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Mathematical modeling for heat conduction in olive fruit

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ABSTRACT

This study aims to develop a numerical model that can simulate the heat transfer in spherical coordinates and predict the temperature of olive fruit during the thermal process. The first step was to measure or estimate the thermophysical properties of olive fruit. The fixed grid finite difference method with an explicit scheme was used to solve the heat transfer equation. The product had an average geometric diameter of 18.18 mm, a bulk density of 556 kg/m^3, a porosity of 48% and a specific heat of 3180 kJ/kg. The inverse method was used to determine the thermal conductivity of olive fruit, which was 0.44 W/m°C. The model was validated by comparing the predicted values with the experimental temperature profiles obtained during the thermal process of the fruit (correlation coefficient higher than 0.99 and mean squared error lower than 1.8°C). The sensitivity coefficient results indicated that the surrounding temperature and the diameter of the product were the most influential parameters on the heat transfer of the product. The model was effective in simulating the thermal processing of olive fruit. The research results can be applied to optimize the pasteurization process of olive fruit.

1. Introduction

Olive belongs to the *Oleaceae* family, Olea genus and Europaea species. Olive fruit contains phenolic compounds including phenolic acids, simple phenols, tocopherols, securidoids and flavonoids. These compounds have anti-carcinogenic, anti-mutation, anti-diabetic and antioxidant properties. Currently, the most important use of this fruit is in the production of edible oil and in the next stage, the preparation of canned food from this fruit. Due to the presence of phenolic compounds with a bitter structure in this fruit (oleuropein), in order to prepare canned olives, the first step is to soak the olives in alkaline solutions, and in the next step, they must be washed several times and finally, for flavoring under fermentation, which occurs naturally in salt water solution [1].

Canning is a common process for preserving the olive fruit in the food industry. During canning, foods are sealed in a sealed container and pasteurized by heat. The main purpose of the thermal process is to destroy microorganisms and deactivate enzymes whose presence causes food spoilage and food unfit for consumption [2].

However, the thermal process applied to the product, as it is often far from optimal conditions, can lead to incomplete processing of the product, which will result in the possibility of the survival of microorganisms and spoilage of the product. On the other hand, following excessive processing of the product, a decrease in the quality of the product can be expected, including a decrease in nutritional value, a decrease in bioactive compounds, softening of the texture, and loss of olive green color [3].

Heat transfer modeling is a mathematical approach to simulate the temperature distribution and heat flux in a food product during thermal processing. Applying these models can help optimize process parameters, such as time and temperature, to ensure food safety and quality. During the thermal process, the temperature inside the food depends on the time as well as the position inside the food system. It is assumed that heat transfer in solid and semi-solid foods such as fruits, viscous solutions, purees, concentrates, is conducted through conduction. For these foods, analytical or numerical solutions of heat conduction equations (Fourier's second law) are used to determine the appropriate processing time [4]. In the stone fruits, the thermal process is slightly different from the solid products. Stone fruits such as olives, cherries, plums, etc., have almost spherical or oval geometries, but inside they contain a lignin core (seed), whose thermophysical characteristics are different from the edible part. In addition, the contact surface between this seed and the pulp is actually the deepest point that can be reached in the fruit and plays the role of the thermal center, which is shown in homogeneous solid objects with a geometric center [5].

Although a lot of research has been done on the thermal process of stone fruits at the global level, little research has been done in our country, and at the industrial level, process optimization is usually based on trial and error. This is despite the fact that by optimizing this process, ensuring the health of the consumer, the duration of the process can be reduced, and at the same time, the loss of nutritional value and the destruction of the quality characteristics of the product (softening of the product or loss of the desired color) be prevented. Therefore, the main goal of this research is to develop a numerical model of heat transfer for the thermal process of the olive fruit. The results of this research will be used in the next step to optimize the pasteurization process.

2- Materials and methods

Physical characteristics of the product

Olives (*Olea Chrysophyla*) that were subjected to the debittering process were used for this research. To determine the size of the fruits, at least 50 samples were randomly selected and their dimensions, length, width, and thickness were measured using calipers. Fruit mass was measured with an electronic scale with an accuracy of 0.001 grams. The pulp moisture content of the olive fruit samples was determined using the oven method. The amount of protein, fat and ash of the fruit tissue was determined by Kjeldhal, Soxhlet and electric furnace methods, respectively. The average diameter (D_a), geometric (D_g) and sphericity (φ) of the fruit was determined using the formulas 1-3. In order to reduce the shape of the sample to the model considered in this paper, the olive was considered as a sphere with the same volume as the real olive. Since the shape of the fruit is almost an ellipse, its equivalent sphere radius (R) was obtained by equation 4 [5].

