

PREDICTION OF FREEZING TIMES IN VEGETABLES USING THE FINITE ELEMENT METHOD AND A COMBINED ENTHALPY AND KIRCHHOFF FORMULATION

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Keywords: Finite element method, Numerical simulations, Freezing, Mushroom, Irregular domains, Kirchhoff transformation, Enthalpy.

Abstract. Mushrooms are widely commercialized products which are very susceptible to enzymatic browning. Therefore their short shelf-life makes their preservation a crucial task. Freezing of previously blanched mushrooms, either whole or sliced, is a common process to obtain longer durability. A numerical model using the finite element technique was applied to predict freezing times of mushrooms considering the actual shape of the product. The original heat transfer equation was reformulated using a combined enthalpy and Kirchhoff formulation in order to obtain accurate numerical results and enhance the computational speed of the program. A three dimensional geometry was used to describe the sliced mushroom shape. Digital image reconstruction was used to obtain the irregular contour of the food product. The numerical predictions agreed with the experimental time-temperature curves during freezing of mushrooms in a tunnel (maximum absolute error < 3.2°C). The codes were applied to determine the required processing times for different operating conditions with minimum computational efforts.

1 INTRODUCTION

The shelf life of mushrooms, such as the commercial button mushroom *Agaricus bisporus*, is limited to a few days, mainly because they have no cuticle to protect them from physical or microbial attack and water loss. In the same way, they have a large content in nutrients and high respiration rate; factors that induce deterioration immediately after harvest (Kotwaliwale et al., 2007). Finally their high tyrosinase and phenolic content makes them very susceptible to enzymatic browning (Aguirre et al., 2009). In view of their highly perishable nature, mushrooms must be processed to extend their commercial shelf life for off-season use (Devece et al., 1999). The conventional conservation process of mushrooms includes washing of the samples and immediate blanching in order to inactivate enzymes, induce a volume contraction, and make the product more pliable to facilitate filling operations (Biekman et al., 1996). During this step shrinking of the tissue samples reaches up to 18%, as reported in Lespinard et al. (2009). Then mushrooms can be submitted either whole or sliced to several processes in order to obtain longer durability, for example low (refrigeration or freezing) or high (sterilization, pasteurization, dehydration, etc.) temperature thermal processes. The process of freezing is generally regarded as being superior to canning or dehydration when judged on the basis of retention of sensory attributes and nutritive properties (Fennema, 1977), and it combines the favorable effect of low temperatures with the conversion of water into ice (Delgado and Sun, 2001). Food engineers are interested in predicting cooling and freezing times in order to estimate the energy requirements for freezing and to design the necessary equipment for effective and rational processing. For this purpose, the evolution and distribution temperatures in the whole dominium of the food during freezing must be known. To this end, finite element method is an established formulation for numerical predictions of the transient temperature in heat conduction problems (Cleland et al., 1984) such as chilling and freezing. It has the great advantage that it can deal better with problems where the object has an irregular geometry (Arce et al., 1983; Pham, 2008). During the freezing process, which involves the phase change of water into ice in the food product, the thermo-physical properties such as specific heat, thermal conductivity, and density undergo abrupt changes due to the latent heat release. The system is then established as a highly non-linear mathematical problem.

Several techniques were applied to deal with the large latent heat release when using the finite element method. One of the traditional methods is the use of the apparent specific heat, where the sensible heat is merged with the latent heat to produce a specific heat curve with a large peak around the freezing point, that can be considered a quasi delta-Dirac function with temperature (depending on the amount of water in the food product). The abrupt change in the apparent specific heat curve requires several iterations for each time step and usually destabilizes the numerical solution. In some commercial simulation softwares that implement the finite element method, such as COMSOL, the use of the apparent specific heat is the only method available (Pham, 2008). Many authors have done approximations by “softening” the peak curve in order to obtain some convergence of the method, modifying the shape of the apparent specific heat curve while maintaining the total latent heat constant. However, this softening method is not recommended, because the actual temperature range around the freezing zone, is altered becoming wider than the actual temperature freezing range.

Sheen and Hayakawa (1991) have simulated freezing of whole mushroom shapes using Tylose gel material with 77% water content. Numerical problems were also reported in this work when applying the finite difference numerical technique caused by an unrealistic heat balance around each surface node on the curvilinear boundary.

Sliced mushrooms which have a T-shaped geometry are also submitted to freezing procedure, however papers considering this type of shape are not present in literature. This shape must be considered as an irregular 3D domain.

