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Additional Information

Non-steady state heat transport: a practical case of a microscopic energy balance in a vegetable

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Abstract

In this paper, the analytical and numerical solutions of a non-steady state mathematical model are developed and analyzed. The mathematical model development of a non-steady state heat transport for a one-dimensional system is shown, and the analytical solution of the model is presented. The numerical solution of the model, using the finite element method, is compared to its analytical solution, proving its consistency. One of the advantages of using numerical tools is that more complex solutions can be obtained, even if the corresponding analytical solution does not exist or is not known, which is useful for engineering students. To demonstrate the applications and possibilities of this work, it is shown that changing the boundary conditions, geometry, or dimension in the system and the mathematical model, it can be solved through a numerical solutions. The paper shows that it is possible to use the finite element method in a university teaching context to complementarily explain the underlying physical phenomena of an engineering problem, here applied to a heat transfer problem in a vegetable.

Keywords: heat transfer, FEM, modelling, methodologies for learning

1. Introduction

The study of heat transfer problems is a research area that has gained importance as it plays a fundamental role in sustainability and environmental care. The application fields of this physics branch are related to both science and engineering, including medicine [1], automotive, thermal management of electronic devices and systems [2], design of refrigeration and air conditioning systems [3], water heating or food preservation [4], and domestic [5] and industrial applications.

When two systems at different temperatures are in contact, there is a heat transfer process until a thermal equilibrium is achieved between them. This transfer process would also occur if one of them was in contact with a third, as stated in the zeroth law of thermodynamics [6]. There are three mechanisms of heat transfer: conduction, convection, and radiation. We are going to study conduction (contact heat transfer without matter transfer) and convection (heat transfer by the transfer of the heat-carrying matter itself). These two mechanisms can be studied in both steady state and nonsteady state. For the steady state, the energetic content of the system remains constant over time as the temperature does, while for the non-stady state, the variation of the energetic content in time must be considered because the temperature changes.

The physical laws describing the property transport mechanisms are simple and easily understandable, but the analytical description is complex. In general, transport phenomena are all those processes in which there is a net transfer or transport of matter, energy, or linear momentum in macroscopic or microscopic quantities.

It is essential to present the phenomenon of heat transfer by exposing the corresponding physical law through the mathematical expression of heat transfer and its analytical resolution, but also offering a numerical resolution [7]. The complexity of the analytical solution of the mathematical expression depends on the number of spatial dimensions considered, the form of the governing equation obtained from the calorific energy balance in the system, and the initial and boundary conditions established. Whether or not there is an analytical solution to the mathematical model, it is possible to solve it numerically by applying simulation methods and tools that make it possible to visualize the evolution of the temperature in the system.

Providing students with all these tools allows them to extrapolate their knowledge to other areas with similar equations, such as the diffusion of a solute in a solvent. Moreover, in this way, they work on computational skills at the same time.

This approach is intended for undergraduate engineering students. It is important that students of engineering degrees more related to the biological part perceive physics as a mundane and useful subject, beyond the mechanical part. Thus, the study case presented considers the problem of heating a vegetable slice for its preservation and subsequent use.

In terms of paper structure, the mathematical model is first explained and detailed. It starts with the theoretical foundations and their simplification for the case of study. Then, the analytical solution for the proposed case study is calculated and the computational model to obtain a numerical solution is developed and validated. The details of the model are based on the formulated theory. Finally, to analyze the importance of different controllable parameters in the solution of the problem, different solutions for changing temperature and thickness are shown.

2. Theory

In this section, the transient heat conduction model is developed from the energy balance for a one-dimensional case considering that the system behaves as an infinite sheet. The situation for the bi- and tri-dimensional case can be solved by applying the superposition principle.

2.1 General equation of heat conduction

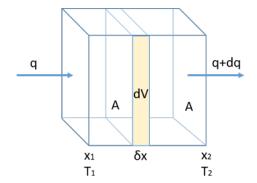


Figure 1. Scheme to obtain heat balance, where A is the area and dV is the differential volume of the sample. The specific heat flux is represented by q.

