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CLL113 - NUMERICAL METHODS IN CHEMICAL ENGINEERING

TERM PAPER

Numerical Investigation of Time Temperature Profile in Microwave Heating Processes

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Abstract
This research employs advanced computational techniques to analyse the relationship between time and temperature during microwave-assisted heating. Using Runge Kutta Fourth Order method, we simulate temperature distributions considering factors like microwave frequency, power levels, and sample geometry. Validation is achieved through controlled experiments, enhancing the accuracy of our models. The study further explores optimization strategies for efficient and uniform heating. This research significantly contributes to advancing microwave heating technologies, offering both enhanced comprehension and practical guidance for industries seeking improved processes through numerical optimization.

Introduction:

The microwave was first built in the early 1940s. Microwave heating provides better efficiency and, better heating rate and uses volumetric heating which means it is converted into heat within the load. C.J. Budd conducted an experiment to calculate temperature distribution and moisture loss using Lambert's Law and found that end and corner effects were a significant source of error in the model. The prediction of temperature distribution and electric field distribution was studied by P K Loharkar and A Ingle. This paper also explored the use of microwave heating in surface engineering. Xin Gao used the FEM Analysis on COMSOL Multiphysics to solve a numerical model to compute numerical work of coupled electromagnetic and heat transfer equations.

The research work of ***Krishnamoorthy Pitchai*** focused on temperature relation of food particle with the power input of the microwave. It also advocated for the development of feedback control modules for modeling tools to re-work the simulation results for multiple constraints of variables. We have made efforts to develop a running code of C++ to solve the differential equation using fourth order Runge- Kutta Method and also to run a simulation of the same on COMSOLE Multiphysics Software.

2. Nomenclature:

T Temperature, deg C

ω Angular frequency of radiations, rads^{-1}

ρ Density, kgm^{-3}

t Heating time, s

D Electric flux density, Cm^{-2}

E intensity of the electric field, Vm^{-1}

J Electric current density, Am^{-2}

ε'' Dielectric loss factor, dimensionless

σ Electrical conductivity , Sm^{-1}

λ Free space wavelength, cm

B Magnetic flux density, Wm^{-2}

ε' Dielectric constant of the material, dimensionless

ρ Volume charge density, Cm^{-3}

H Intensity of magnetic field, Am^{-1}

C_p Specific heat capacity at constant stress, $\mathrm{Jkg^{-1}\ K^{-1}}$

E_{rms} Root mean square (rms) value of Electric field intensity, $\mathrm{Vm^{-1}}$

ε_0 Permittivity of free space, $8.852 \times 10^{-12}\mathrm{Fm^{-1}}$

Q_{em} Power dissipated or Heat generated per unit volume, $\mathrm{Wm^{-3}}$

Input Parameters used in the COMSOL Simulation:

Parameter	Value
Oven interior dimensions (cm)	$29 \times 28.5 \times 20$
Potato dimension (cm)	$3.6 \times 4.7 \times 2.1$
Placement of potato	Turntable center
Heating time (s)	35
Thermal properties of potato	
Thermal conductivity $(\mathrm{W/mK})$	0.4
Density $(\mathrm{kg/m^3})$	1000
Specific heat $(\mathrm{J/kgK})$	3900
Dielectric properties of potato	
Dielectric constant	50
Dielectric loss	15
Heat transfer coefficient $(\mathrm{W/m^2\ K})$	
All surfaces except bottom	2
Oven air temperature $({}^\circ\mathrm{C})$	25
Initial food and air temperature $({}^\circ\mathrm{C})$	25
Microwave frequency (MHz)	2450
Waveguide dimensions, width $(\mathrm{a}) \times$ height $(\mathrm{b})(\mathrm{cm})$	8×3.5
Microwave excitation $(\mathrm{A/m})$	20

3. Problem Formulation

Microwaves are Electromagnetic waves (EM Waves) that abide by the Maxwell's equations. The Maxwell's equations for constant permittivity and permeability and with no sources can be written as:

$$\nabla \times \mathbf{E} = -j\omega\mu\mathbf{H} \qquad \text{---(3.1)}$$

$$\nabla \times \mathbf{H} = j\omega\epsilon_0\epsilon\mathbf{E} \qquad \text{---(3.2)}$$

$$\nabla \cdot \mathbf{E} = 0 \qquad \text{---(3.3)}$$

$$\nabla \cdot \mathbf{H} = 0 \qquad \text{---(3.4)}$$

The Electric field intensity, E and Magnetic field intensity, H are both defined as time harmonics as:

$$\mathbf{E}(x, y, z, t) = \mathbf{E}_0(x, y, z)e^{j\omega t} \qquad \text{---(3.5)}$$

$$\mathbf{H}(x, y, z, t) = \mathbf{H}_0(x, y, z)e^{j\omega t} \qquad \text{---(3.6)}$$

It needs to be noted that the Tangential component of electric field is continuous at an interface. The walls of the cavity being perfect conductors, this condition must hold. Also, the Field vectors are zero inside a perfect conductor. These govern the following boundary condition.

$$E_{\text{tangential}} = 0$$

We also use the formula for power absorbed per unit volume, P, by dielectric food from microwave which is given by the expression:

$$P(x, y, z, t) = \frac{1}{2}\omega\epsilon_o\epsilon''|\mathbf{E}|^2$$

The expression for Fourier's law of heat conduction for one-dimensional heat conduction is as follows:

$$\dot{Q}_{\text{cond}} = -kA\frac{dT}{dx}$$

Here k is the thermal conductivity of the material, which is a measure of the ability of a material to conduct heat, and dT/dx is the temperature gradient in the material. Although the thermal conductivity of a material varies with temperature, it stays almost constant for temperature changes that are not significant.

