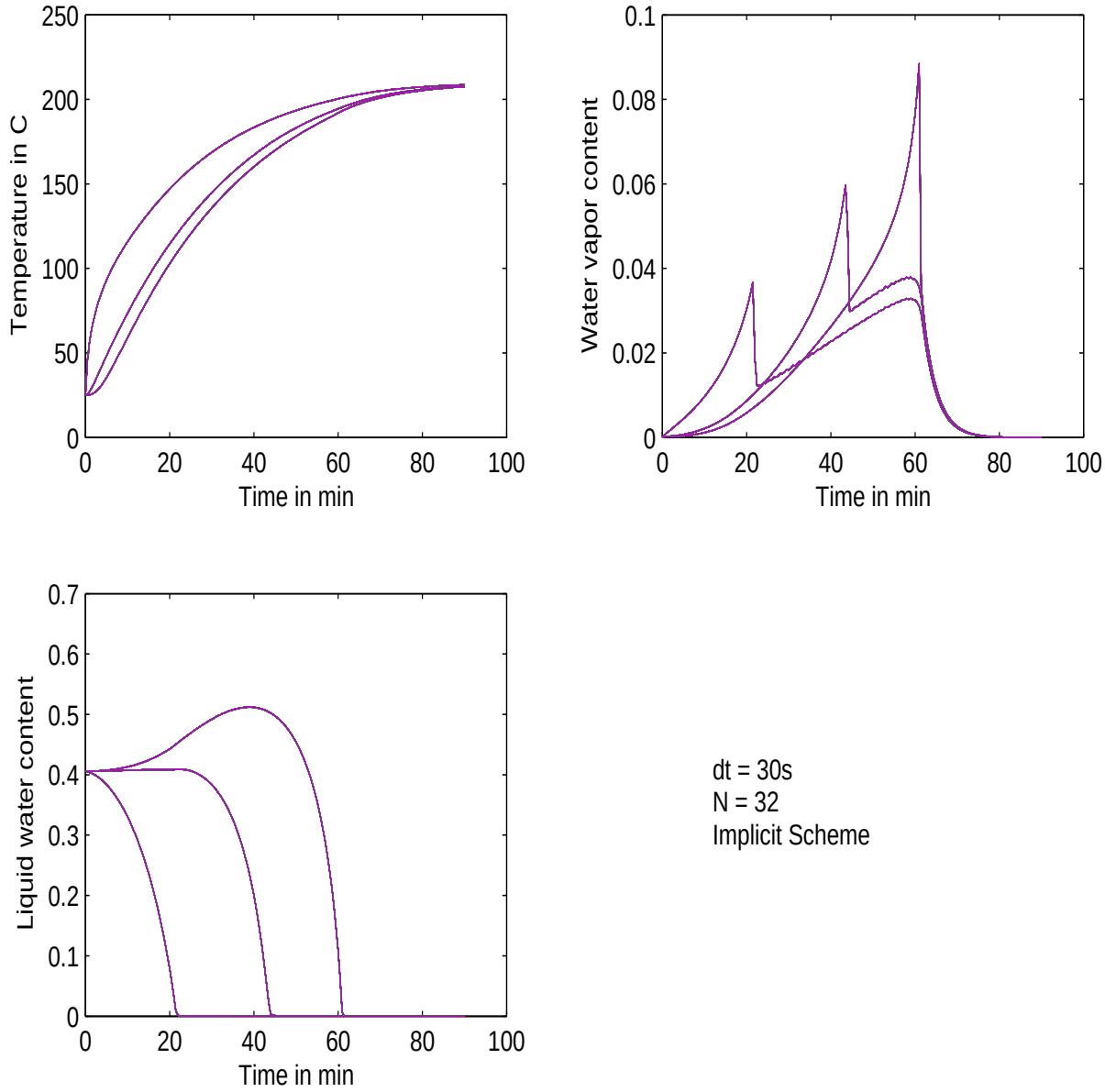

Figure 3.5: Temperature and Moisture profiles for model simulated through Implicit Scheme - Profiles for smaller spatial intervals(Surface, halfway to center, center)

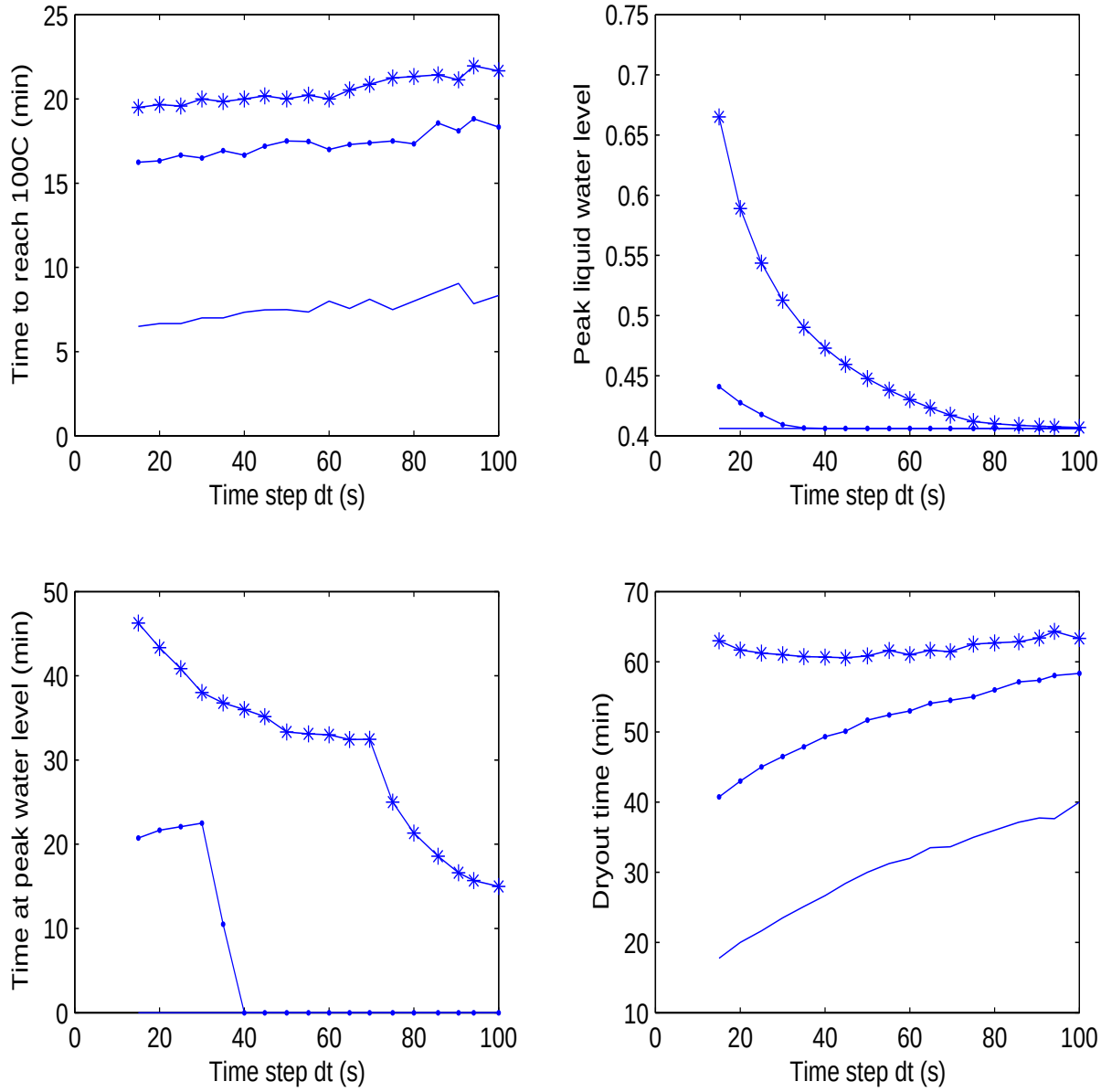

Figure 3.6: Sensitivity of Finite Difference Scheme to the size of time intervals (N=32):- Line - surface; Dotted line - half way to center; Starred line - center