The implementation of the enthalpy method, which can be obtained through the integration of the specific heat with temperature (Comini, 1974; Mannapperuma and Singh, 1988, 1989; Pham, 2008), and the Kirchhoff function, which is the integral of the thermal conductivity, allows the reformulation of the heat transfer differential equation into a transformed partial differential system with two mutually related dependent variables H (enthalpy) and E (Kirchhoff function) (Scheerlinck et al., 1997, 2001; Fikiin, 1996, 1998). The combined enthalpy and Kirchhoff transformation has been previously applied in Santos et al. (2010) to simulate the freezing process of irregular 3D bakery products (croissants). Even though it generates great advantages to the resolution of the phase change problem, there are few works in literature which apply this method to simulate either freezing or thawing of other foodstuffs. Combining both transformations helps to avoid inaccuracies and/or divergence of the numerical method, caused by the latent heat peak release and the jump of the thermal conductivity at the phase transition, with the great numerical advantage of minimizing the execution speed of the program, since the resulting finite element matrices are constant.

The goals of this work are:

1. To develop a finite element code that simulates: the freezing process of an irregular shaped food using a combined enthalpy and Kirchhoff transformation method.
2. To apply the numerical model during freezing of sliced mushrooms considering a 3D geometry.
3. To validate the numerical solutions comparing the temperature predictions with experimental data during the freezing process of sliced mushrooms in a tunnel.
4. To predict processing times for different operating industrial conditions; different external fluid temperature and surface heat transfer coefficients.

2 MATERIALS AND METHODS

2.1 Finite element simulation during the freezing process of a 3D geometry (mushroom slice)

During the phase change transition in the freezing process the thermo-physical properties are strongly dependent on temperature. This constitutes a highly non-linear mathematical problem. A mushroom slice represents an irregular three dimensional geometry, therefore the heat conduction equation in Cartesian coordinates with phase change transition can be written as follows:

$$\rho(T) C_p(T) \frac{\partial T}{\partial t} = \nabla \cdot (k(T) \nabla T) \quad t \geq 0 \quad \text{in } \Omega \quad (1)$$

Eq. (1) is valid in the domain Ω , where T is the temperature, k is the thermal conductivity, C_p the apparent specific heat, and ρ the density (Carslaw and Jaeger, 1959). The initial (Eq. (2)) and boundary conditions (Eq. (3)) are:

$$T = T_0 \quad t = 0 \quad \text{in } \Omega \quad (2)$$

$$-k \left(\frac{\partial T}{\partial x} \cdot n_x + \frac{\partial T}{\partial y} \cdot n_y + \frac{\partial T}{\partial z} \cdot n_z \right) = h(T - T_{\text{ext}}) \quad t \geq 0 \quad \text{in } \delta\Omega \quad (3)$$

where $\delta\Omega$ is the domain of the convective interface which corresponds to external surface in contact with the cooling air, n_x , n_y , and n_z are the normal outward vector components, T_{ext} is the external air temperature; T_0 is the initial food temperature and h is the surface heat transfer coefficient.

The following change of variables is performed:

$$H(T) = \int_{T^*}^T \rho(T) \cdot C_p(T) dT \quad (4)$$

$$E(T) = \int_{T^*}^T k(T) dT \quad (5)$$

where H is defined as the volumetric specific enthalpy (Comini et al., 1990), E is the Kirchhoff function that represents the thermal conductivity integral (Comini et al., 1990; Fikiin, 1996), and T^* is a reference temperature that corresponds to a zero value of H and E . By combining Eq.(1), Eq. (4) and Eq. (5), and the initial and boundary conditions represented by Eq. (2) and Eq. (3) the following equations were obtained:

$$\frac{\partial H}{\partial t} = \nabla^2 E \quad t \geq 0 \quad \text{in } \Omega \quad (6)$$

$$-(\nabla E) \cdot \mathbf{n} = h \cdot (T - T_{\text{ext}}) \quad t \geq 0 \quad \text{in } \Omega \quad (7)$$

$$H = H_0 \quad t = 0 \quad (8)$$

Applying the finite element technique described in Santos et al. (2010) the following system of ordinary differential equations must be solved:

$$CG \cdot \frac{dH}{dt} + FG \cdot T(H) + KG \cdot E(H) = m \quad (9)$$

where:

$$CG = \sum_{e=1}^{ne} \int_{\Omega_e} (N^T N) d\Omega_e \quad \text{is the global capacitance matrix}$$

$$KG = \sum_{e=1}^{ne} \int_{\Omega_e} (B^T B) d\Omega_e \quad \text{is the global conductance matrix}$$

$$FG = \sum_{s=1}^{ns} \int_{\Omega_s} (N^T h N) d\delta\Omega_s \quad \text{is the global convection matrix}$$

$$m = \sum_{s=1}^{ns} \int_{\delta\Omega_s} (N^T h T_{\text{ext}}) d\delta\Omega_s \quad \text{is the global thermal load vector}$$