If we assume $\boldsymbol{n}$ is the normal of the isothermal surface at point P, then the rate of heat conduction at that point can be expressed by Fourier's law as:

$$\dot{Q}_n = -kA\frac{\partial T}{\partial n}$$

The Heat Conduction Vector $\boldsymbol{Q}_n$ in rectangular cartesian coordinates, can be expressed in terms of its components as

$$\overrightarrow{Q_n} = \dot{Q}_x \vec{\imath} + \dot{Q}_y \vec{\jmath} + \dot{Q}_z \vec{k}$$

where $\vec{\imath}, \vec{\jmath}$, and $\vec{k}$ are the unit vectors in x,y, and z directions, and $\dot{Q}_x, \dot{Q}_y$, and $\dot{Q}_z$ are the magnitudes of the heat transfer rates in the x-, y-, and z-directions, which again can be determined from Fourier's law as

$$\dot{Q}_x = -kA_x \frac{\partial T}{\partial x}, \ \dot{Q}_y = -kA_y \frac{\partial T}{\partial y}, \ \text{and} \ \dot{Q}_z = -kA_z \frac{\partial T}{\partial z}$$

Also, we use A_x, A_y and A_z are heat conduction areas normal to the x-, y-, and z-directions, respectively.

$$\begin{pmatrix} \text{Rate of heat} \\ \text{conduction at} \\ x, y, \text{and } z \end{pmatrix} - \begin{pmatrix} \text{Rate of heat} \\ \text{conduction} \\ \text{at } x + \Delta x, \\ y + \Delta y, \text{and } z + \Delta z \end{pmatrix} + \begin{pmatrix} \text{Rate of heat} \\ \text{generation} \\ \text{inside the} \\ \text{element} \end{pmatrix} = \begin{pmatrix} \text{Rate of change} \\ \text{of the energy} \\ \text{content of} \\ \text{the element} \end{pmatrix}$$

The above expression can be formulated mathematically as shown below. Notations as written in the Nomenclature part have been used.

$$\dot{Q}_x + \dot{Q}_y + \dot{Q}_z - \dot{Q}_{x+\Delta x} - \dot{Q}_{y+\Delta y} - \dot{Q}_{z+\Delta z} + \dot{E}_{\text{gen, clement}} = \frac{\Delta E_{\text{element}}}{\Delta t}$$

Without loss in generality, we assume the control volume as a cuboid with dimensions Δx, $\Delta y \ and \ \Delta z. Thus, the$ volume of the volume element is $V_{\text{element}} = \Delta x \Delta y \Delta z$. The change in the energy content of the element and the rate of heat generation within the element can be expressed as

$$\begin{aligned} \Delta E_{\text{element}} &= E_{t+\Delta t} - E_t = mc(T_{t+\Delta t} - T_t) = \rho c \Delta x \Delta y \Delta z (T_{t+\Delta t} - T_t) \\ \dot{E}_{\text{gen, element}} &= \dot{e}_{\text{gen}} V_{\text{element}} = \dot{e}_{\text{gen}} \Delta x \Delta y \Delta z \end{aligned}$$

Substituting it into Equation given above, we get,

$$\dot{Q}_x + \dot{Q}_y + \dot{Q}_z - \dot{Q}_{x+\Delta x} - \dot{Q}_{y+\Delta y} - \dot{Q}_{z+\Delta z} + \dot{e}_{\text{gen}} \Delta x \Delta y \Delta z = \rho c \Delta x \Delta y \Delta z \frac{T_{t+\Delta t} - T_t}{\Delta t}$$

We divide Equation above by $\Delta x \Delta y \Delta z$ which gives

$$-\frac{1}{\Delta y \Delta z} \frac{\dot{Q}_{x+\Delta x} - \dot{Q}_x}{\Delta x} - \frac{1}{\Delta x \Delta z} \frac{\dot{Q}_{y+\Delta y} - \dot{Q}_y}{\Delta y} - \frac{1}{\Delta x \Delta y} \frac{\dot{Q}_{z+\Delta z} - \dot{Q}_z}{\Delta z} + \dot{e}_{\text{gen}} = \rho c \frac{T_{t+\Delta t} - T_t}{\Delta t}$$

The cross-sectional area bearing heat transfer in x direction is $A_x = \Delta y \Delta z$. Similarly, the heat transfer areas for y and z directions is$A_y = \Delta x \Delta z\ and\ A_z = \Delta x \Delta y\ respectively.$ We take limit as $\Delta x, \Delta y, \Delta z$ and $\Delta t \rightarrow 0$, which gives