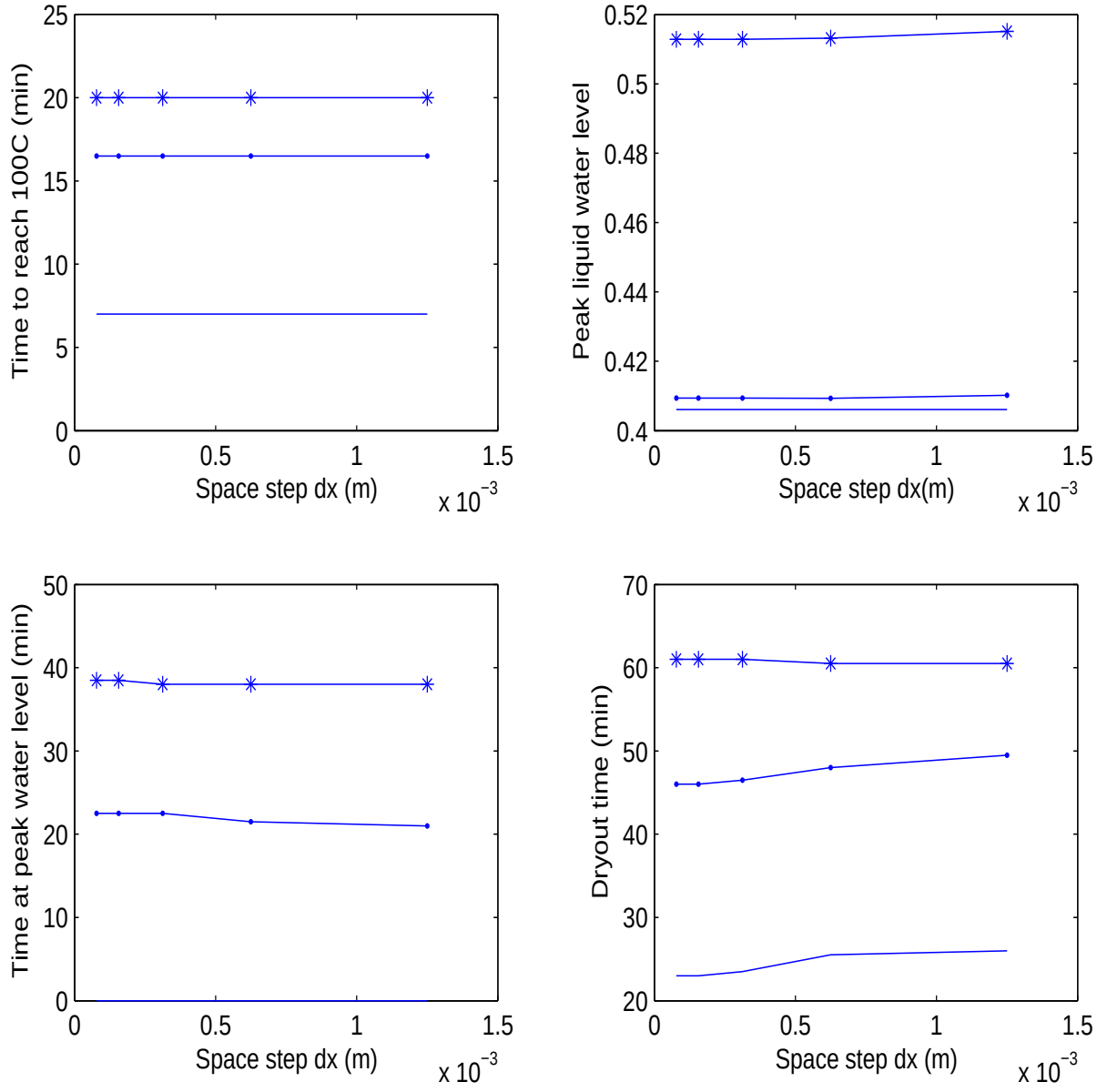

Figure 3.7: Sensitivity of Finite Difference Scheme to the spatial increment ($\Delta t = 30$):- Line - surface; Dotted line - half way to center; Starred line - center

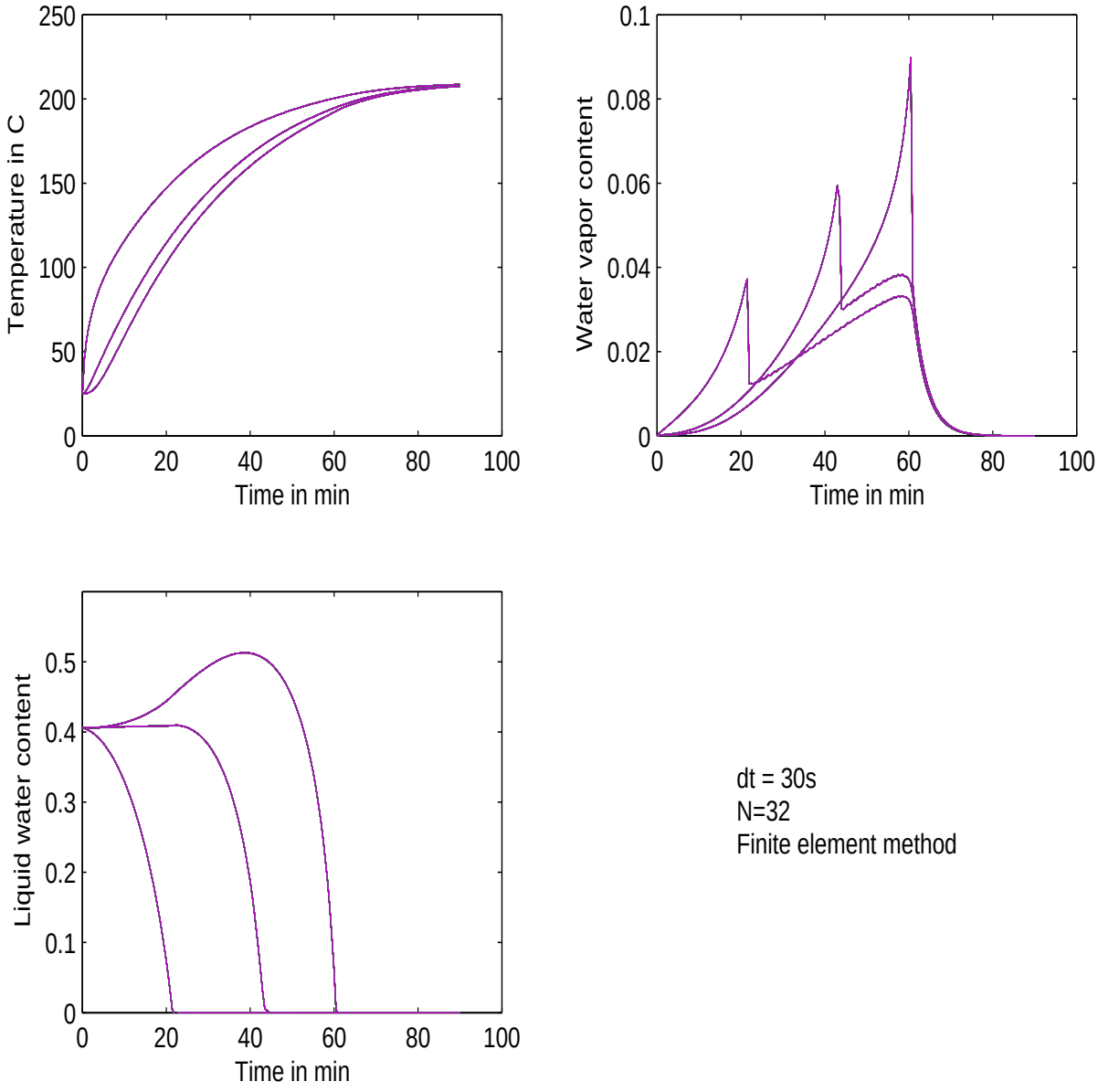

Figure 3.8: Temperature and Moisture profiles for model simulated through Finite Element Scheme (Surface, halfway to center, center)

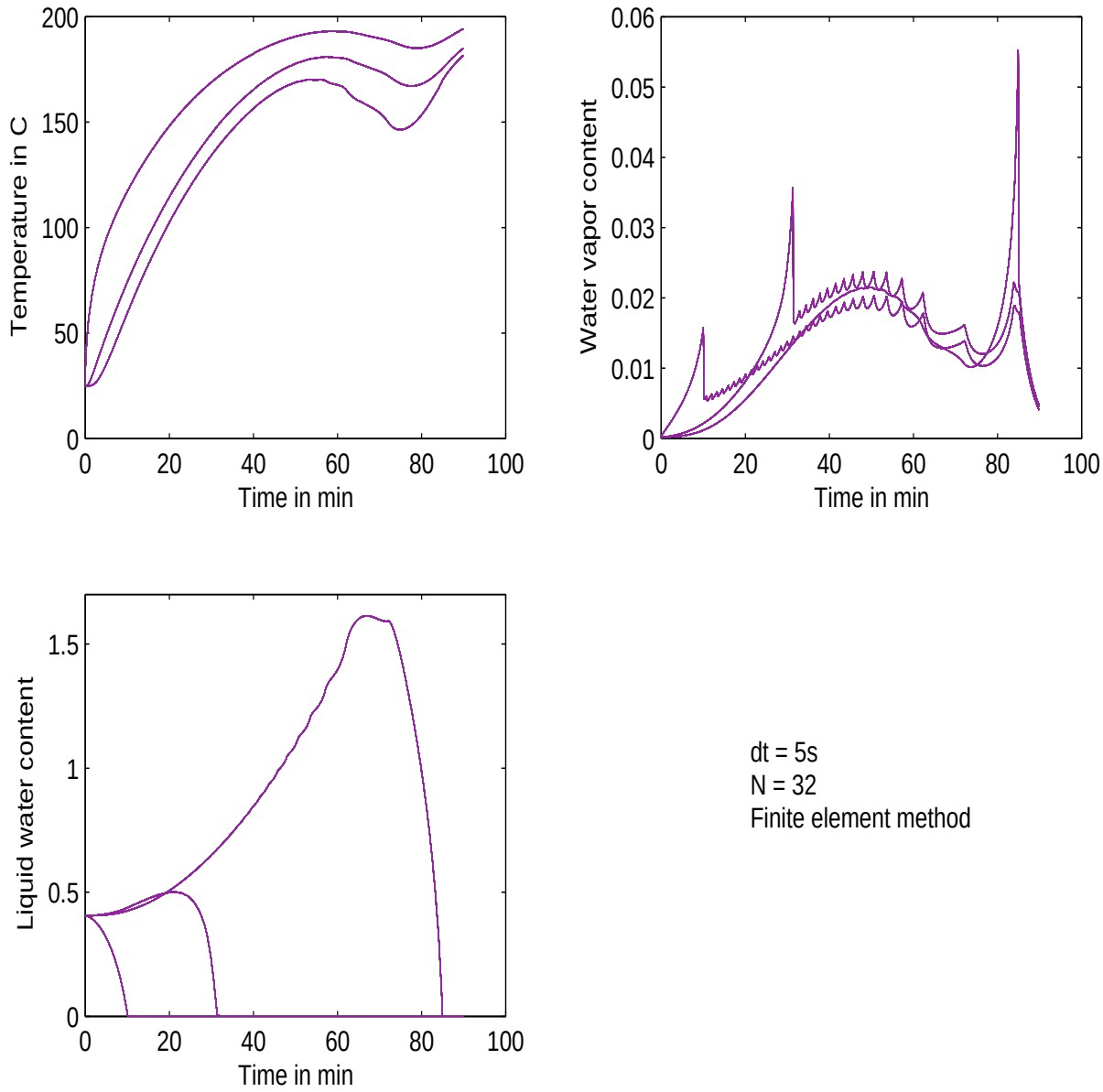

Figure 3.9: Temperature and Moisture profiles for model simulated through Finite Element Scheme -Diverged solutions when $\Delta t = 5s$ (Surface, halfway to center, center)

3.2.2 Finite Element Scheme

The simulation of the one dimensional model was also carried out using the finite element scheme and the profiles were drawn to illustrate the results. (Fig 3.8 and Fig 3.9)

3.3 Two Dimensional Model

The two dimensional model which is developed as an extension of the one dimensional model is simulated using finite difference scheme.