To measure the heat transfer in the fruit, a type (K) thermocouple was placed in the central point of the sample, but due to the soft texture of the product, the exact location of the thermocouple was rechecked after the treatment using calipers. The temperature was measured at intervals of 20 seconds and measured by Testo model 1763. The test was performed in a hot water bath with the temperatures of 65, 75 and 85 degrees Celsius (accuracy ± 2 degrees Celsius). In order to make the temperature uniform, the bath was turned on for 20 minutes before the start of the test and the mixing and disturbance of the bath during the test was prevented [6].

$$D_a = \frac{(L+W+T)}{3} \quad [1]$$

$$D_g = (LWT)^{1/3} \quad [2]$$

$$\varphi = \frac{(LWT)^{1/3}}{L} \quad [3]$$

$$R = \frac{1}{2}\sqrt[3]{D^2L} \quad [4]$$

$$\varepsilon = 100\left(1-\frac{\rho_b}{\rho_t}\right) \quad [5]$$

Determination of thermophysical properties

Density

The apparent density (mass) of olive fruits was measured by weighing a specific amount (100 grams) of olive fruits filled inside a box with a certain volume, and the apparent density was calculated by dividing the mass of the olive fruits by the volume of the box. The real density and the real volume were determined using the toluene displacement method, and the porosity was obtained from equation 5 [7,8].

1.1.1. Coefficient of thermal conductivity and specific heat

In order to determine the thermal conductivity of olives, the inverse method was used. The inverse method is a transient method that uses an optimization algorithm to minimize the difference between the measured temperature and the calculated temperature [9]. The specific heat of olive was also determined according to the chemical composition of the product and using equation 6. In the following relation, Cp and Cp_i are respectively the specific heat of the product and the specific heat of each component of the product, and x_i is the mass fraction of the ingredients of the product [10].

$$Cp = \sum Cp_i x_i \quad [6]$$

Convective heat transfer coefficient

The average convective heat transfer coefficient on the surface was determined using the transient mode method. In this method, an aluminum sphere with a weight of 8.22 grams and a radius of 10 mm, in which a thermocouple was located in the centre portion, was used. The average convective heat transfer coefficient on the surface was estimated using the slope of the linear section of the time graph relative to ln ($T-T_{Al}$), by the equation 7.

$$h = \frac{M_{Al}Cp_{Al}}{Sm} \quad [7]$$

In the above relationship, M_{Al} is the mass of the aluminum sphere, Cp_{Al} is the specific heat of aluminum, S is the slope of the graph line ln ($T-T_{Al}$) with respect to time and the mass of the sphere [11].

Modeling

In order to reduce the shape of the sample to the model considered in this paper, the olive was considered as a sphere with the same volume as the real olive. The heat transfer equation in an unsteady state for a sphere can be written in the following form [5].

$$\frac{\partial T}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\alpha\frac{\partial T}{\partial r}\right) \quad [8]$$

The initial condition (IC) and boundary conditions (BCs) for this equation are:

$$IC: T(r,0)=T_0 \quad [9]$$

$$BC_1: \frac{dT}{dr}=0 \quad at \quad r=0, \quad [10]$$

$$BC_2: -k\frac{dT}{dr}=h(T-T_a) \quad at \quad r=R, \quad [11]$$

Analytical modeling of heat transfer

In order to solve the heat transfer equation in transient (unsteady) conditions, the analytical solution of Fourier's second equation was used, and according to the assumption of spherical shape of the sample, the following equation was used [9].

$$\frac{T-T_a}{T_o-T_a}=\sum_{n=1}^{\infty}\left[C_n(x)\exp\left(-\mu_n^2\frac{\alpha.t}{L^2}\right)\right] \quad [12]$$

In the above relationship, the term C_n is different according to the desired geometric shape and the equation 13 is used for the sphere shape [12].

$$C_n(x)=\frac{2[\sin(\mu_n)-\mu_n.\cos(\mu_n)]}{\mu_n-\sin(\mu_n)\cos(\mu_n)}.\frac{\sin\left(\mu_n.\frac{x}{L}\right)}{\mu_n.\frac{x}{L}} \quad [13]$$

In relation 13, μ_n are the roots of equations 12 and in equation 14 Bi is Biot's number [13].

$$N_{Bi}=1-\frac{\mu}{\tan(\mu)} \quad [14]$$

Numerical modeling (finite difference)

The governing equation of heat transfer was solved numerically by applying the initial and boundary conditions and using the finite difference method based on the explicit scheme. In this study, the olive fruit was divided into 10 nodes with a radius of 0.009 m. The inputs used in the model are shown in Table 1 and programming was done on MATLAB R2016b software. From solving the above equation based on the explicit scheme in the finite difference method, the following equation can be estimated for the internal points of the sample, for the nodes located in the center and surface of the sample, similar equations can be obtained according to the boundary conditions (11-10) of the sample [3].

$$T_{i,j+1}=\frac{\alpha\Delta t}{\Delta r^2}\left[\left(\frac{i-2}{i-1}\right)T_{i-1,j}+\left(\frac{\Delta r^2}{\alpha\Delta t}-2\right)T_{i,j}+\left(\frac{i}{i-1}\right)T_{i+1,j}\right] \quad [15]$$

Statistical Analysis

Two statistical criteria, coefficient of determination (R^2) and mean square error (MSE) were used to evaluate the fit between the model and experimental data [14].

$$R^2=1-\left[\frac{\sum_{i=1}^{N}\left(T_{pre,i}-T_{\exp,i}\right)^2}{\sum_{i=1}^{N}\left(T_{pre,i}-T_{pre,i}\right)^2}\right] \quad [16]$$

$$MSE=\frac{\sum_{i=1}^{N}\left(T_{\exp,i}-T_{pre,i}\right)^2}{N} \quad [17]$$

Where $T_{exp,i}$ stands for the experimental temperature found in any measurement and $T_{pre,i}$ is temperature predicted for this measurement and N is the number of observations.