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+\dot{e}_{\text{gen}}=\rho c\frac{\partial T}{\partial t}$$

since, from the definition of the derivative and Fourier's law of heat conduction,

$$\lim_{\Delta x\to 0}\frac{1}{\Delta y\Delta z}\frac{\dot{Q}_{x+\Delta x}-\dot{Q}_x}{\Delta x}=\frac{1}{\Delta y\Delta z}\frac{\partial Q_x}{\partial x}=\frac{1}{\Delta y\Delta z}\frac{\partial}{\partial x}\left(-k\Delta y\Delta z\frac{\partial T}{\partial x}\right)=-\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)$$
$$\lim_{\Delta y\to 0}\frac{1}{\Delta x\Delta z}\frac{\dot{Q}_{y+\Delta y}-\dot{Q}_y}{\Delta y}=\frac{1}{\Delta x\Delta z}\frac{\partial Q_y}{\partial y}=\frac{1}{\Delta x\Delta z}\frac{\partial}{\partial y}\left(-k\Delta x\Delta z\frac{\partial T}{\partial y}\right)=-\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)$$
$$\lim_{\Delta z\to 0}\frac{1}{\Delta x\Delta y}\frac{\dot{Q}_{z+\Delta z}-\dot{Q}_z}{\Delta z}=\frac{1}{\Delta x\Delta y}\frac{\partial Q_z}{\partial z}=\frac{1}{\Delta x\Delta y}\frac{\partial}{\partial z}\left(-k\Delta x\Delta y\frac{\partial T}{\partial z}\right)=-\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)$$

This results in the simplified expression as given in Equation below:

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+\dot{e}_{\text{gen}}=\rho c\frac{\partial T}{\partial t}$$

We now implement the definition of second derivative to arrive at Equation given below where $\alpha = k/\rho c$ is the thermal diffusivity of the material. This equation is is known as the Fourier- Biot

$$\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}+\frac{\dot{e}_{\text{gen}}}{k}=\frac{1}{\alpha}\frac{\partial T}{\partial t}$$

equation can also be written in terms of Laplacian operator as follows:

$$\rho C_p\frac{\partial T}{\partial t}=k\nabla^2 T+P_v(x,y,z,t)$$

We have used this form of the Fourier- Biot equation to develop our codes.

4. Numerical Analysis:

In this research study, we have employed the Runge-Kutta Method of 4th order as the numerical approach for solving nonlinear coupled ordinary differential equations described by the final equations (3.1-3.7). The method has been applied to obtain solutions while considering the corresponding boundary conditions (3.8-3.14). Additionally, the differential equations have been transformed into initial value problems to facilitate the numerical solution using the Runge-Kutta Method. This methodology contributes to the robust and accurate numerical analysis undertaken in this study.

Description of Runge Kutta method: -

We favor 4th order Runge-Kutta for its superior accuracy and stability, striking an optimal balance in solving differential equations compared to other orders as in this case the truncation error is of order $O(h^5)$.

Suppose, to approximate the solution to a first-order differential equation given by

$$\frac{dy(t)}{dt} = f(y(t), t), \text{ with } y(t_0) = y_0 \, dt \qquad ..4$$

(starting from some known initial condition, $y(t_0)=y_0$). The development of the Fourth Order Runge-Kutta method closely follows those of the Second Order, and will not be covered in detail here. As with the second-order technique, there are many variations of the fourth-order method, and they all use four approximations of the slope. We will use the following slope approximations to estimate the slope at some time *t0* (assuming we only have an approximation to $y(t_0)$ (which we call $y^*(t_0)$).

$$K_1 = f(y^*(t_0), t_0) \qquad ...4.1$$

$$K_2 = f\left(y^*(t_0) + k_1 + \frac{h}{2}, t_0 + \frac{h}{2}\right) \qquad ...4.2$$

$$K_3 = f\left(y^*(t_0) + k_2 + \frac{h}{2}, t_0 + \frac{h}{2}\right) \qquad ...4.3$$

$$K_4 = f\left(y^*(t_0) + k_3 + \frac{h}{2}, t_0 + \frac{h}{2}\right) \qquad ...4.4$$

Each of these slope estimates can be described verbally.

k_1 is the slope at the beginning of the time step (this is the same as k_1 in the first and second order methods).

If we use the slope k_1 to step halfway through the time step, then k_2 is an estimate of the slope at the midpoint. This is the same as the slope, k_2, from the second order midpoint method. This slope proved to be more accurate than k_1 for making new approximations for y(t).

If we use the slope k_2 to step halfway through the time step, then k_3 is another estimate of the slope at the midpoint.

Finally, we use the slope, k_3, to step all the way across the time step (t_0+h), and k_4 is an estimate of the slope at the endpoint.

We then use a weighted sum of these slopes to get our final estimate of $y^*(t_0+h)$

$$y^*(t_0+h) = y^*(t_0) + \frac{\frac{1}{6}k1+\frac{1}{3}k2+2k3+k4}{6}\, h \qquad \text{...4.5}$$

$$y^*(t_0) + \left(\frac{1}{6}k1 + \frac{1}{3}k2 + \frac{1}{3}k3 + \frac{1}{6}k4\right)h \qquad \text{...4.6}$$

$= y^*(t_0) + mh$ where m is a weighted average slope approximation.

We have implemented this method in solving this problem using C++.Our code consists of four major function one main driver function, one for calculating the electric field ($E_{(x,y,z,t)}$), one for calculating the power($P_{(x,y,z,t)}$) and one for solving the differential equation in which we used R.k method of 4^{th} order to convert the ordinary differential equation to an initial value problem. We have assumed step size to be small (h = 0.1) in order to get more precise result.All the computational data are fed into the main function in the form of vectors, from there other three functions were called.