3.3.1 Finite Difference Scheme

Finite difference scheme is used to validate the model in two dimensional case. The above explained "θ" method is used here also and interestingly like one dimensional case, except "$\theta = 1$" ie implicit scheme, all other values of "θ" give wrong results (Fig 3.10-12). The time interval also plays a vital role in the simulation. The lower (Fig 3.13-15) and higher time intervals beyond a range leave out some unsatisfactory results. In general the model reflects same behavior that of one dimensional model. The critical values are also calculated at different points to analyze the performance of the numerical scheme(Fig 3.16).

3.4 Profile Discussions

The simulated profiles are discussed in detail below. The profiles give the behavior of the temperature and moisture during the process of baking.

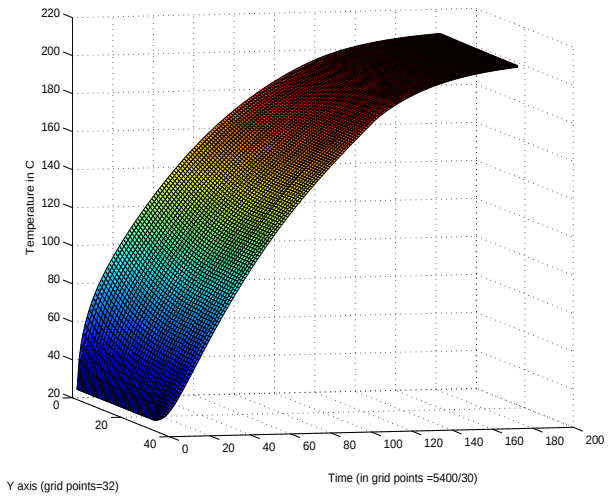

Figure 3.10: Temperature profile for 2-D model simulated through Finite Difference Scheme($\Delta t = 30s$ and X axis fixed for surface, halfway to center and center).

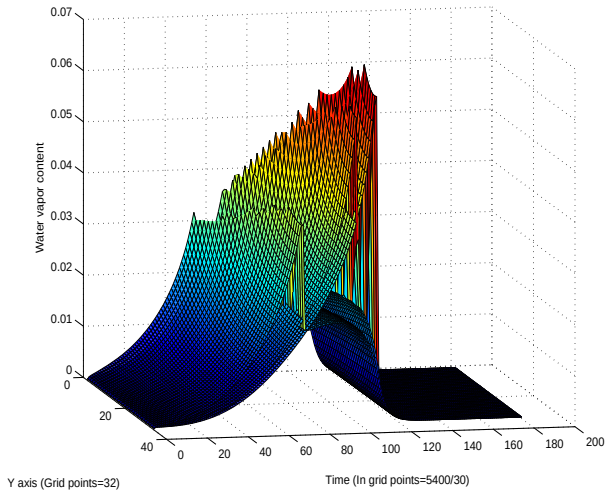

Figure 3.11: Water vapor profiles for 2-D model simulated through Finite Difference Scheme($\Delta t = 30s$ and X axis fixed for surface, halfway to center and center).

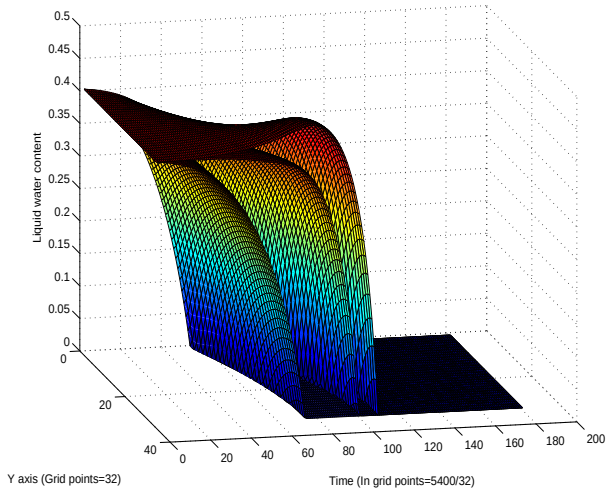

Figure 3.12: Liquid water profiles for 2-D model simulated through Finite Difference Scheme($\Delta t = 30s$ and X axis fixed for surface, halfway to center and center).

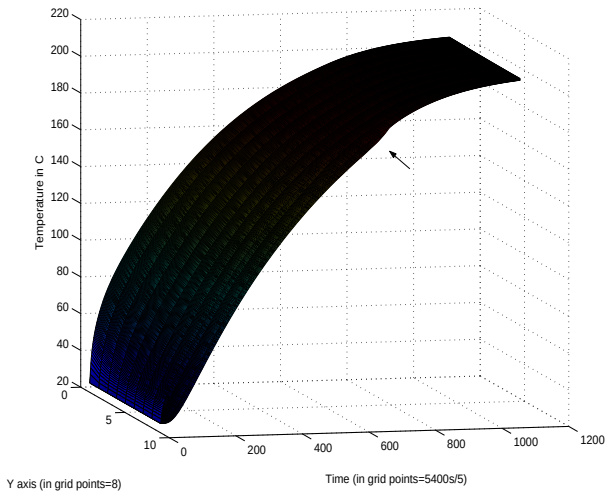

Figure 3.13: Temperature profile for 2-D model simulated through Finite Difference Scheme ($\Delta t = 5s$ and X axis fixed for surface, halfway to center and center, Divergent result).

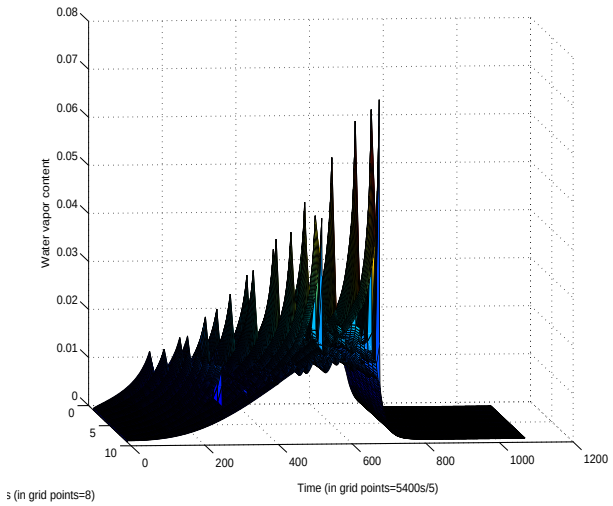

Figure 3.14: Water vapor profiles for 2-D model simulated through Finite Difference Scheme($\Delta t = 5s$ and X axis fixed for surface, halfway to center and center, Divergent result).

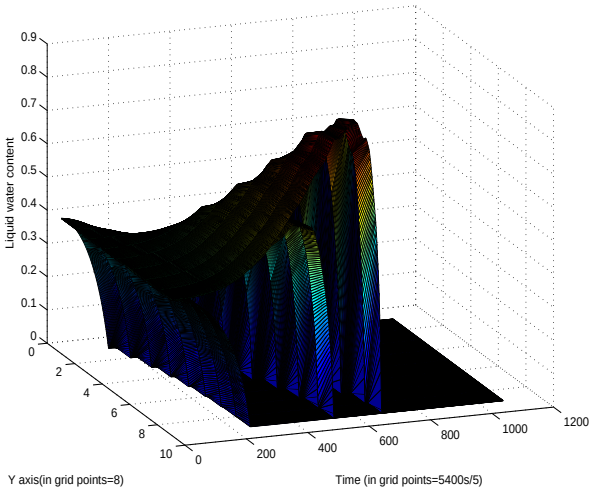

Figure 3.15: Liquid water profiles for 2-D model simulated through Finite Difference Scheme($\Delta t = 5s$ and X axis fixed for surface, halfway to center and center, Divergent result).