H , E , and T are the nodal values of enthalpy, the Kirchhoff function and temperature, respectively. N is the vector of dimensions $[1 \times 4]$ containing the shape functions (N_j) with $j=1-4$ for the reference tetrahedron element, N^t is the transpose vector (dimension 4×1), ne is the total number of elements, ns is the number of boundary elements, Ω_e is the integration

domain, $\delta\Omega_s$ is the boundary integration domain. The matrix B (dimension 3x4) is defined as follows:

$$B = \begin{bmatrix} N_{1x} & N_{2x} & N_{3x} & N_{4x} \\ N_{1y} & N_{2y} & N_{3y} & N_{4y} \\ N_{1z} & N_{2z} & N_{3z} & N_{4z} \end{bmatrix} \quad \text{where} \quad N_{ix} = \frac{\partial N_i}{\partial x}, \quad N_{iy} = \frac{\partial N_i}{\partial y} \quad \text{and} \quad N_{iz} = \frac{\partial N_i}{\partial z} \quad \text{for } i=1, 2, 3, \text{ and } 4.$$

It can be observed that the thermal properties of the foodstuffs are not present in the calculations of the matrices; therefore these matrices need to be calculated only once, which reduces the computer time significantly. If the surface heat transfer coefficient is considered constant during the process, FG and m also remain constant.

Eq. (9) is also a system of ordinary differential equations with three unknown variables, H, E, and T that are interrelated through non-linear algebraic functions (H(T), E(T), H(E), T(H), T(E), E(H)). Incorporating the functions E(H) and T(H) in Eq. (9) the system can be rewritten as:

$$\frac{dH}{dt} = f(H) \quad (10)$$

The system was solved using the standard Matlab routines ODE (Ordinary Differential Equations).

In order to obtain the temperatures, the function T(H) was used, since the solution is given in enthalpy values at the mesh nodes.

2.2 Reconstruction of mushroom shape and mesh generation

3D geometry of the mushroom slices were built from images of samples (Figure 1a). These images were digitally processed to obtain a binary image. In this regard, Image Processing Toolbox, MATLAB (MathWorks, Natick, Massachusetts), was used according with the following steps (Goñi et al., 2007):

- Conversion of original RGB images to grey-scale format,
- Noise reduction through a 3 x 3 median filter to enhance image quality,
- Segmentation through a threshold value which was obtained by analyzing the grey-scale image histogram. A binary image was obtained where black colour (pixel value equal to 0) represented the background and white colour the sample (pixel value equal to 1).

The contour of the binary image was approximated with a B-Spline curve, which was used as a base for the construction of the simulation domain. To construct the axial-symmetric two-dimensional domain, the B-Spline curve was transformed into a solid object. The three-dimensional domain was obtained by extrusion of the two-dimensional irregular image.

To run the finite element model the three-dimensional domain was imported into a mesh generator and discretized using tetrahedrons (Figure 1b). The mesh information was preprocessed and used as input into the main finite element code.

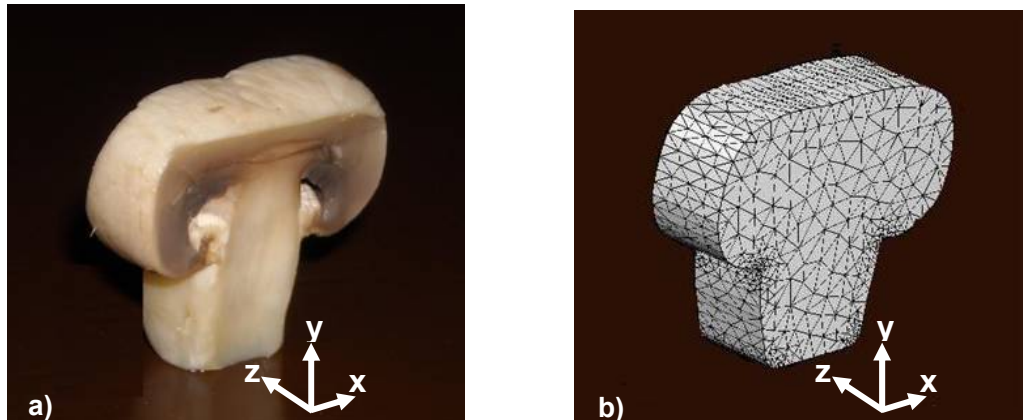


Figure 1: a) Digital photograph of the mushroom slice and b) 3D mesh using tetrahedral elements (7689 elements, 1881 nodes).