Applying the general equation of the property balance in the differential element considered (Input + Generation = Output + Accumulation), the governing equation obtained from the energy balance (1) is:

$$q_{x+\delta x} - q_x + \frac{\partial \left(\rho C_p T dV\right)}{\partial t} = g dV \tag{1}$$

If no heat is generated (g = 0) then

$$dq_x + \frac{\partial \left(\rho C_p T dV\right)}{\partial t} = 0 \tag{2}$$

For one-dimensional heat transfer conduction in the x direction, the temperature of each point depends on both the time and its position so it can be expressed as T(x, t) as in equation (3), and it is possible to apply the Fourier's law in one dimension [8],

$$q_x = -kA\frac{\partial T}{\partial x} \tag{3}$$

Considering that $dV = A\delta x$, and applying the Fourier's Law in equation (2), it remains,

$$\alpha \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t} \tag{4}$$

where α is the thermal diffusivity of the sample [9] ($\alpha = \frac{k}{\rho C_p}$).

To conclude the formulation of the mathematical model and solve equation (4) analytically, initial and boundary conditions must be established accounting for some considerations such as:

1. Temperature T_0 is initially uniform throughout the system.

$$\mathbf{t} = \mathbf{0} \land \forall \mathbf{x} \to T(\mathbf{x}, \mathbf{0}) = T_0 \tag{5}$$

2. The conduction heat flux that arrives at the surface of the system is interchanged by convection with the fluid around the system (figure 2).

$$t > 0 \rightarrow -k \frac{\partial T(L,t)}{\partial x} = h[T(L,t) - T_{\infty}]$$
 (6a)

or
$$T(L,t) = T_{\infty}$$
, (6b)

3.if h is very high, i.e., when external resistance to heat transfer is negligible, there is a symmetrical distribution of temperature in the system with respect to the central axis (figure 2).

$$t > 0 \rightarrow \frac{\partial T(0,t)}{\partial x} = 0$$
 (7)

- 4. The temperature surrounding the system (T_{∞}) does not change with time.
- 5. The physical properties remain constant throughout the process.
- 6. The system material is not shrinking.

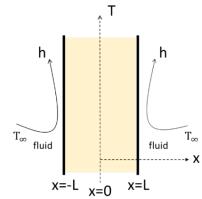


Figure 2. Transversal section of the system; h is the convective heat transfer coefficient.

2.2. Analytical solution

By making the following variable change,

$$\psi(x,t) = \frac{T(x,t) - T_{\infty}}{T_o - T_{\infty}}$$
(8)

the mathematical model (equations 4, 5, 6, 7) result in:

$$\alpha \frac{\partial^2 \psi}{\partial x^2} = \frac{\partial \psi}{\partial t} \tag{9}$$

$$\psi(x,0) = 1 \tag{10}$$

$$-k\frac{\partial\psi(L,t)}{\partial x} = h\,\psi(L,t) \tag{11}$$

$$\frac{\partial \psi(0,t)}{\partial x} = 0 \tag{12}$$

This model meets the conditions for applying the method of separation of variables (all the equations, except one, are homogeneous and of constant coefficients),

$$\psi(x,t) = F(x)G(t) \tag{13}$$

resulting:

$$\frac{1}{F(x)}\frac{d^2F(x)}{dx^2} = \frac{1}{G(t)}\frac{dG(t)}{dt} = -\omega^2$$
(14)

The equation G(t) is a first order equation and F(x) is a second order, so by integrating them, it results:

$$\begin{cases} G(t) = C_1 e^{-\alpha \omega^2 t} \\ F(x) = C_2 \sin(\omega x) + C_3 \cos(\omega x) \end{cases}$$
(15)

Now, substituting equation (15) into equation (13), results in:

$$\psi(x,t) = e^{-\alpha\omega^2 t} [A\sin(\omega x) + B\cos(\omega x)] \quad (16)$$

where A and B are integration constants obtained from the boundary conditions.