The initial conditions that we had taken is that, at t = 0s the temperature of the material is 25℃.

Our code outputs the following things:-

a. What is the approximate temperature of a substance at any given time.
b. How temperature is changing with time at any given(x,y,z).

Results and Discussions:

The results that we obtained via solving the differential equation using various step sizes of h are C++:-

Figure 1:

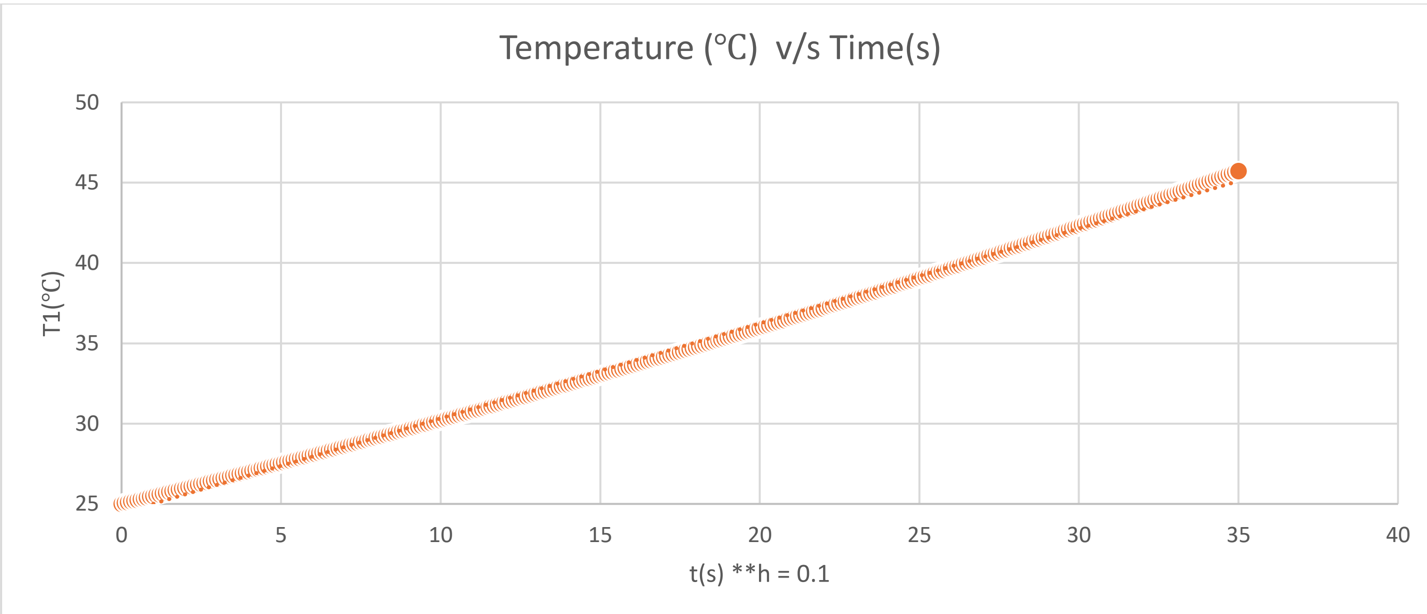


Figure 2:

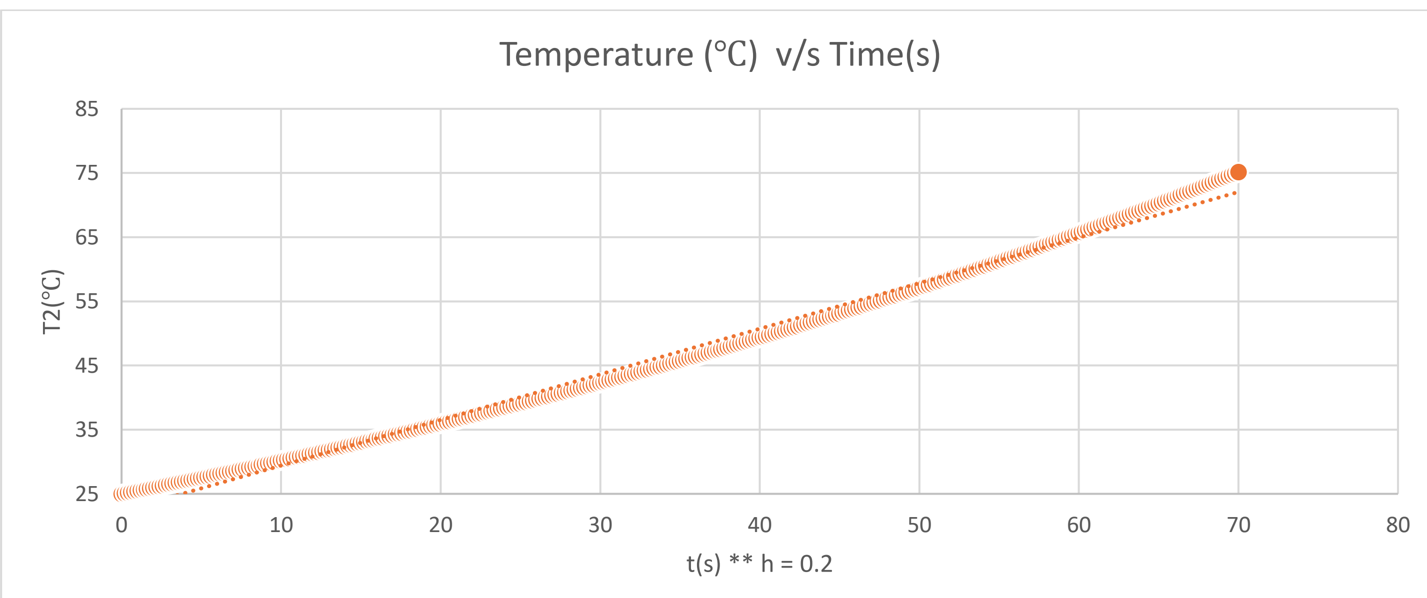
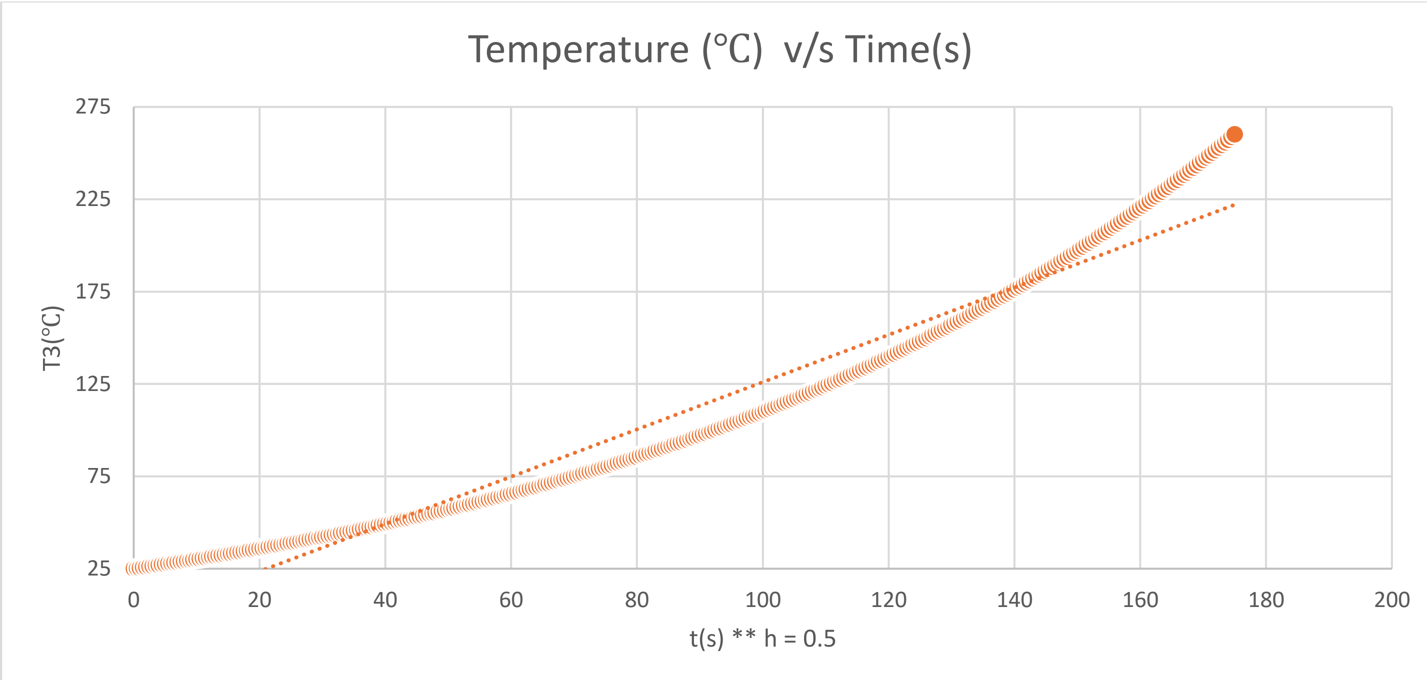


Figure 3:



The results that we obtained via simulating the electromagnetic heating:-

We have used COMSOL Multiphysics 5.5 to simulate the electric field, temperature variation with time respectively.

In the study mode of model wizard, we used frequency transient one way electromagnetic heating sequence then we generated the geometry of the microwave oven along with the material selection. After checking the boundary conditions ,port properties and building mesh we generated all the results. The results were generated in the form of plots for eg . electric field intensity with z direction.