2.3 Thermo-physical properties of the product

The specific heat, thermal conductivity and density of the mushroom (between -40 and 20 °C) was considered dependent with temperature. The typical composition of the *Agaricus bisporus* mushrooms considered to estimate the thermal properties were: 90.5% moisture content, 4.9% carbohydrates, 0.3% fat, 3.5% protein and 0.8% ash, as given by Bernás et al. (2006). The moisture contents (%) of the *Agaricus bisporus* mushrooms used in the present work were verified experimentally by drying triplicate samples in an oven at 80 °C until reaching constant weight. The models proposed by Choi and Okos (1986) were implemented to estimate the thermal properties as a function of temperature and composition of the foodstuff. The thermal conductivity was:

$$k(T) = \sum x_i^v \cdot k_i(T) \quad (11)$$

where k is the global conductivity, k_i is the thermal conductivity of the component i (where i corresponds to the different components: water, ice if the temperature is lower than the initial freezing temperature T_f , carbohydrate, fat, etc.), x_i^v corresponds to the volumetric fraction of each component.

The density of the product was calculated using:

$$\rho(T) = \frac{1}{\sum \frac{x_i}{\rho_i}} \quad (12)$$

where $\rho(T)$ is the global density and ρ_i is the density of the component i (water, carbohydrates, ice, ash, etc). The fractions “ x_i ” correspond to the mass fraction of each component.

The specific heat of the mushroom was estimated using the following Eq. (13) (Miles, 1983):

$$Cp(T) = \sum x_i Cp_i - Lx_w \frac{T_f}{T^2} \quad (13)$$

The ice content as a function temperature (at $T < T_f$) was estimated using the equation proposed by [van Beek \(1979\)](#):

$$x_{ice} = x_w \cdot \left(1 - \frac{T_f}{T}\right) \quad (14)$$

where x_{ice} is the mass fraction of ice, x_w is the mass fraction of water in the foodstuff, and T_f is the initial melting point of the product. The initial freezing point of the mushroom obtained from the freezing curves using the tangent method was -1.2°C ([Fennema, 1973](#)); this value was in agreement with initial freezing temperatures for mushrooms values reported in [Wang et al. \(2007\)](#); $T_f = -1.870 \pm 0.8$. [Figures 2a, 2b and 2c](#) show the functional relationships of the thermo-physical properties with temperature. The volumetric specific heat in Eq. (13) was obtained by multiplying the $\rho(T)$ by the $C_p(T)$, and then numerically integrated using Eq. (4) to obtain the enthalpy function ([Figure 3a](#)). The same procedure was carried out with the $k(T)$ in order to obtain the Kirchhoff function ($E(T)$) according to Eq. (5) ([Figures 3b](#)). [Figure 3c](#) shows the function $E(H)$.

2.4 Experimental procedure

The freezing experiments were applied to previously blanched whole Mushrooms, which were afterwards placed over a metal mesh in a tunnel freezer at -15°C . The blanching procedure was carried out, according to [Lespinard et al. \(2009\)](#), during 7 minutes at 90°C in a water bath. One group of the blanched whole samples were sliced and introduced in a tunnel (FRIOTECNOLOGÍA, Argentina) in order to be frozen individually at an external air temperature of -15°C .

Thermocouples type T (copper-constantan (Cu-CuNi)), inserted in the mushrooms, were connected to an acquisition system (Testo 175, Testo AG, Germany) in order to record the time-temperature evolution in the product and cooling medium every 10 s.

The cooling air velocity in the tunnel freezer was measured using a hot wire anemometer (TSI model 1650); the value obtained was $v=2.5$ m/s.

2.5 Determination of the surface heat transfer coefficient (h)

In order to estimate the surface heat transfer coefficient the transient method was used; the numerical solution of heat conduction equation is the most appropriate method when dealing with heterogeneous foodstuffs, complex 3D geometries or variable boundary conditions ([Arce et al., 1983](#); [Rahman et al., 2005](#)).