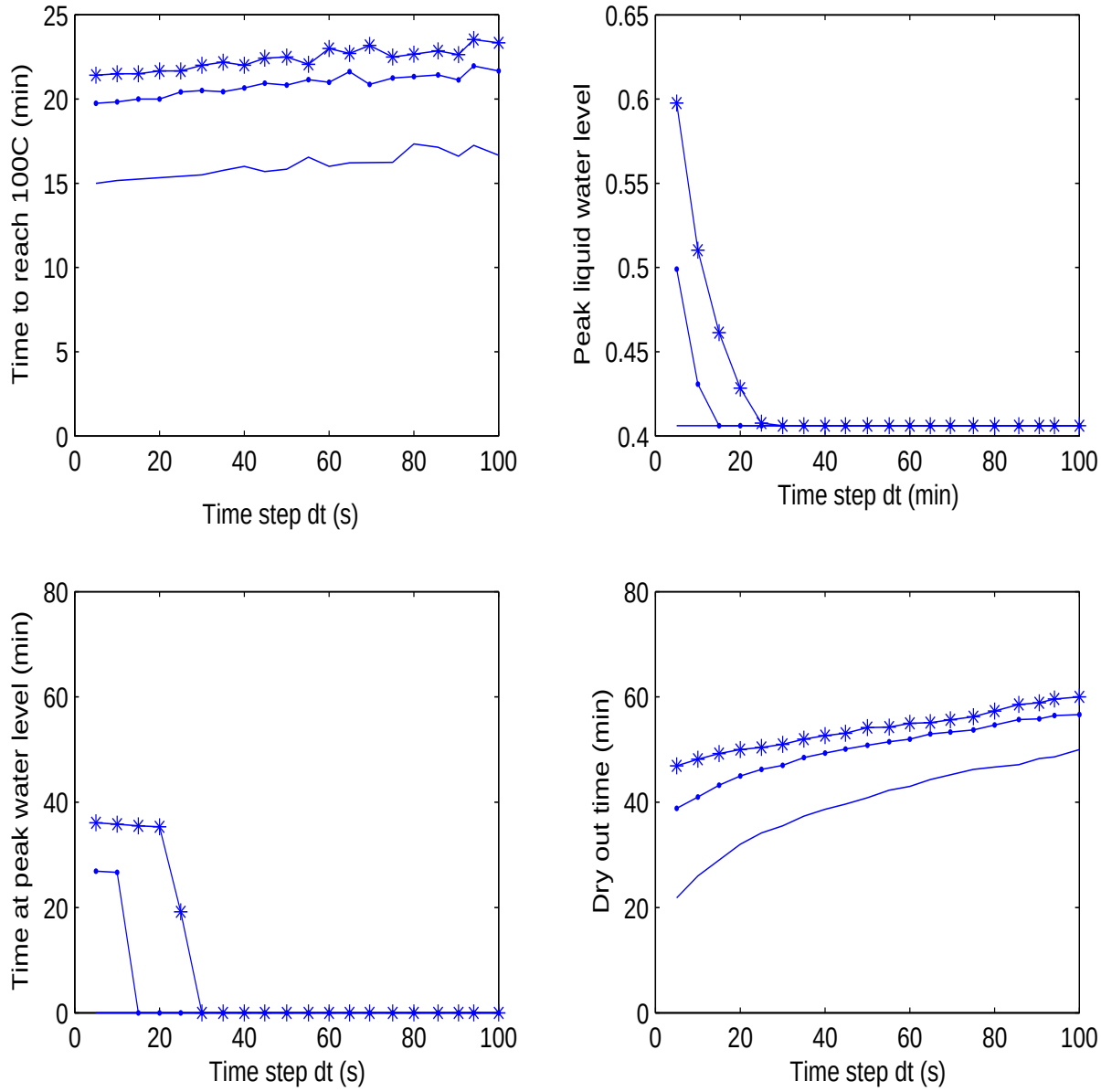

Figure 3.16: Sensitivity of Finite Difference Scheme to time intervals (N=32):- center slice with respect to y axis (Line - surface; Dotted line - half way to center; Starred line - center).

3.4.1 Discussion on the Temperature Profile

As it is mentioned earlier, the result of the simulation of the present model gives satisfactory results only when the time increment is greater than 15s (The reason for this will be elaborated in Chapter 4). So the profile when $\Delta t = 30s$ is taken for analysis.

The dough is placed in the oven which is maintained at a constant temperature of 210^oC. As time increases, the temperature of the dough rises due to natural convection, conduction and radiation. Since the surface of dough is exposed to oven heat more than any other parts of the dough, temperature on the surface increases much faster. When surface temperature increases, heat is transferred within the dough through conduction and also due to diffusion of water vapor. The center of dough does not attain the maximum temperature until the end of the baking process. Mechanism that accounts for the slower rise of temperature in center is the greater rate of heat loss caused by evaporation of water as compared with the rate of heat absorption by the dough. While temperature on the surface rises fast and in the center rises slow, the temperature halfway to center rises in a moderate level, a little faster than the center portion. By around 65-70 minutes, temperature of the dough, i.e., on surface, center and halfway to the center becomes a steady value which means that the dough is baked completely.

3.4.2 Discussion on the Liquid Water and Water Vapor Profiles

The mass transfer during baking is due to the diffusion of liquid water and water vapor content. The profiles show that liquid water content decreases rapidly on the surface while water vapor content increases since both are interrelated. The sudden

rise in temperature on the surface accounts for this rapid change since the increased temperature evaporates liquid water into water vapor. The vapor diffuses towards center and surface and at the center it condenses back into water since interior is in lower temperature compared to the surface. This explains the rise in water levels at center and towards center before it drops down to zero. It can also be seen that at around 45-50 min, though center holds temperature more than 100^oC the profile shows large amount of water levels. The reason for this can be explained as below, since the water vapor diffusion is slower than evaporation, the heat is used to increase the temperature rather than evaporating water. Or when the partial water vapor pressure is satisfied, the evaporation ends and the temperature increased [Thorvaldsson et.al, 1999]. Depending on liquid water profile, the vapor profile also changes since water is evaporated to vapor. The changes in vapor profile is also due to the diffusion of water vapor into air where the pressure gradient is high because of higher temperature.

3.4.3 General Discussion

Baking process is explained here with the help of temperature and moisture profiles drawn from the simulation of the mathematical model [Thorvaldsson et.al, 1999].

The bread sample is placed in an oven which is at a constant temperature of 210^oC and baked for about 90 minutes. The temperature close to the surface increases rapidly whereas it rises slowly inside the dough and this higher temperature vaporizes liquid water into water vapor which in turn raises the gradient of the water vapor content close to the surface. This creates a difference in the gradient of the vapor content between the surface and center, and vapor starts to move towards the center, where the vapor content gradient is low, and to the surface to reduce the vapor pressure. The temperature at the center is low compared to that of the

area close to the surface which makes water vapor condense back to liquid water.

The oven is at a much higher temperature than the dough, so in order to satisfy the water vapor pressure gradient, vapor diffuses out of the surface and the surface starts to dry out. Water left over is then evaporated to satisfy the vapor pressure and diffuses towards the surface and center till it dries out. The condensation of diffused vapor at the center build up water gradient at the center which in turn makes it diffuse towards the surface. This entire process continues till the the entire water and vapor content dries out and the dough is baked into bread.

The analysis of critical points reveals that the model is very much sensitive towards time interval (mesh size) while they are stable with respect to the spatial interval(Fig 3.6-7). Except one, other critical points vary drastically with respect to time interval. The first critical point C1, which gives the time to reach 100^oC is almost stable with time interval and it indicates that the profile for temperature distribution during baking is not very sensitive. It can be seen from the profile that the surface temperature reaches 100^oC in around 6 minutes whereas the center portion takes 20 minutes. Other profiles show that they vary with the time intervals. For smaller time interval the peak water content at the center is much above than that for higher intervals and as the length of time interval increases, the amount of peak water content reduces. The increase in time interval also results in reduction of time period to reach the peak water level. The dry-out time remains almost constant at the center but on the surface and halfway to the center, it goes higher with the increase in time intervals.

The two dimensional model shows almost the same behavior as that of one dimension, which was previously unknown. The critical values taken at the center

slice is showing a little more stable behavior than that of one dimensional model except for a few beginning time intervals. With the increment in time intervals, the peak water level decreases from a higher value to a constant value one which is the initial amount. The similar trend is seen in the time factor for peak water content also. The graphs plotted for two dimensional simulation also shows similar behavior with one dimensional case. This indicates that the study and the results on one dimensional model can also be applied to two dimensional model. This fact may help in further studies since it is more easy and takes less computational effort to study a one dimensional model.

The non-convergent behavior of the simulations of these one and two dimensional mathematical models for smaller time intervals is the negative aspect of this model which other researchers are also encountered ([Zhou, 2004], in the case of one dimensional model). This encouraged to do further analysis of the model and to develop some procedure to overcome this difficulty which is explained in the next chapter.

Chapter 4

Improved Methodology for Simulation

4.1 Introduction

As it is concluded in last chapter, the convergence of the implicit scheme, only for a particular range of values [Zhou, 2004] encouraged to do the further analysis of this model. The simulations of the model with respect to different sets of parameters gave an indication that the algebraic inequalities which are inserted between the governing equations to deal with the phase change might have caused this non-convergent behavior. It seems that this algebraic inequalities are causing some discontinuity in the interdependence of governing differential equations.

To clarify this inference and to test the stability of the governing partial differential equations, some simulations are done without using these algebraic inequalities. Though the results are meaningless with respect to baking theory, it showed that the governing differential equations are stable with respect to time and space. So it became clear that the introduction of algebraic inequalities to adopt tabled values make the system inconsistent. Here some suggestions are given to improve the convergence range of the model as all previous schemes are sensitive towards

the size of the time interval. The suggested procedure is also implemented using computer codes and results of the simulation are discussed section 4.2.