Imposing the boundary condition of symmetry (equation 7) on equation (16) we get,

$$\frac{\partial \psi(0,t)}{\partial x} = \left\{ e^{-\alpha \omega^2 t} [A\omega \cos(\omega x) - B\omega \sin(\omega x)] \right\}_{x=0} = 0$$
(17)

Then, it is obtained A = 0 and equation (16) is rewritten as:

$$\psi(x,t) = e^{-\alpha \omega^2 t} [B\cos(\omega x)]$$
(18)

Imposing the boundary condition represented in equation (6a) or (6b) on equation (18), results in:

$$\frac{\partial \psi(L,t)}{\partial x} = \left\{ e^{-\alpha \omega^2 t} [-B\omega \sin(\omega x)] \right\}_{x=L}$$
(19a)
$$= -\frac{h}{k} e^{-\alpha \omega^2 t} [B\cos(\omega L)]$$

$$or \psi(L,t) = e^{-\alpha \omega^2 t} [B \cos(\omega x)] = 0,$$
(19b)

if h is very high:

$$tan(\omega L) = \frac{hL}{k\omega L} = \frac{N_{Bi}}{\omega L},$$

$$being N_{Bi} \ the \ Biot \ number = \frac{hL}{k}$$
(20a)

$$or \ cos(\omega L) = 0 \tag{20b}$$

The eigenvalues ω_n are the positive roots of the equation (20a)

$$\omega_n L = f(N_{Bi})$$
 with $n = 1, 2, ...$ (21)

or of the equation 20b if h is very high,

$$\omega_n L = (2n-1)\frac{\pi}{2}$$
 with $n = 1, 2, ...$

Therefore, the function $\psi(x, t)$ will be a lineal combination of all possible solutions:

$$\psi(x,t) = \sum_{n=1}^{\infty} B_n e^{-\alpha \omega_n^2 t} \cos(\omega_n x)$$
(22)

To solve the coefficients B_n the initial condition is applied,

$$\psi(x,0) = \sum_{n=1}^{\infty} B_n \cos(\omega_n x) = 1$$
(23)

And, by orthogonality of eigenfunctions:

$$\int_{0}^{L} \cos(\omega_{n}x) \cos(\omega_{m}x) dx =$$

$$= \begin{cases} 0 \text{ if } n \neq m \\ \frac{L}{2} + \frac{1}{4\omega_{n}} \sin(2\omega_{n}L) \text{ if } n = m \end{cases}$$
(24)

At this point, introducing the $cos(\omega_n x)$ on both sides of equation (23) and integrating, equation (25) is obtained.

$$B_n\left(\frac{L}{2} + \frac{1}{4\omega_n}\sin(2\omega_n L)\right) = \frac{1}{\omega_n}\sin(\omega_n L)$$
(25)

Then:

$$B_n = \frac{2 \sin(\omega_n L)}{\omega_n L + \sin(\omega_n L) \cos(\omega_n L)}$$
(26)

where the eigenvalues ω_n are the positive roots of the transcendent equation (20), being

$$B_n = \frac{2(-1)^{n-1}}{\omega_n L}$$
(27)

when h is very high.

The resulting equation is

$$\psi(x,t)$$
(28a)
= $2\sum_{n=1}^{\infty} \frac{\sin(\omega_n L)}{\omega_n L + \sin(\omega_n L) \cos(\omega_n L)} e^{-\alpha \omega_n^2 t} \cos (\omega_n x)$

with ω_n such that $tan(\omega_n L) = \frac{N_{Bi}}{\omega_n L}$, or

$$\psi(x,t) = 2\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{\omega_n L} e^{-\alpha \omega_n^2 t} \cos (\omega_n x)$$
(28b)

with $\omega_n L = (2n - 1)\frac{\pi}{2}$, when h is very high.