To estimate the heat transfer coefficient, a bronze mushroom shaped object was manufactured. Bronze was chosen as a test material due to its high thermal diffusivity, which assures an almost instantaneous uniform temperature profile. A thermocouple was inserted at the centre of object to sense the time-temperature history during cooling in the tunnel freezer, which operated under the same conditions as the mushrooms freezing experiments. The following thermo-physical properties for bronze were used: $\rho = 8470 \text{ kg m}^{-3}$, $C_p = 376.81 \text{ J kg}^{-1} \text{ K}^{-1}$, $k = 122.87 \text{ W m}^{-1} \text{ K}^{-1}$.

Different heat transfer coefficients were used to simulate temperature profiles; experimental and predicted temperatures for each proposed h coefficient were compared. The heat transfer coefficient that minimized the residual sum of squares (RSS) given by Eq. (15) was selected.

$$RSS = \sum (T_{\text{exp}} - T_{\text{sim}})^2 \quad (15)$$

The heat transfer coefficient (h) obtained by Eq. (15) was 17 W/(m² °C).

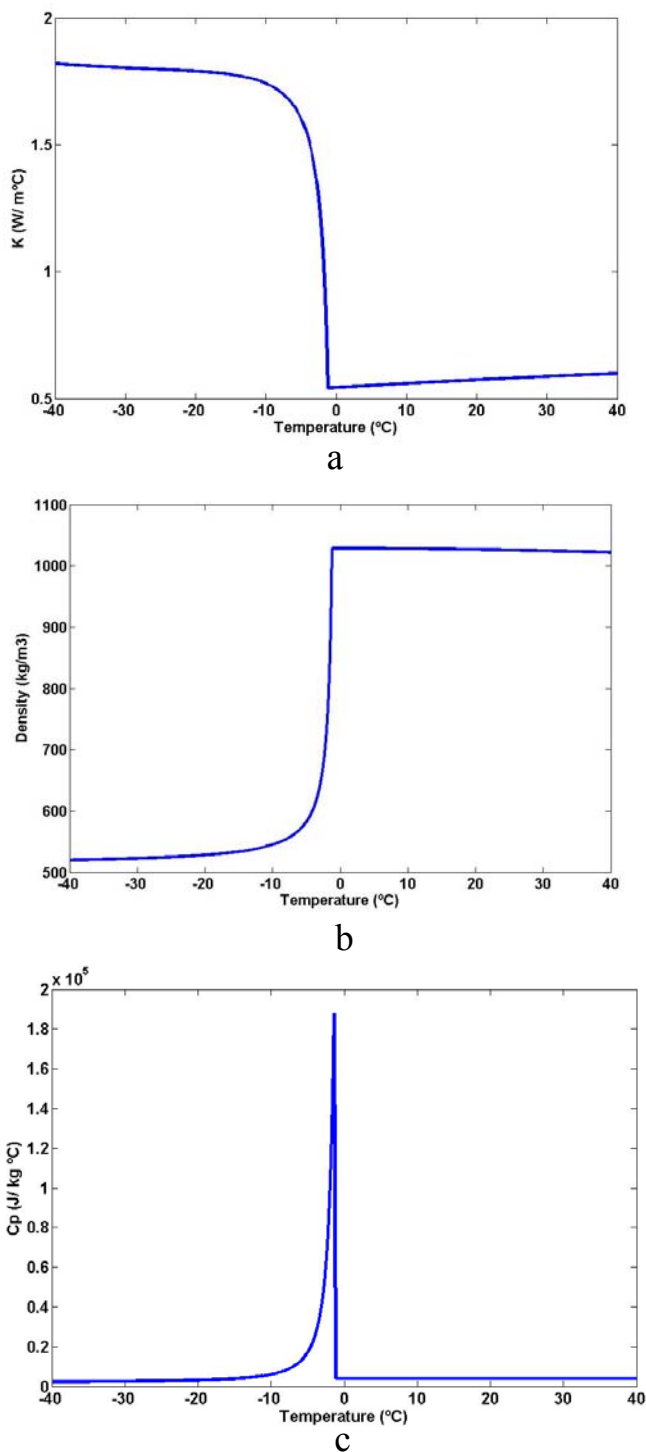


Figure 2: Thermo physical properties of the mushrooms used for the freezing process as a function of temperature a) thermal conductivity b) density and c) specific heat.