4.2 Methodology, Simulation and Results

Simulation using the algorithm mentioned in chapter 2 results in a non-convergent behavior of the model with respect to the size of the time intervals. More precisely, the numerical scheme gives satisfactory results only in a particular range of time intervals and when the interval or mesh size is less than 15 seconds, say at $\Delta t = 10s$ and $\Delta t = 5s$, numerical computation gives divergent results for temperature and moisture profiles (Fig 3.4). The simulations show that sudden rise in liquid water and water vapor contents and hence higher values for vapor and water for the following time steps, can be one of the reasons for this unsatisfactory results for smaller time intervals.

When the time interval is large, these higher values of moisture contents does not have a great influence on the system of governing equations since for the next time step, the increase in moisture values matches with the increase in temperature with respect to the large time interval. It means that when the time increment is longer, the temperature is getting higher in each steps and hence the moisture values has to be higher. But in the case of smaller time intervals, the time is increasing slowly and hence the temperature, so the moisture is also expected to grow in a slow rate but the adoption of inequalities for updating scheme using the tabled values makes the moisture growth more faster than expected or actual growth, and this accumulated error gives a bad result for the whole system towards the final time which can be clearly visible in the profiles with small time interval (Fig 3.4).

In the case of small time intervals, the algebraic inequalities makes the phase change more instantly than the reality. So for these time intervals, the problem of this sudden rise can be reduced by relaxing the saturated vapor content which is derived from the table for saturated vapor pressure. This relaxation allows some time for the phase change process to complete. This is done by introducing the equation

$$\frac{\partial V}{\partial t} = \gamma(V^* - V), \tag{4.1}$$

where V^* is the amount of vapor corresponding to the saturated vapor pressure and γ is a rate constant.

The relaxation using above differential equation can be justified because in the real baking process, evaporation to the saturation point is not instantaneous. Liquid water vaporizes to water vapor to satisfy the vapor pressure and this process is a time consuming simultaneous process with increase in temperature. The rate constant γ can be viewed as a relaxation parameter which should be selected carefully so as to relax the vaporization process in a satisfactory way. In the present simulation, the relaxation parameter is taken in the range of 0.01 - 0.015.

Equation (4.1) is solved as below,

$$\begin{aligned} V^* - V &= C\exp(-\gamma t) \\ &= (V^* - V^0)\exp(-\gamma t) \end{aligned}$$

or

$$V = V^0\exp(-\gamma t) + V^*(1 - \exp(-\gamma t)) \tag{4.2}$$

where V^0 is the initial water vapor content (at the $(n+1)^{th}$ step of V, V^0 is the value of V atvn^{th} step). For each time step the above equation can be written as,

$$V_{correction} = V^n \exp(-\gamma \Delta t) + V^*(1 - \exp(-\gamma \Delta t)) \tag{4.3}$$

This $V_{correction}$ is used instead of *saturated vapor content* in the procedure of updating water and vapor with respect to the increased temperature as described in section 2.4.

Simulations are then done with this new procedure and the results obtained are more satisfactory than previous results for smaller values of time intervals. The graphs below show the results for $\Delta t = 10s$, $\Delta t = 5s$ and $\Delta t = 2s$. Interestingly it is observed that this relaxation technique works for semi-implicit numerical method ie., when $\theta = 0.25$ also.

4.3 Discussions

This new approach is based on the assumption that the baking is a slow continuous process with simultaneous heat and mass transfer where the transition from one phase to another occur slowly. So in the case of small time steps, the updating scheme may increase the values of vapor and water more than the expected or actual values (the phase transition is done instantly). Therefore in this relaxation approach the tabled values for saturated vapor are relaxed before using them for updating the water and vapor values. This relaxation approach for solving one dimensional model for baking, almost succeeded in getting more meaningful results for small time intervals where the original approach failed. Since the adoption of algebraic inequalities is one of the reason for this time step size sensitiveness, a well chosen differential equation in the place of these algebraic values may reduce this sensitiveness of the model and make it more reliable.

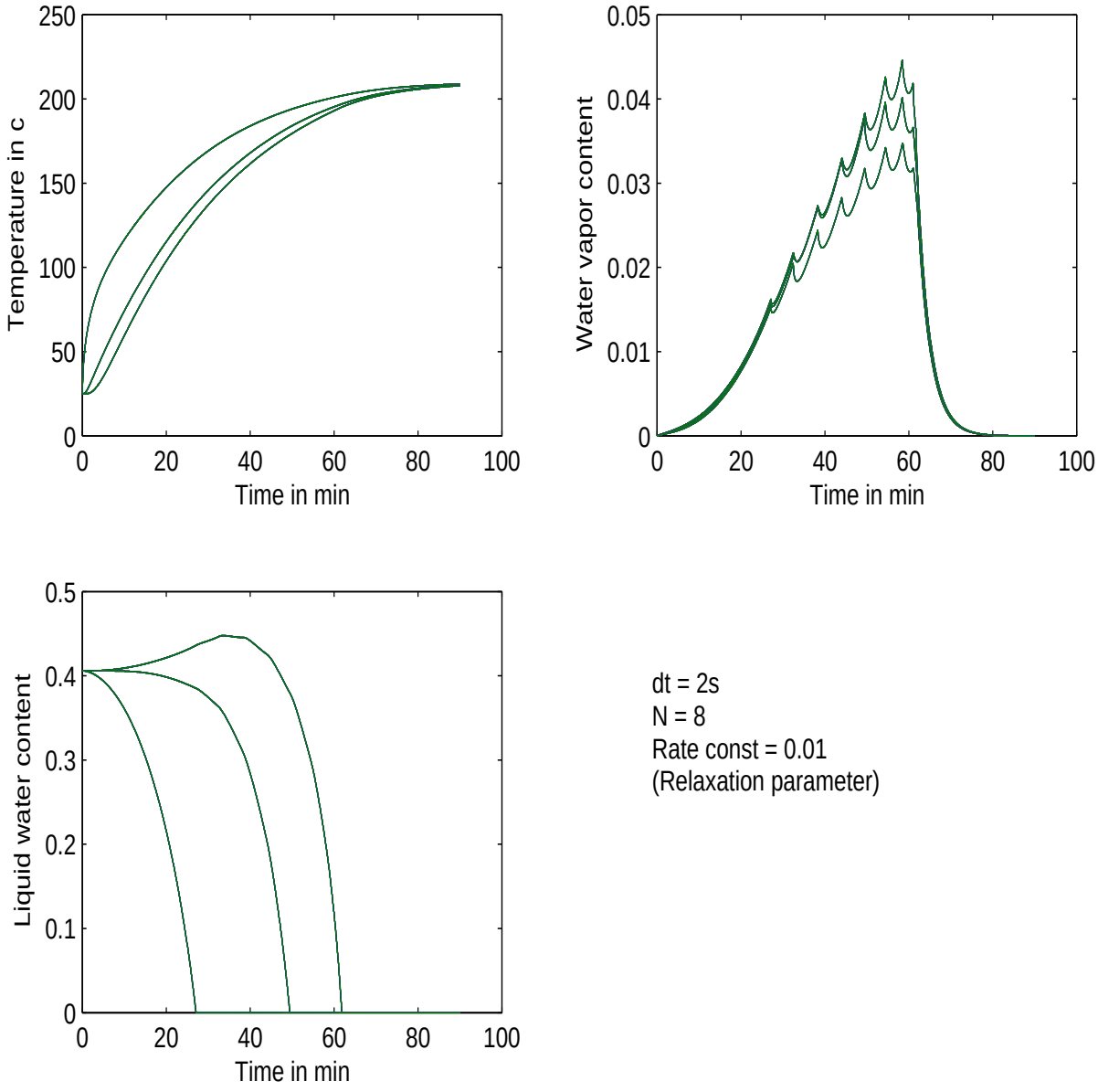

Figure 4.1: New improved results for Temperature and Moisture profiles using relaxation scheme when $\Delta t = 2s$. (Surface, halfway to center, center)