3. Modelling

One of the most widely used methods to perform simulations is the Finite Element Method (FEM). It is a flexible method that can be used in multiple areas of science and engineering [10-14]. Through the FEM, it is possible to generate numerical solutions to problems of different complexity. To do this, it is necessary to know the initial and boundary conditions of the problem to be solved. The commercial software COMSOL Multiphysics [15] allows applying the FEM, working with problems of various dimensions and degrees of freedom. In order to simulate a non-steady state heat problem, the geometry (1D, 2D or 3D) must first be defined. In order to reduce the degrees of freedom, and therefore the computational cost, it is important to start with simple problem approaches that allow to obtain valid solutions. Once the geometry of the problem is defined, by selecting the module - in this case the one containing the heat equation -, the physical conditions of the problem are defined.

COMSOL Multiphysics has several modules that allow solving heat transport problems. One of the available options is to use the specific heat transport module. This module can be used to solve many types of problems with various boundary conditions. In our case, since this is a simple problem, the mathematical module can be used directly. In the mathematical module, classical partial differential equations (PDEs) can be added. In this case, the equation to be solved (for 1D case for example) is:

$$d_a \frac{\partial T}{\partial t} + \nabla \cdot (-c \nabla T) = f; \quad \nabla = \frac{\partial}{\partial x} \quad (i)$$

Where $d_a = \rho \cdot c_p$ and $c = k = d_a \cdot \alpha$. To solve the governing equation (9); the conditions that we must introduce are: $d_a = 1$; f = 0. Therefore, $k = \alpha$.

Once the physical module to be used has been defined, boundary and initial conditions have to be specified. In the case of the one-dimensional system, an initial temperature $T = T_0$ is set on the whole line defining the sheet. The boundary conditions defined at the two ends of the line are as follows:

- At the point in contact with the fluid, a Dirichlet condition is used with a temperature $T = T_{\infty}$.

- At the other end, a zero flow condition is used.

Once the physics of the problem is configured, the size and typology of the mesh is selected. The mesh generates a finite number of points called nodes where the equations with partial derivatives will be solved to obtain the numerical solution of the problem. In the 1D case, the mesh consists of a number of points. When the problems become twodimensional, different geometries can be used, such as triangular geometry. The number of nodes to solve has to fulfill certain conditions for the solution to be convergent and robust; it needs a minimum number of elements limiting the maximum element size. In the case of the one-dimensional system, there are uniformly distributed points every 30 µm. In the two-dimensional case, a triangular type mesh is used. There is a maximum element size of 125 µm and a minimum element size of 0.25 µm. This results in an element size of 1600 elements. These sizes are enough to avoid any error-causing numerical dispersion. In the end, it is a compromise between the number of points and the computational cost (the higher the number of points, the higher the computational cost). Once the mesh type and the number of elements has been stablished, the solver is defined. The solver of choice is MUMPS. This solver is of the direct type and has a high memory consumption but is very robust. COMSOL allows the use of other solvers (direct and indirect) with less memory consumption. For non-steady state problems, a temporary solver is used. Therefore, the time range as well as the time steps must be configured. In the case of the proposed problem, time solutions between 0 and 5 seconds have been calculated in steps of 50 ms. It is important to define a proper time step to avoid excessively increasing the computational cost and, at the same time, obtaining a good time solution that allows to see and understand the physics of the problem.

4. Food conservation: Practical application.

In the food industry, the importance of thermal treatment of food, both heating and cooling, is trivial ([3], [4], [16]). For the design of such processes, the optimisation of their operation, or the layout and sizing of the related equipment, it is essential to know the mechanisms of heat and matter transfer that take place ([1], [2], [3], [9]). Simulating processes or equipment operation mathematically is a powerful tool for their design and optimisation. This requires knowledge on the development of mathematical models applying general and particular laws of energy and matter. It is also necessary to use calculation tools for solving the mathematical models and, consequently, simulating the processes ([10], [12], [17], [18]). All this is necessary for students to comprehend the heat transfer phenomenon for food preservation and how it is distributed through the food, even if it is a homogeneous food. Furthermore, the approach presented offers a way for them to visualise it and to see how the different parameters affect the heat transfer phenomenon, which can be helpful in the first courses of the degree.