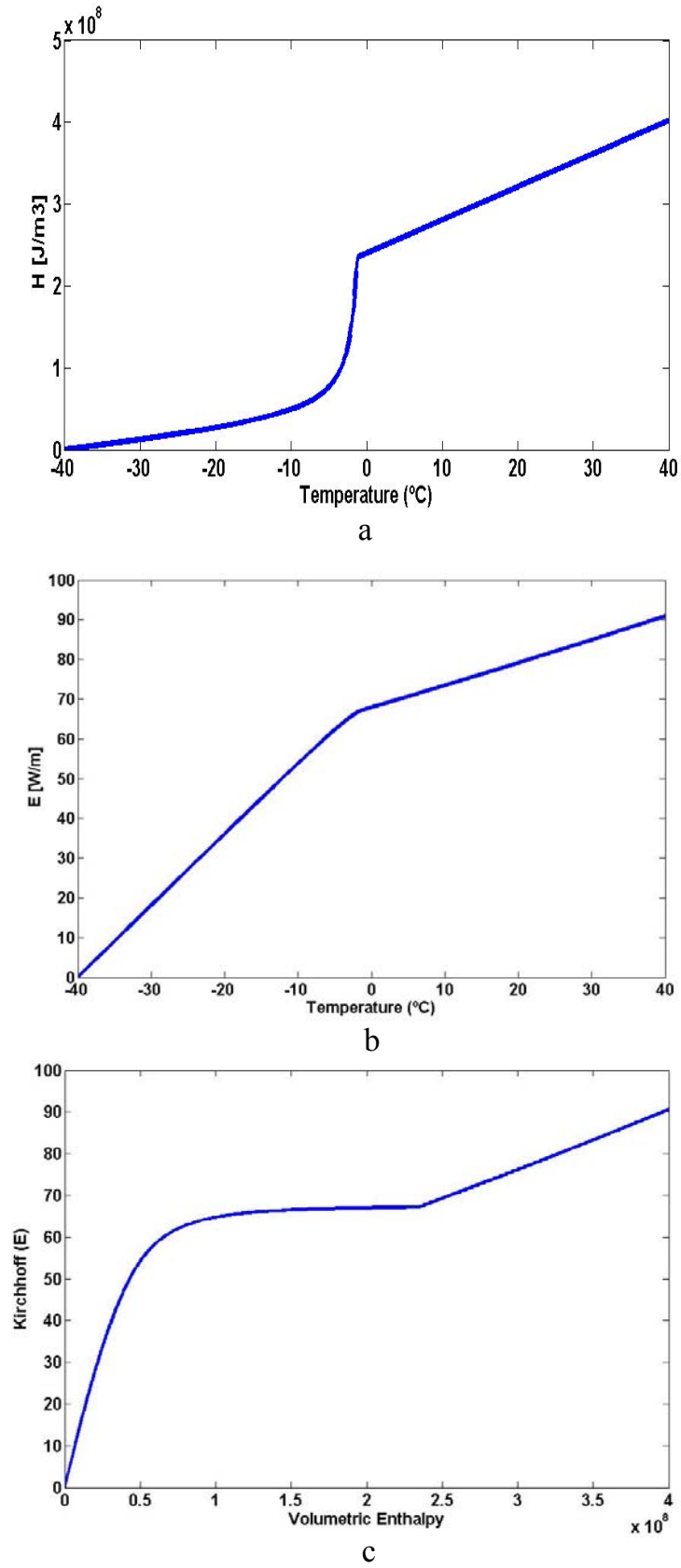


Figure 3: Functional relationships used in the combined formulation of the freezing process a) Enthalpy vs. temperature b) Kirchhoff function vs. temperature c) Kirchhoff function vs. enthalpy.

3 RESULTS AND DISCUSSION

3.1 Comparison of the numerical model with experimental results for the freezing process

The numerical simulations obtained with the code, were contrasted with experimental time-temperature freezing curves of mushrooms. Figure 4 shows the predicted and experimental temperatures for the sliced mushroom. It can be seen from the results that a good agreement was obtained between the experimental measurements and the numerical predictions. The absolute maximum difference (infinite norm of the error= $\|T_{\text{exp}} - T_{\text{sim}}\|_{\infty}$) for all experiments was less than 3.10°C .