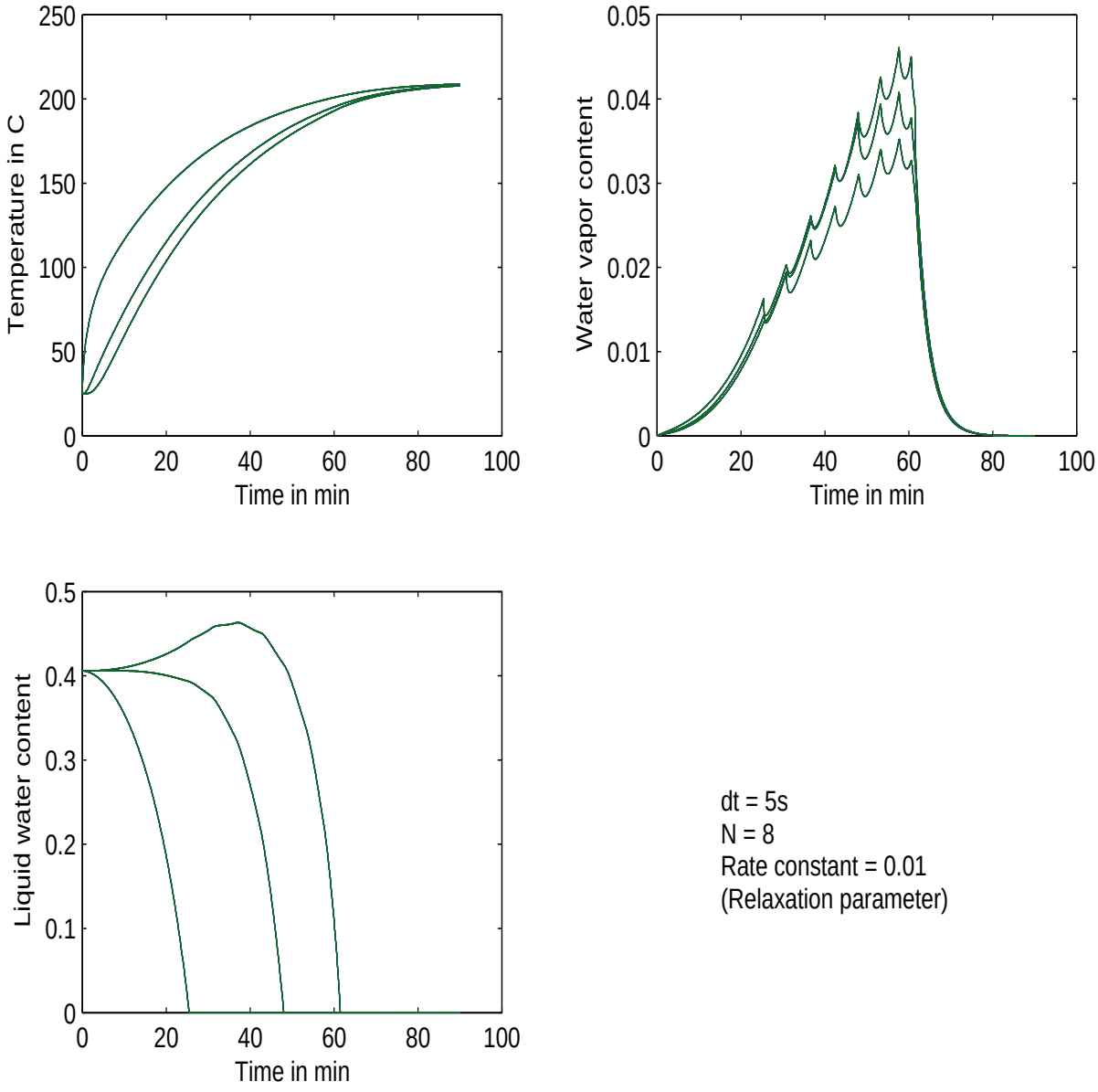

Figure 4.2: New improved results for Temperature and Moisture profiles using relaxation scheme when $\Delta t = 5s$. (Surface, halfway to center, center)

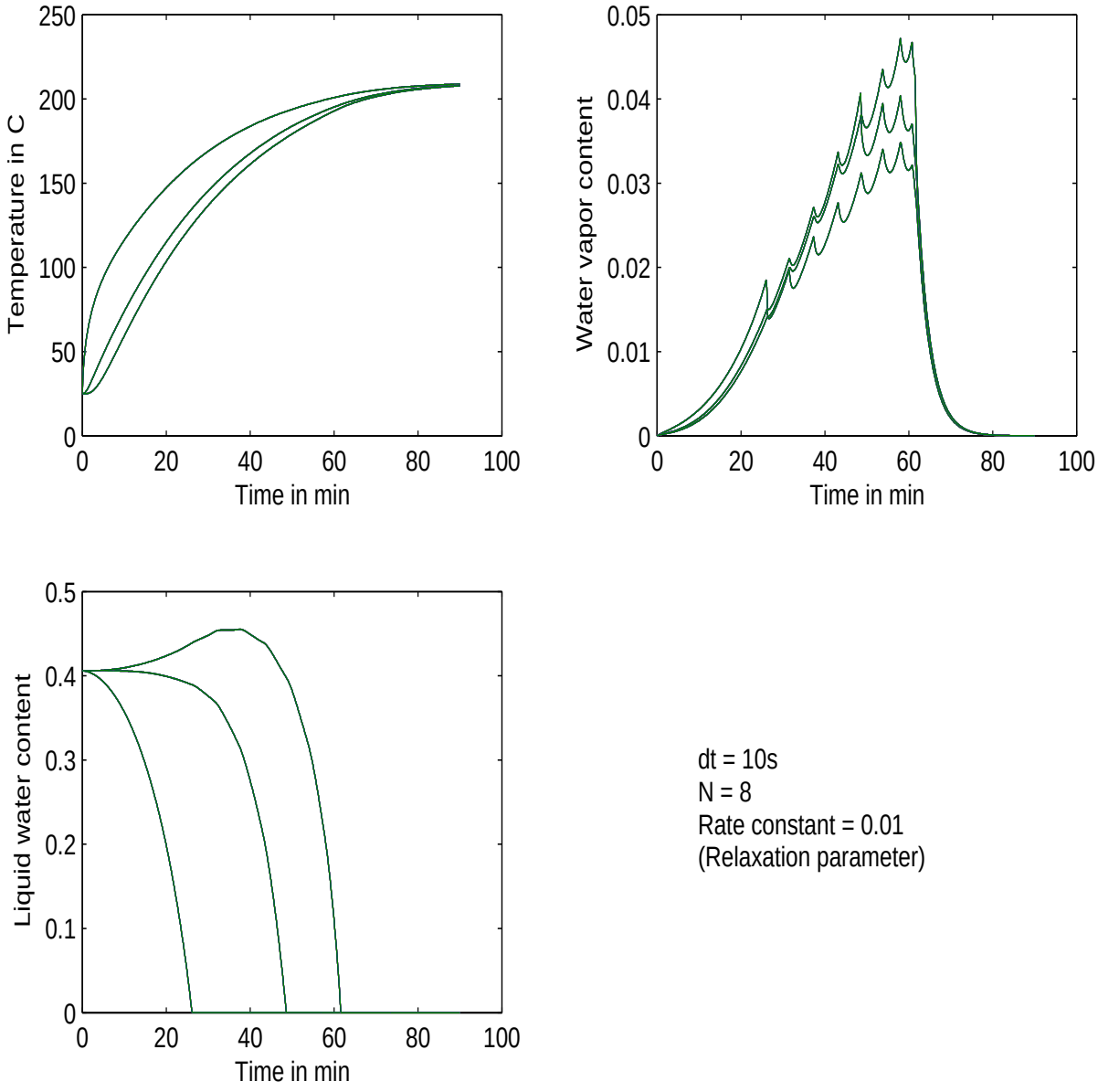

Figure 4.3: New improved results for Temperature and Moisture profiles using relaxation scheme when $\Delta t = 10s$. (Surface, halfway to center, center)

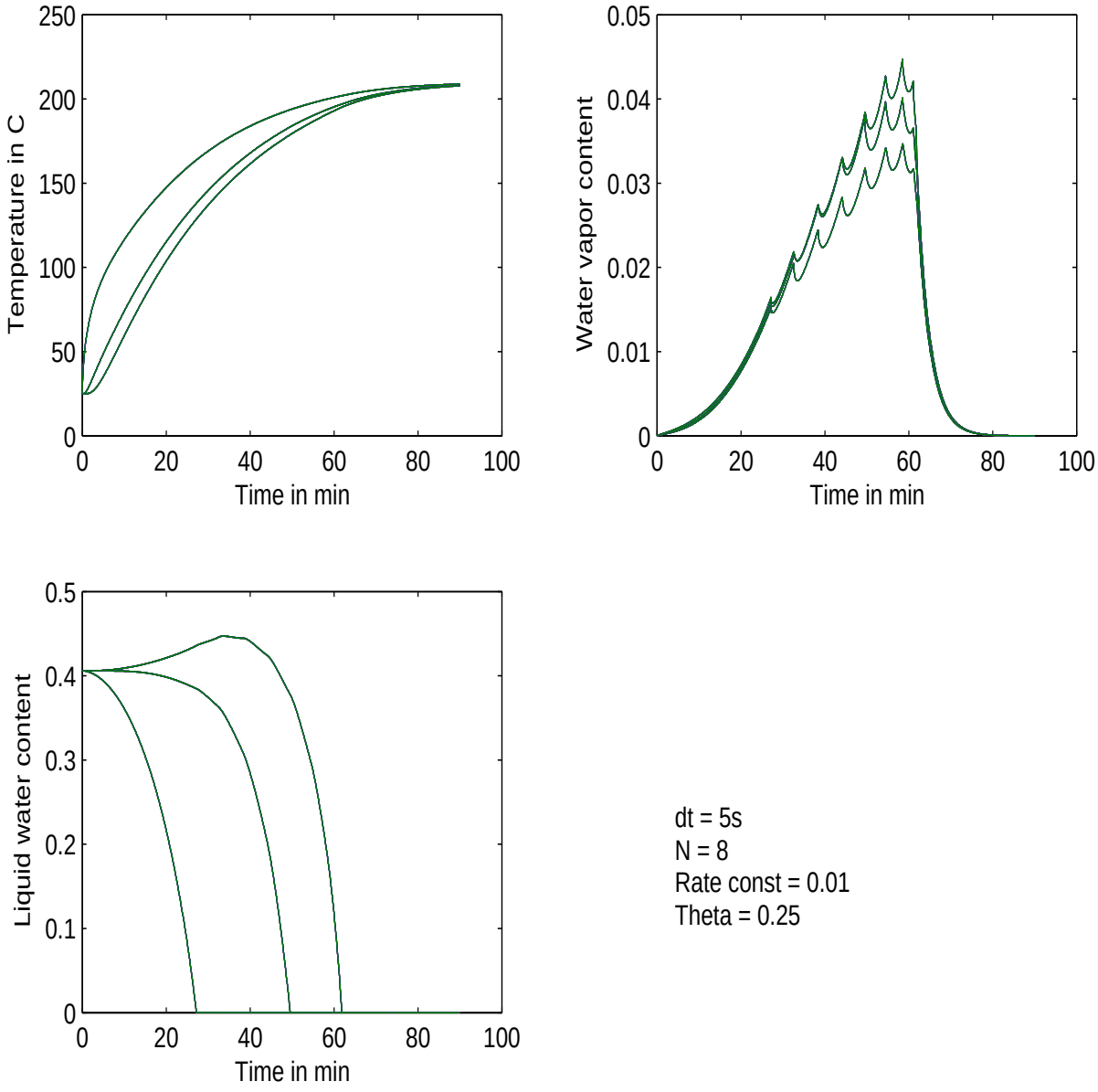

Figure 4.4: New improved results for Temperature and Moisture profiles using relaxation scheme when $\theta = 0.25$. (Surface, halfway to center, center)