An excellent example of non-steady state heat transfer is a practical case for food preservation, as we mentioned before. Thus, we raise the following issue: Let us consider that we want to produce slices of a vegetable to be used in salads. In this particular case, we will choose carrots in order to assign a numerical value to the characteristic parameters of the material. The manufacturing procedure consists of immersing the slices in a solution of different compounds and at 25°C to prevent vegetable browning.

In addition, the slices must be kept at a temperature of 1°C. For this reason, after the previous treatment, they are placed in another bath with other preservatives at a temperature of 1°C. The slices will remain in this second bath until all its points reach a temperature less than or equal to the desired temperature (1°C); therefore, we will have to determine how long they have to be.

We will consider that the slices are cylindrical in shape with a diameter of 2.5 cm and a thickness (2L) of 1.5 mm; the thermal diffusivity (α) of the carrot is 0.002 cm²/s [16]; the convective heat transfer coefficient is very high (i.e., the external resistance to convective heat transfer is negligible).

4.1 Analytic Solution

Since the diameter of the slice is much greater than its thickness, the heat that the slice exchanges with the water through its peripheral surface could be neglected with respect to the heat that it exchanges through its other surfaces. Therefore, the problem is simplified to a heat transfer in a single direction. Because of this high convective heat transfer coefficient (h) and, therefore, a high value of N_{Bi} , equation (28b) was used.

The objective is to determine the time required for the center of the carrot slice to reach 1°C:

$$t/\psi(0,t) = \frac{\mathbf{1} - (-\mathbf{1})}{\mathbf{25} - (-\mathbf{1})} = 2\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{\omega_n L} e^{-\alpha \omega^2 t}$$
(29)

The time required for the center of the carrot slice to reach 1°C is obtained by iterating equation (29). To determine an initial value of t, it was assumed that considering only the first term would be sufficient:

$$\frac{1}{13} = \frac{4}{\pi} e^{-0.002 \left(\frac{\pi}{0.15}\right)^2} t$$
$$t = 3.2s$$

As the Fourier number to the calculated time ($Fo = \frac{\alpha t}{L^2} = 1.138$) is higher than 0.2 [1], the error produced by considering the first term of the series and disregarding all the others is less than 2%, a margin that is more than valid for making the calculations. Therefore, the result will be:

t = 3.2s

4.2 Numerical Solution and modelling

First, given the type of problem, a one-dimensional system is proposed to obtain the solution initially. As explained in section 3, it is first necessary to define the geometry of the problem. In this case, it is a line of length half the thickness of the carrot. The next step is to define the physics of the problem. Using the heat module, the initial and boundary conditions must be set. In this sense, the initial condition for all points on the initial temperature line is the proposed one (25°C). The boundary conditions are defined as follows: the heat equation must be configured with a diffusion coefficient of $2 \cdot 10^{-7}$ W/(m·K); symmetry at the 0 coordinate of the line that acts as the center of the carrot; and, the Dirichlet condition at the other end of the straight line that behaves as a fixed temperature value is, in this case, -1°C. Regarding the meshing, a number of equidistant nodes detached along the 25 µm line are selected. results were shown in figure 3. The convergence graph of the solution as a function of the time steps is shown in figures (3i).

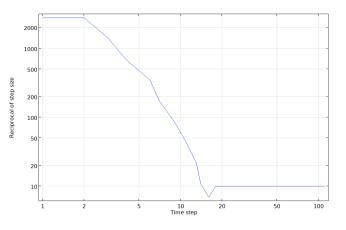


Figure 3i. Convergence plot of the one-dimensional numerical solution as a function of time steps.