Additionally the sliced mushroom, which corresponds to a 3D geometry, was analyzed considering a one-directional heat transfer flow, i.e. the heat flow ($q = \nabla T \cdot n$) perpendicular to the z axis is not significant. In order to compare both results a one-dimensional phase change problem taking into account the thickness of the mushroom ($e=0.0072$ m) was coded using Matlab 6.5. Figure 4 shows the experimental measurements and the predicted temperature for the 1D and 3D models. As can be seen the experimental freezing curve satisfactorily agrees with the three dimensional model proposed, therefore it can be concluded that the freezing of sliced mushrooms cannot be approximated as a one-dimensional problem. If a sliced mushroom shape is considered a one-dimensional heat flow problem, the calculated freezing times would be overestimated with respect to the actual 3D model, resulting in a much higher energy demand and quality loss.

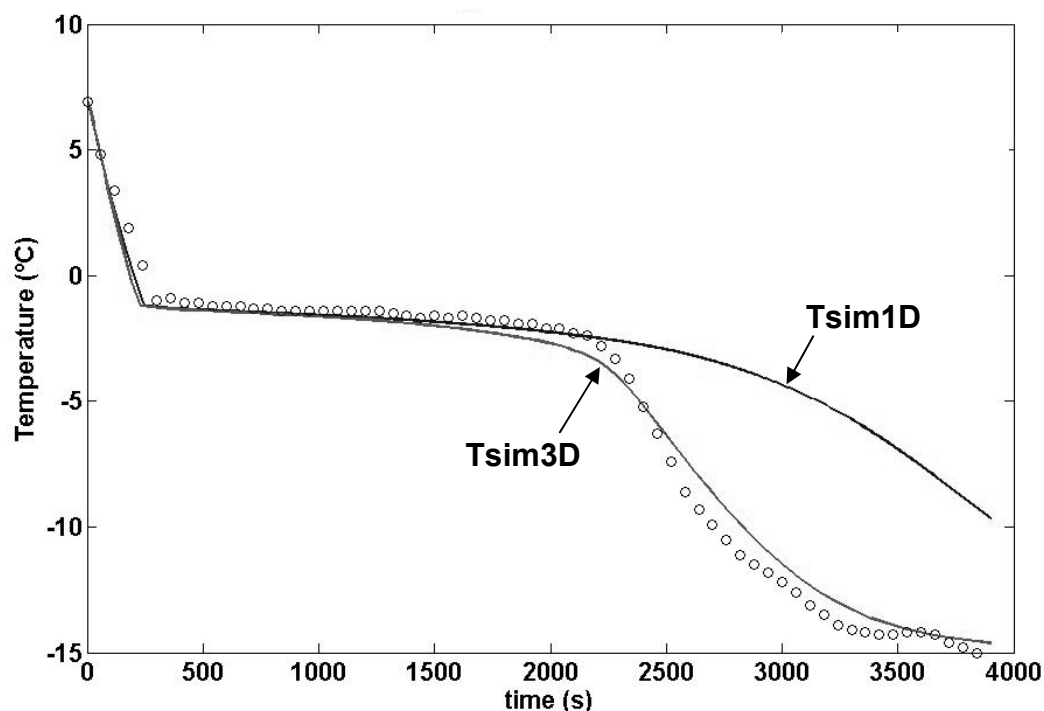


Figure 4: Experimental and predicted temperature values using a 1D (at $x=0.0036$ m) and 3D model at an internal point ($(x,y,z)=(-0.001,0.0245,0.0036)$ in m), $T_i=6.9^{\circ}\text{C}$. For all experiments $T_{\text{ext}} = -15^{\circ}\text{C}$, $h=17$ W/(m² °C).

Figure 5a shows the temperature distribution of the irregular shaped body after 972 s inside the tunnel freezer. It can be observed that the corners of the mushrooms reached lower temperatures much faster than the thicker central zone.