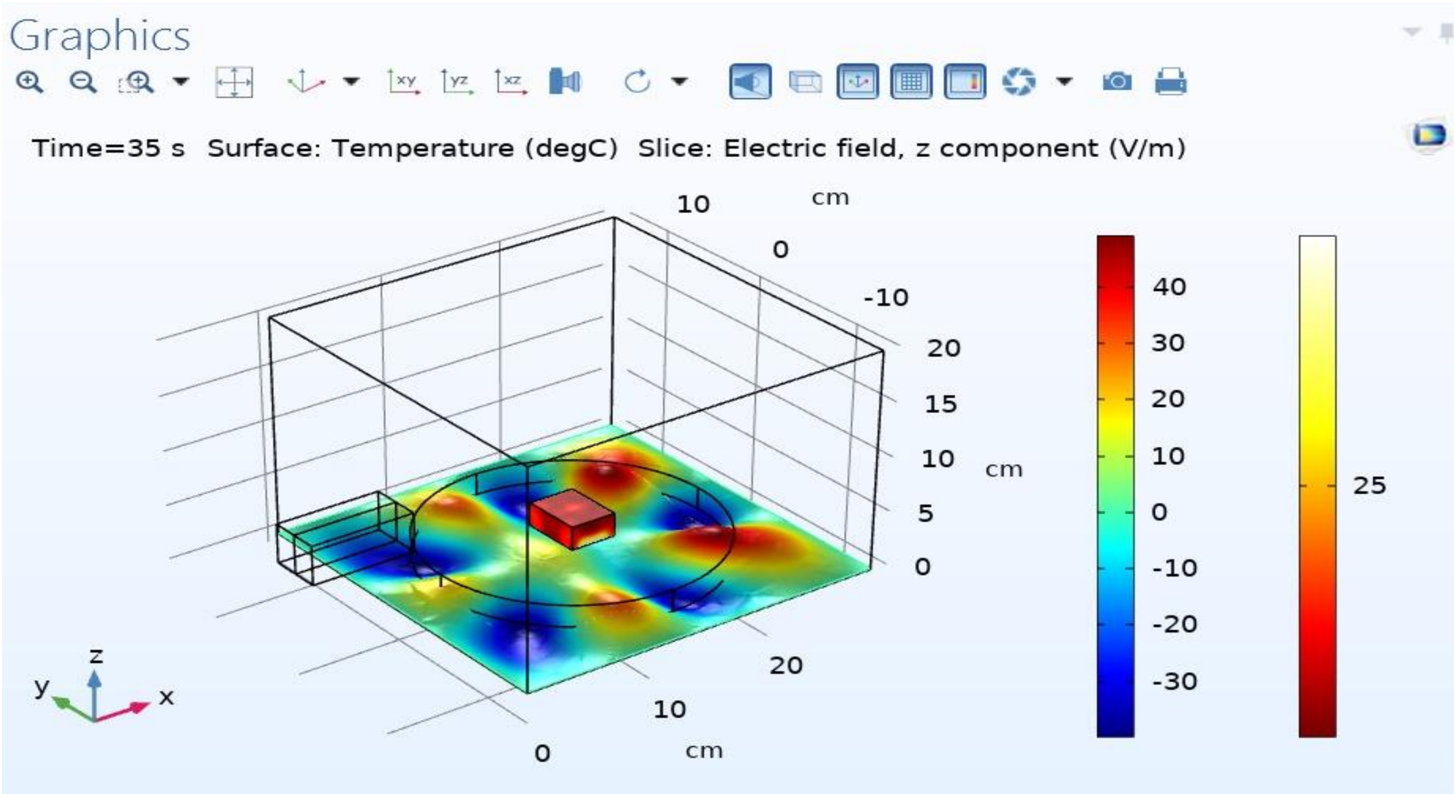


Fig.4 :- Surface Temperature Modelling.