Chapter 5

Conclusion

The present study is focussed on the mathematical model for simultaneous heat and mass transfer during bread baking. One dimensional model is taken as suggested by Thorvaldsson and Janestad and from it a two dimensional model is developed to examine the behavior of the problem in a two dimensional environment. Two different numerical schemes, implicit finite difference scheme and finite element scheme are used to implement this mathematical model for baking and an efficient code is written in MATLAB to simulate the model and then to study its behavior. Then the profiles for temperature and moisture distribution during baking are plotted. Some critical values are also calculated to study the performance of the schemes used.

The results of simulations show that the model is very much sensitive towards the time interval rather than spatial interval. It gives satisfactory results only when the size of time interval is of the range Δt= 15 - 90s. When it goes below 15s, the profile becomes non-convergent. The computational experiments with different parameters indicated that the adoption of an updating scheme with the help of tabled values and a set of algebraic equations to handle the phase change during

baking may be one of the reason for this time sensitiveness. So in order to reduce this non-convergent behavior or the time step size sensitiveness of the model, a new procedure is adopted in the methodology to relax the sudden change in vapor and water and thus to allow sometime to complete this phase change process. The results obtained through this new procedure shows that this relaxation procedure almost succeeded in obtaining meaningful results for smaller time intervals.

Within the workable range of the time intervals, the results obtained satisfactorily explain the heat and mass movements during baking to convert raw dough into an eatable, flavored bread. The developed two dimensional model also explains the transfer as similar to that of one dimensional model. The critical values calculated for two dimensional model indicate that it is also sensitive towards the size of the time intervals but shows slightly better behavior. In general the two dimensional model mimics the behavior of the one dimensional model and this fact may help in the study of the model in future, since it is easier and computationally less complex to study one dimensional model.

As it is mentioned the divergent results obtained when $\Delta t < 15s$ may be due to the algebraic conditions applied for simulating evaporation and condensation of water vapor. The satisfactory results obtained using the improved procedure (i.e., when the tabled value is relaxed) indeed points out that these algebraic equations may be a cause. A differential equation in the place of these algebraic inequalities and equations may solve this problem and further new methodology can be adopted to solve these system of equations simultaneously since the actual baking is a simultaneous heat and mass transfer problem.

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Appendix A

Flowchart for the Matlab Code

The mathematical models for baking are implemented numerically using the finite difference and the finite element methods and then they are solved computationally with the help of a code which is written in Matlab. The Matlab code consists of five subprograms which are joined together with the help of a main program. The subprograms are,

1. To evaluate the temperature at $(n+1)^{th}$ time step by solving the heat equation using the values for n^{th} time step.

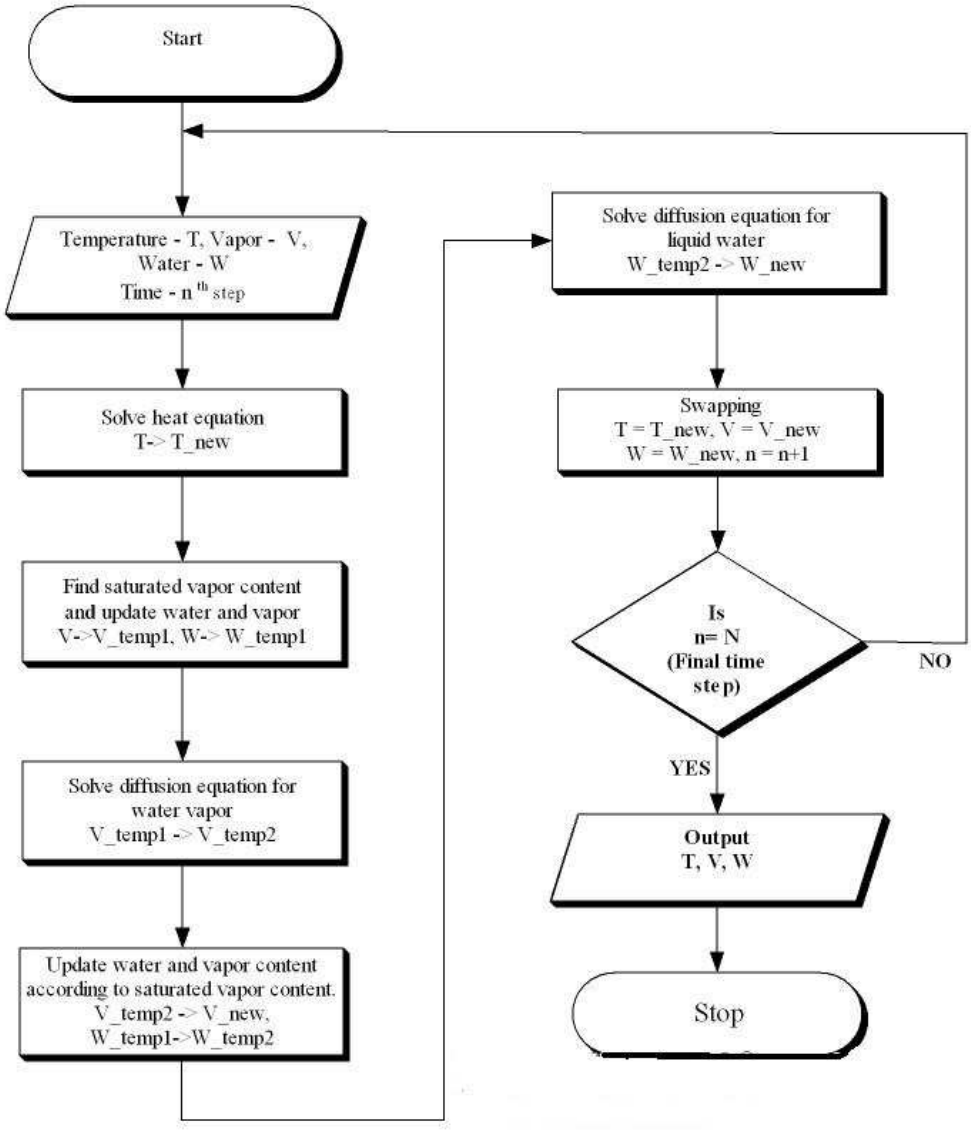
2. To calculate the saturated vapor content for new temperature and then to update the liquid water and vapor content.

3. To evaluate the vapor content after diffusion by solving the diffusion equation for water vapor with updated water vapor content.

4. To update the liquid water and the water vapor content after diffusion using the saturated vapor content and algebraic inequalities

5. To evaluate the liquid water content after diffusion by solving the diffusion equation for liquid water using the updated water content.