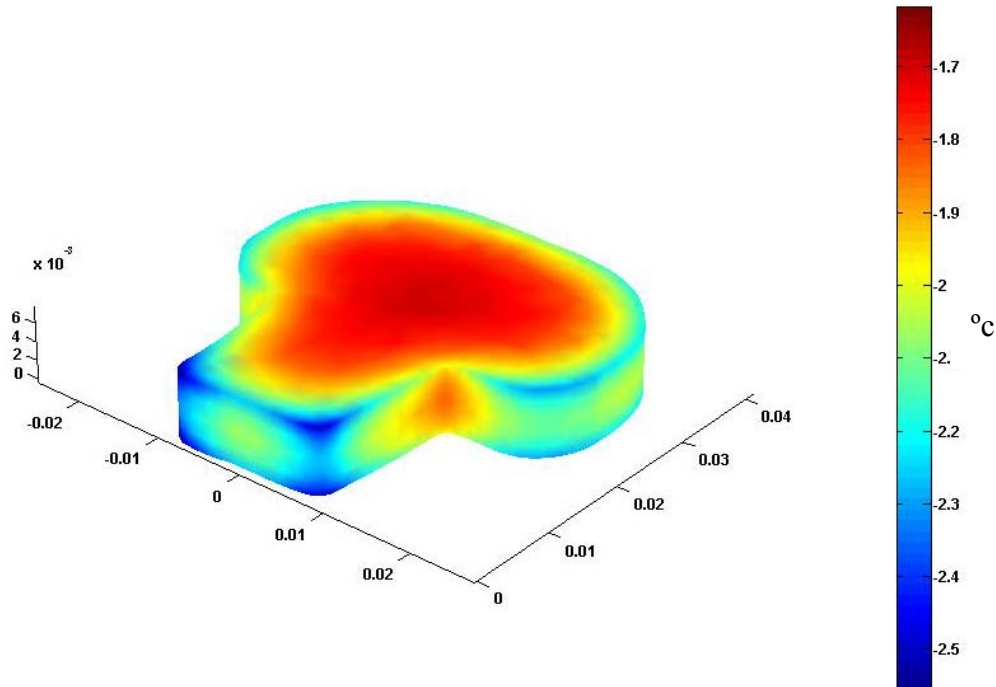


Figure 5: Temperature distribution of the mushroom after 972 s inside the tunnel freezer ($h=17 \text{ W}/(\text{m}^2 \text{ }^\circ\text{C})$, $T_i=10 \text{ }^\circ\text{C}$) at the surface.

3.2 Application of the numerical model to predict freezing times

Since the temperature distribution within a product varies considerably during freezing process, freezing time must be defined with respect to a position. The thermal centre is generally taken as reference, which is the location where the temperature changes most slowly. The freezing time is usually defined as the time to reach a particular temperature at the slowest cooling point (the thermal centre) (Hossain et al., 1992). For freezing, a number of final centre temperatures have been used: -5°C , -10°C and -18°C .

In this way, simulations were carried out in order to obtain the freezing times for different external fluid temperatures and surface heat transfer coefficients values, considering an initial temperature of $10 \text{ }^\circ\text{C}$. The time needed to reach a value of $-10 \text{ }^\circ\text{C}$ in the warmest point was calculated for sliced mushrooms (Table 1).

All the numerical runs were tested for their computational speed, the maximum CPU time were less than 9 minutes using a PC Intel(R) Core(TM) 2 6300 with a processor speed of 1.86 GHz and a RAM of 2GB.

It is noteworthy that the computational speed of the numerical simulations of the freezing process is low, due to the simultaneous Kirchhoff and enthalpy transformation. Using this combined transformation the conductance, capacitance, and convective matrices as well as the thermal load vector in the finite element formulation remained independent of the time variable.

h (W/(m ² °C))	T _{ext} = -20 °C	T _{ext} = -30 °C
5	106.9	69.11
10	54.57	35.49
20	27.9	18.52
100	7.04	4.73
10000	0.91	0.61

Table 1: Freezing times (in minutes) considering different operating conditions: surface heat transfer coefficients and external fluid temperatures. Initial uniform temperature of 10°C. Maximum CPU time for all numerical runs was 9 minutes.

4 CONCLUSIONS

Finite element codes were developed to simulate the phase change transition during freezing of an irregular foodstuff. A combined Kirchhoff and Enthalpy formulation of the heat transfer equation was applied to deal with the highly non-linear mathematical problem and to enhance the computational speed of the numerical runs, resulting in a minimum CPU. The finite element code was found to be convergent, no oscillations of the temperature predictions were encountered in the solutions.

The numerical model was compared with experimental freezing curves of sliced mushrooms. The numerical runs agreed well with experimental time-temperature curves. The freezing of sliced mushroom was also compared with a one-dimensional heat flow model, in order to verify that the mushroom slice object must be approximated as a 3D heat transfer problem.

The code was applied to obtain freezing times of mushrooms considering different operating conditions. This information can be useful for food processors to obtain valuable information to design freezing equipment and optimize processes.

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