Figure 3 shows the solution to the first one-dimensional model. In this case, the temperature is shown as a function of time, and it can be stated that the solution is consistent in obtaining the value of t = 3.2 seconds to achieve the target temperature. Thus, the analytical and numerical results are in agreement and therefore the model is validated.

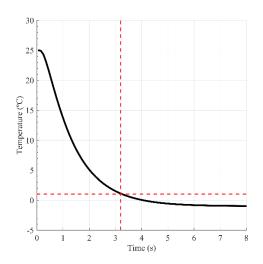


Figure 3. Numerical solution for 1D FEM model T(t).

The model was obtained by performing energy balance in a controlled volume, applying Fourier's particular law, and making the corresponding simplifications and assumptions. In addition, a logical value for the thermal diffusivity parameter was determined from experience and the literature. The objective was to develop, in a reasoned way, the mathematical model, to apply the mathematical knowledge and the tools to solve it analytically and numerically to compare both results. Based on the literature and experience, the derived model reliably explains what happens in reality [16]. The aim is not to develop an innovative model or a model for a specific food but to describe the methodology to create the model and use methods and tools to solve it. The aim is for the student to

compare and visualise the most significant parameters in the model and the process.

One of the advantages of FEM is that the degrees of freedom can be increased easily. The solution for a two-dimensional model is shown below (Figure 4). In this case, in order to reduce the degrees of freedom, a simplification using the geometry of the carrot cut was preferred. The boundary conditions remain the same as in the previous model, except that a single point on the line is no longer defined, but a contour in each zone that meets the conditions of the problem. As in the one-dimensional case, the convergence graph of the solution as a function of time steps is shown (Figure 4i)skype

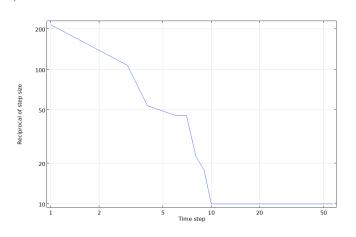


Figure 4i. Convergence plot of the one-dimensional numerical solution as a function of time steps.

Figure 4 shows the 2D solution of the proposed problem for time t=3.2 seconds. It is possible to obtain a picture of how the heat is distributed at each instant of time. Later, the possibility of generating an animation such as the one provided in supplementary material is discussed.

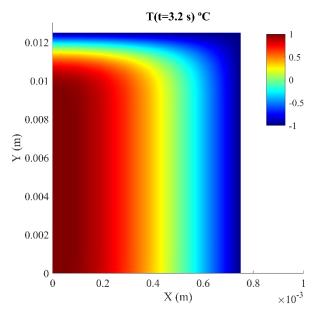


Figure 4. Numerical solution using two-dimensional FEM for time t = 3.2 seconds.

Finally, the solving of the same problem is proposed in a three-dimensional way. In this case, one has to take advantage of the geometric characteristics of the carrot. In this sense, It can be stated that a cross section can be reproduced by generating a revolution. That is, it has 2D-axisymmetric geometry. To define the proposed model, a rectangle has been prepared; when rotated 360°, it generates a carrot slice. In this case, Figure 5 shows a two-dimensional XY slice for the solution time.

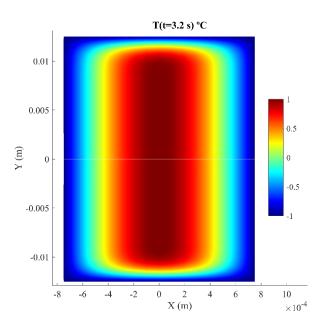


Figure 5. Numerical solution generating a 3D-solution using 2D-axisymmetric FEM model for time t = 3.2 seconds.

An animation showing all the temporary solutions of the 3D model has been included in the supplementary material (S1), so that the cooling of the carrot cut can be appreciated and the evolution of the problem can be seen.