Program Flowchart



Appendix B

Matlab Code for One Dimensional Simulation

```
                    %#######################
                       %MAIN PROGRAMME
                    %#######################
close all; clear all;
N=32;       theta=0;   dt=30;  Time=5400;    % N is number of spacial nodes
dx=0.01/N;  M=Time/dt;                       % M is number of temporal nodes
%*********************************
% inputting the initial values
%*********************************
for i=1:1:N+1
    T(i)=25;
    V(i)=0;
    W(i)=0.4061;
    T1(1,i)=T(i);
    V1(1,i)=V(i);
    W1(1,i)=W(i);
```

```
end
%***********************************
% loop for time step starts
%***********************************
for t=1:1:M
    [T_new]=Tnew(T,V,W,N,dt,dx,theta);
    [V_temp,W_temp,V_s,P]=correction(T_new,V,W,N,P) ;
    [V_new]=Vnew(T_new,V_temp,W_temp,dx,dt,N,theta);
    [V_new,W_temp]=Correction2(T_new,V_new,W_temp,V_s,N,P);
    W_new=Wnew(T_new,V_new,W_temp,dx,dt,N,theta);
    T=T_new;
    V=V_new;
    W=W_new;
   for i=1:1:N+1
       T1(t+1,i)=T(i);
       V1(t+1,i)=V(i);
       W1(t+1,i)=W(i);
   end
end
%*****************************************
% writing the output into a file
%*****************************************
fid=fopen('output.m','w');
for t=1:M+1
  for i=1:N+1
      l=(t-1)*dt/60;
      x=(i-1)*dx;
      format short e;
      fprintf(fid,'\n Time(%d,%d)=%e; T(%d,%d)=%e;  V(%d,%d)=%e;  W(%d,%d)=%e; '
```

```
                                ,t,i,l,t,i,T1(t,i),t,i,V1(t,i),t,i,W1(t,i));
  end
  fprintf(fid,'\n');
end
fclose(fid);
%**************************************
%Plotting the graphs
%**************************************
clear all;
output;
figure(1);
subplot(2,2,1)
plot(Time,T)
subplot(2,2,2)
plot(Time,V)
subplot(2,2,3)
plot(Time,W)

                %#####################################
                % Function to calculate New Temperature.
                %#####################################
function [T_new,a] = Tnew(T,V,W,N,dt,dx,theta)
%*********************************
%constants below
%*********************************
k=0.07;                 cp=3500;            lam=2.261*10^(6);       hc=0.5;
sig=5.670*10^(-8);      Dw=1.35*10^(-10);
T_air=210;              T_r=210;            W_air=0;
esp_p=0.9;              esp_r=0.9;
```

```
%*******************************
%        loop starts
%*******************************
a=zeros(N+1,N+1);
for i=2:N
    r=k*dt/((170+284*W(i))*cp*dx*dx);
    a(i,i-1)=-r*(1-theta);
    a(i,i)=1+2*r*(1-theta);
    a(i,i+1)=-r*(1-theta);
    b(i)=r*theta*T(i-1)+(1-2*r*theta)*T(i)+r*theta*T(i+1)
                                    +lam*Dw*dt/(cp*dx*dx)*(W(i+1)-2*W(i)+W(i-1));
end
%*********************************************
%for temp at 1st node where T_f is fictious node
%*********************************************
a1=(12/5.6);              b1= (12/5.6);
a2=1+a1*a1;               b2=1+b1*b1;
F_sp=(2./(pi*a1*b1))*(log(sqrt(a2*b2/(1+a1*a1+b1*b1)))+a1*sqrt(b2)*atan(a1/sqrt(b2))
                          +b1*sqrt(a2)*atan(b1/sqrt(a2))-a1*atan(a1)-b1*atan(b1));
hr=sig*((T_r+273.5)^(2)+(T(1)+273.5)^(2))*((T_r+273.5)+(T(1)+273.5))
                                                        /(1/esp_p+1/esp_r-2+1/F_sp);
hw=1.4*10^(-3)*T(1)+0.27*W(1)-4.0*10^(-4)*T(1)*W(1)-0.77*W(1)^(2);
temp=lam*(170+284*W(1))*Dw*hw;
T_f=T(2)+2*dx/k*(hr*(T_r-T(1))+hc*(T_air-T(1))-temp*(W(1)-W_air));
w_f=W(2)-2*dx*hw*(W(1)-W_air);
r=k*dt/((170+284*W(1))*cp*dx*dx);
a(1,1)=1+2*r*(1-theta)*(1+dx*hr/k+dx*hc/k);
a(1,2)=-2*r*(1-theta);
b(1)=r*theta*T_f+(1-2*r*theta)*T(1)+r*theta*T(2)+lam*Dw*dt/(cp*dx*dx)
```

```
     *(W(2)-2*W(1)+w_f)+r*(1-theta)*2*(dx/k)*(hr*T_r+hc*T_air-temp*(W(1)-W_air));
%************************************
%for Temp at last node
%************************************
T(N+2)=T(N);
r=k*dt/((170+284*W(N+1))*cp*dx*dx);
a(N+1,N)=-2*r*(1-theta);
a(N+1,N+1)=1+2*r*(1-theta);
b(N+1)=r*theta*T(N)+(1-2*r*theta)*T(N+1)+r*theta*T(N)+lam*Dw*dt/(cp*dx*dx)
                                                        *(W(N)-2*W(N+1)+W(N));
%************************************
%solving
%************************************
T_new=a\b';
T_new=T_new';

                    %################################################
                     %Function to correct vapour and water content.
                    %################################################
function [V_temp,W_temp,V_s,P]=correction(T_new,V,W,N)
R=8.314;
%*******************************
% data points for interploation
%*******************************
x=0:2:100;
y=[.611 .705 .813 .934 1.072 1.226 1.401 1.597 1.817 2.062 2.337 2.642 2.983
  3.360 3.779 4.242 4.755 5.319 5.941 6.625 7.377 8.201 9.102 10.087 11.164
  12.34 13.61 15. 16.5 18.14 19.92 21.83 23.9 26.14 28.55 31.15 33.94 36.95
  40.18 43.63 47.33 51.31 55.56 60.11 64.93 70.09 75.58 81.43 87.66 94.28 101.31];
x=[x 105:5:180];
```

```
y=[y 120.82 143.27 169.06 198.53 232.1 270.1 313. 361.2 415.4 475.8 543.1 617.8
    700.5 791.7 892.0 1002.1];
x=[x 190 200 225 250 275 300];
y=[y 1254.4 1553.8 2548 3973 5942 8581];
%************************************************************
% interploation and calculation of saturated amount of vapor
%************************************************************
for i=1:1:N+1
    P(i)=interp1(x,y,T_new(i),'spline')*1000;
    V_s(i)=18.*10^(-3)*P(i)/(R*(T_new(i)+273.5)*(170+281*W(i)))*0.7*3.8;
end
%****************************************
% correction in vapour and water content
%****************************************
for i=1:1:N+1
    if W(i)+V(i)<V_s(i)
        V_temp(i)=W(i)+V(i);
        W_temp(i)=0;
    else
        V_temp(i)=V_s(i);
        W_temp(i)=W(i)+V(i)-V_s(i);
    end
end


                    %###################################
                       % Function to find new Vapour
                    %###################################
function [V_new]=Vnew(T_new,V_temp,W_temp,dx,dt,N,theta)
V_air=0;
```

```
%*********************************
% V at internal points
%*********************************
for i=2:1:N
    r=dt*9.0*10^(-12)*(T_new(i)+273.5)^(2)/(dx*dx);
    a(i,i-1)=-r*(1-theta);
    a(i,i)=1+2*r*(1-theta);
    a(i,i+1)=-r*(1-theta);
    b(i)=r*theta*V_temp(i-1)+(1-2*r*theta)*V_temp(i)+r*theta*V_temp(i+1);
end
%************************
% V at 1st boundary
%************************
temp=2*dx*3.2*10^(9)/((T_new(1)+273.5)^(3));
r=dt*9.0*10^(-12)*(T_new(1)+273.5)^(2)/(dx*dx);
V_f=V_temp(2)-temp*(V_temp(1)-V_air);
a(1,1)=1+r*(1-theta)*(2+temp);
a(1,2)=-2*r*(1-theta);
b(1)=r*theta*V_f+(1-2*r*theta)*V_temp(1)+r*theta*V_temp(2)+temp*r*(1-theta)*V_air;
%************************
%V at last boundary
%************************
V_temp(N+2)=V_temp(N);
r=dt*9.0*10^(-12)*(T_new(N+1)+273.5)^(2)/(dx*dx);
a(N+1,N)=-2*r*(1-theta);
a(N+1,N+1)=1+2*r*(1-theta);
b(N+1)=r*theta*V_temp(N)+(1-2*r*theta)*V_temp(N+1)+r*theta*V_temp(N+2);
```

```
%********************
%solving
%*********************
V_new=a \b';
V_new=V_new';

              %##############################################
              %second correction of vapour and water content.
              %##############################################
function [V_new,W_temp]=Correction2(T_new,V_new,W_temp,V_s,N,P)
R=8.314;
for i=1:1:N+1
    V_s(i)=18.*10^(-3)*P(i)/(R*(T_new(i)+273.5)*(170+281*W(i)))*0.7*3.8;
end
for i=1:1:N+1
    if W_temp(i)+V_new(i)<V_s(i)
        V_new(i)=W_temp(i)+V_new(i);
        W_temp(i)=0;
    else
        W_temp(i)=W_temp(i)+V_new(i)-V_s(i);
        V_new(i)=V_s(i);
    end
end

              %########################################
              %Function to calculate new water content.
              %########################################
function [W_new]=Wnew(T_new,V_new,W_temp,dx,dt,N,theta)
W_air=0;              Dw=1.35*10^(-10);
```

```
%*****************************
%Internal nodes
%*****************************
for i=2:1:N
    r=dt*Dw/(dx*dx);
    a(i,i-1)=-r*(1-theta);
    a(i,i)=1+2*r*(1-theta);
    a(i,i+1)=-r*(1-theta);
    b(i)=r*theta*W_temp(i-1)+(1-2*r*theta)*W_temp(i)+r*theta*W_temp(i+1);
end
%*****************************
% W at 1st boundary
%*****************************
temp=2*dx*(1.4*10^(-3)*T_new(1)+0.27*W_temp(1)-4.0*10^(-4)*T_new(1)*W_temp(1)
                                                    -0.77*W_temp(1)*W_temp(1));
w_f=W_temp(2)-temp*(W_temp(1)-W_air);
r=dt*Dw/(dx*dx);
a(1,1)=1+r*(1-theta)*(2+temp);
a(1,2)=-2*r*(1-theta);
b(1)=r*theta*w_f+(1-2*r*theta)*W_temp(1)+r*theta*W_temp(2)+r*(1-theta)*temp*W_air;
%*****************************
%W at last boundary
%*****************************
W_temp(N+2)=W_temp(N);
r=dt*Dw/(dx*dx);
a(N+1,N)=-2*r*(1-theta);
a(N+1,N+1)=1+2*r*(1-theta);
b(N+1)=r*theta*W_temp(N)+(1-2*r*theta)*W_temp(N+1)+r*theta*W_temp(N+2);
```

```
%***************************
%solving
%***************************
W_new=a\b';
W_new=W_new';
                              %########## END ##########
```

A HEAT AND MASS TRANSFER MODEL FOR BREAD BAKING: AN INVESTIGATION USING NUMERICAL SCHEMES

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