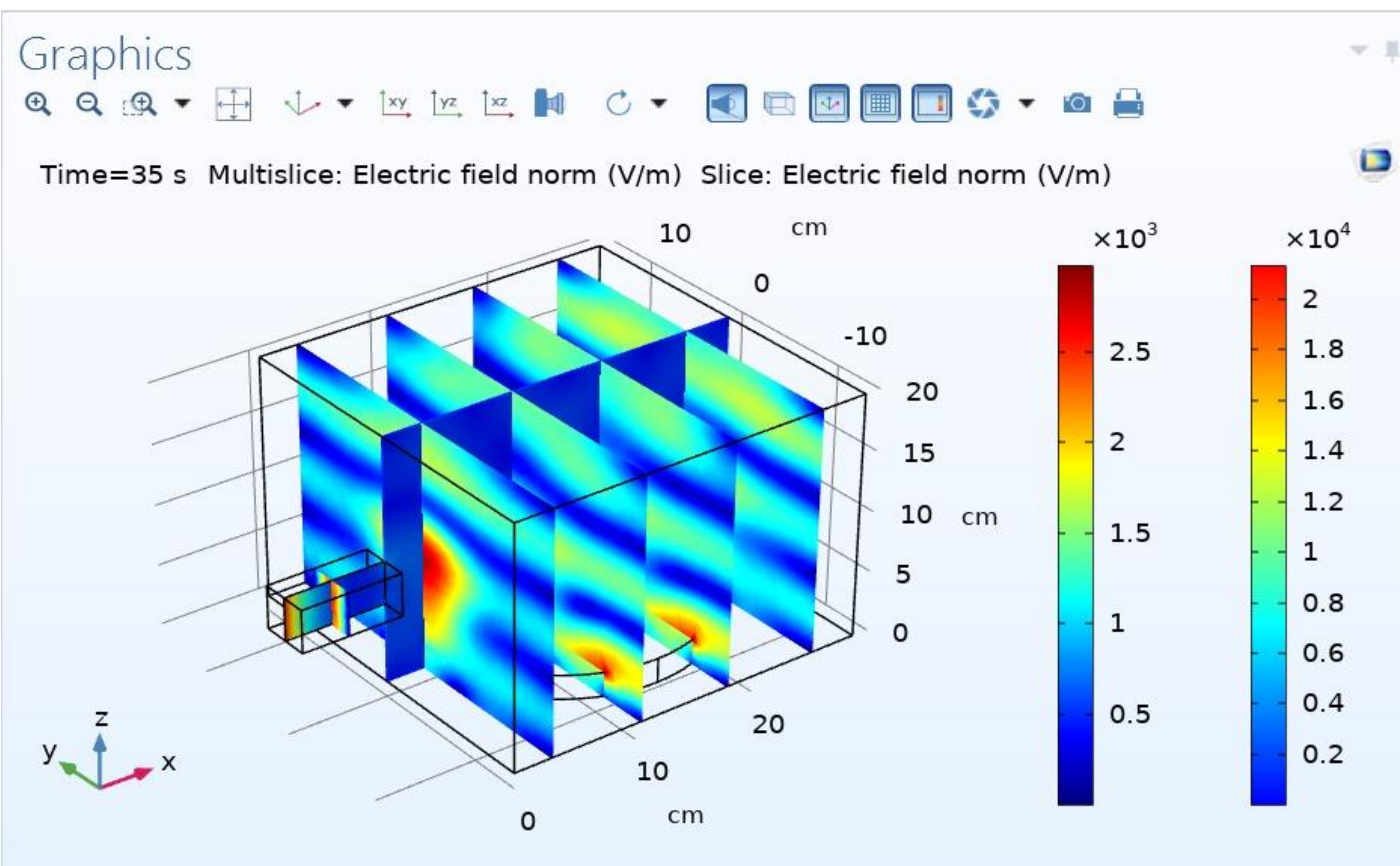


Fig.5:- Electric Field Intensity

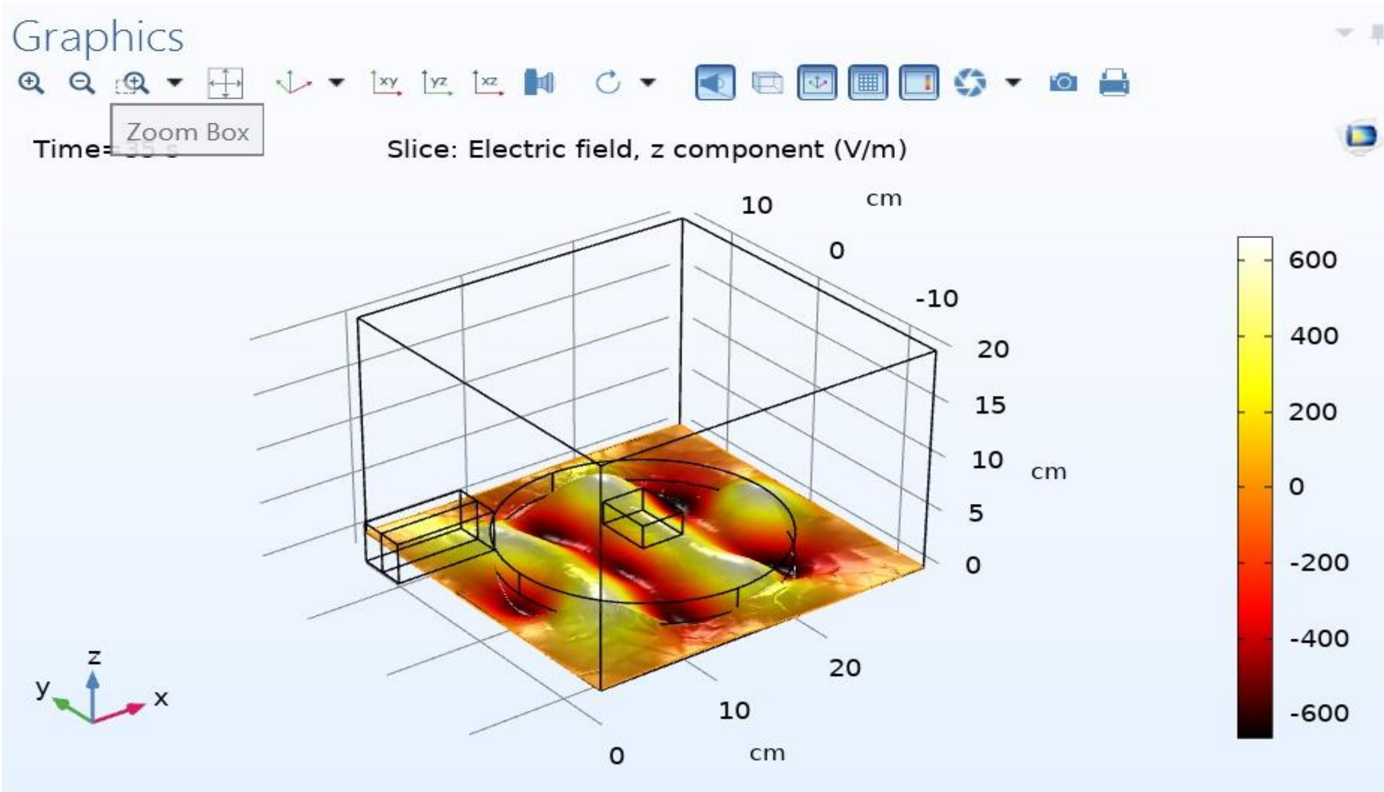


Fig.6:- Magnitude of Electric field in z direction.