In view of the foregoing, heat transfer problems can be understood intuitively. However, finding in the equations which are the most relevant parameters for the solution is not trivial. We propose that the student will be able to deduce which parameters are influential by modifying the conditions of the problem - at the numerical level, once the model has been validated with consistent analytical and numerical results -. Two additional types of simulations are shown below. In the first one, different vegetation thickness values are used (Figure 6), while in the second one, different initial temperatures of the vegetable have been considered (Figure 7).

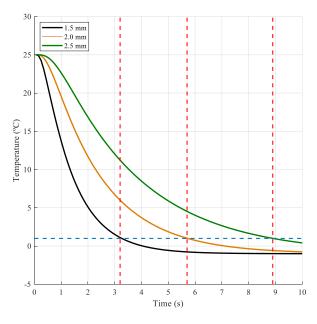


Figure 6. Numerical solutions for different thicknesses. The dashed red lines mark the desired temperature point (1°C). The time values achieved are shown in Table 1.

It can be observed that if the thickness of the plant is increased by 1 mm, the increase in cooling time almost triples, from 3.2 s to 8.9 s (Table 1).

Table 1. Numerical solutions for different thicknesses

Thickness (mm)	Time (s)
1.5	3.20
2.0	5.70
2.5	8.90

Contrarly, changing the initial temperature of the vegetable from 20 °C to 35 °C with 5 °C steps does not make much difference in the cooling time (Figure 7 and Table 2).

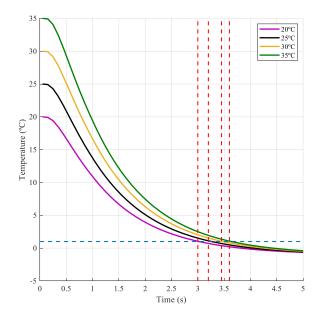


Figure 7. Numerical solutions for different temperature. The dashed red lines mark the time cut-off at the desired temperature. The time values achieved are shown in Table 2.

 Table 2. Numerical solutions for different initial temperatures (T₀).

Temperature (°C)	Time (s)
20	3.00
25	3.20
30	3.45
35	3.60

In this case, the student can see that the thickness of the plant is much more influential in heat transport and cooling than the initial temperature of the vegetable. Therefore, the learning outcome related to the analysis of the factors influencing this type of problem is achieved.

5. Conclusions

A non-steady state heat transport problem has been proposed in order to understand such an important phenomenon in the field of engineering and science. The underlying physics has been explained for the case of an infinite sheet. A proposed problem related to this type of physics has been solved analytically. Using FEM, we have solved the same problem both one-dimensionally, 2D and 3D, obtaining a consistent solution that validates the model. One of the advantages of using FEM is that it allows starting from a simple model explained theoretically, as proposed in this work. Subsequently, 2D or 3D models can be generated, whose solution is more complicated to demonstrate and validate analytically. Furthermore, allowing to change boundary and initial conditions, FEM offers students a complete and comprehensive way to see the time evolution and understand the physical behaviour of the problem.

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Data Availability Statement:

Not applicable.

Abbreviations

- A: Area that is traversed by the heat flow (m²)
- V: Sample volume analysed (m³)
- Q: Heat flow per unit time (J/s)

qx:Heat flow per unit time in the x-direction (J/s)

k : diffusion coefficient (W/m·K)

- ρ : volume density (kg/m³)
- Cp: Specific heat at constant pressure (J/kg·K))
- T: Temperature (K)
- T(x,t): Temperature as a function of time and position (K)
- To: Initial temperature (K)
- T∞: Steady-state temperature (K)
- α : Thermal conductivity (m²/s)
- t: Time (s)
- h: Convective heat transfer coefficient (W/m²·K)

L: Position of the separation surfaces between the sample and the surrounding fluid (air) (m)

 $\psi(x,t)$: Normalised function heat flow per unit time

- F(x): Position-dependent function
- G(t): Time-dependent function
- ω: Angular frequency (rad/s)

ωn: Eigenvalues

NBi: Biot number

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