As we know that, electric field generated by the magnetron is trapped between the metal boundary plates stationary waves which has nodes and antinodes at different point and spaces which is justified by crest and trough in the above mentioned graph. Crest shows high electric field intensity in the region which implies high energy transfer to the water molecule and vice versa.

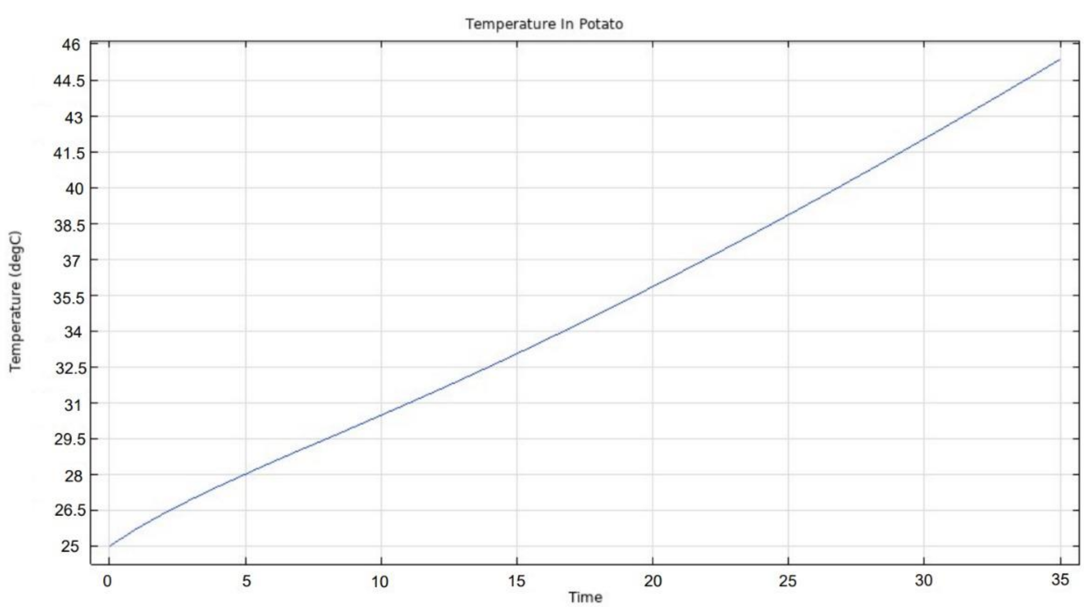


Fig.7:- Plot obtained via simulation.

6. Path Forward

After working out the paper and formulating the graphs we began to think what else could be done to increase the value and applicability of the research. We noticed that the paper originally does not include the effect of heat loss via walls of microwave and turntable rotation. This effect has to be considered if we are studying the model. Since this model has an application in many fields like temperature prediction, we cannot ignore it.

$$-k \cdot \partial T / \partial n = h \cdot (T_{microwave} - T_{\mathrm{atmp}})$$

$$\rho Cp(w\partial T/\partial z + u\partial T/\partial r) = [\partial(\kappa\partial T/\partial z)/\partial z + \partial(\kappa\partial T/\partial r)/\partial r + \kappa/r\partial T/\partial r] - \partial(qr)/\partial z$$
$$+\mu[4/3(dw/dr)^2+(dv/dr)^2+(du/dz)^2+(dw/dr)^2$$
$$+1/r^2(dv/dz)^2+2u^2/r-\tfrac{2}{3}(du/dz)(dw/dr)+4/3\ (du/dr)^2]$$

Due to complexities offered by this equation, we were not able to design a working code in the given amount of time. This equation could have been used instead of the simplified equation of the original paper. The results obtained by similar experiments would have been more accurate.

7. Conclusion

For the simulation process We have used a hypothetical substance which has almost similar density and specific heat capacity as potato. We assumed the shape of this hypothetical substance as a cuboid. We have here assumed the electric field vector to be changing in the z direction due to changes in y coordinate. The magnetic field vector has a negligible value in comparison to the Electric Field Vector and therefore has been neglected. There is no turntable rotation considered in our simulation testing. Applied the boundary conditions on the object such as Electric field diminishes to zero at the metal boundary plates which are the boundary surface of our simulation microwave.

The developed C++ code majorly consists of four functions for evaluating the parameters Electric Field using Equation given above, Power consumed by the microwave, a function for solving the Differential equation using the Fourth order Runge Kutta Method {RK-4} which delivers an error of 5th order.

8. Self Assessment

Level-2

Working on this term paper turned out to be a valuable learning experience for our team. During our research we paid close attention to choosing a topic of research such that we had the basic knowledge of the applied numerical method and the physics and mathematics used. Our selected topic on Microwave heating ensured that we had the basic knowledge such as our core courses as Transport Phenomena (CLL110) and Material and Energy Balances (CLL111).

To make our research papers more authentic, we have simulated our model on **COMSOL Multiphysics 5.5** (A totally new software) and have achieved some original and ground-breaking work. We have developed the codes on **C++**. The codes developed are all working. The results obtained are exactly in accordance with the results of the original paper. ***The Runga- Kutta Method of 4th order*** was utilized for this equation. The exact boundary conditions have been applied and original results have been achieved. The differential equation upon solution gave the relation between Surface temperature of the particle with reference to coordinates and Power Supplied by the microwave.

9.References

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