3-Results and discussion

Physical and thermophysical properties of the product

Table 1 shows the physical properties of the olive fruit in experiments. The size of the fruit was different in the range of 18.04-21.65 mm. The mean arithmetic, geometric diameter, and equivalent radius of the olive fruit were calculated as 18.46, 18.18 and 8.83 mm, respectively. The sphericity of the olive fruit was estimated at 80.5%. The amount of the bulk and the real density was also found to be about 556 and 1082 kg/m3, and the amount of porosity obtained using equation 5 was estimated as 48.6% [8, 15].

Table 1. Physical and thermal properties of olive fruit

Properties	Olive fruit
Moisture, % (wb)	57.6±1.48
protein % (wb)	5.12±0.65
Fat % (wb)	17.8±1.23
Ash % (wb)	1.74±0.35
Length (mm)	22.65±3.25
Width (mm)	15.68±2.32
Arithmetic mean diameter (mm)	18.46±1.75
Geometric mean diameter (mm)	18.18±1.65
Sphericity (%)	0.805±2.71
Equivalent radius	8.83±0.64
Unit mass (g)	3.7±1.21
Bulk density (kg/m^3)	556±4.15
True density (kg/m^3)	1082±3.4
Porosity (0-1)	0.48±0.81
Specific heat (J/kg.K)	3180
Thermal diffusivity (m^2/s)	2.49E-07
Heat transfer coefficient (W/m.K)	410
Initial temperature (ºC)	20±2
Ambient Temperature (ºC)	85±2

The accuracy of experimental data for thermophysical properties of food can be doubted due to defects in the methods used to measure such values, and this problem is more evident in the case of thermal conductivity due to the need to create a uniform heat flux in the product during measurement. As Simpson and Cortés (2004) suggested, the thermophysical properties may be determined more accurately by predicting them using the accurate model instead of measuring them [16]. In this research, the inverse method was used to determine the thermal conductivity of the sample. The inverse method is a method to estimate the thermal conductivity of food by solving the second Fourier conductivity equation and fitting the solution with the experimental temperature-time data. This method has been successfully used to estimate the thermal conductivity of other food products including bread [17]. As can be seen in the Figure 1, the lowest MSE, which is an estimate of the error between the experimental data and the model data, was found to be around 0.44, and therefore this value is considered as the thermal conductivity coefficient of the sample in the model.

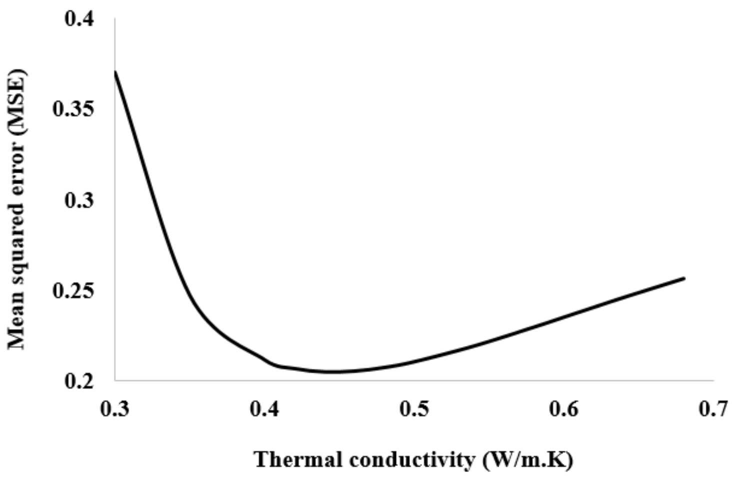

Figure 1. The relationship curve of mean squared error and thermal conductivity

Verification and validation of the model

In order to verify the model, the results of the numerical modeling (finite difference method) were compared with the results of the analytical solution for spherical coordinates [18]. The Figure 2 shows the comparison between the results of the numerical model (finite difference) and the analytical model. As can be seen from the Figure 2, there is a complete agreement between the two models, so that for three points (center (r/R=0), middle (r/R=0.5) and surface (r/R=1)), the error estimated by MSE was equal to 0.182, 0.049 and 0.157, respectively, and the determination coefficient (R^2) for all three points was determined to be above 99%. In order to validate the model, a comparison between the experimental results and the model data was used. As it is clear from the figure, there is an acceptable agreement between the temperature measured in the center of the sample and the temperature measured by the numerical model, so that the mean square error between the experimental data and the model data is equal to 1.8 and the coefficient of determination was 99%.

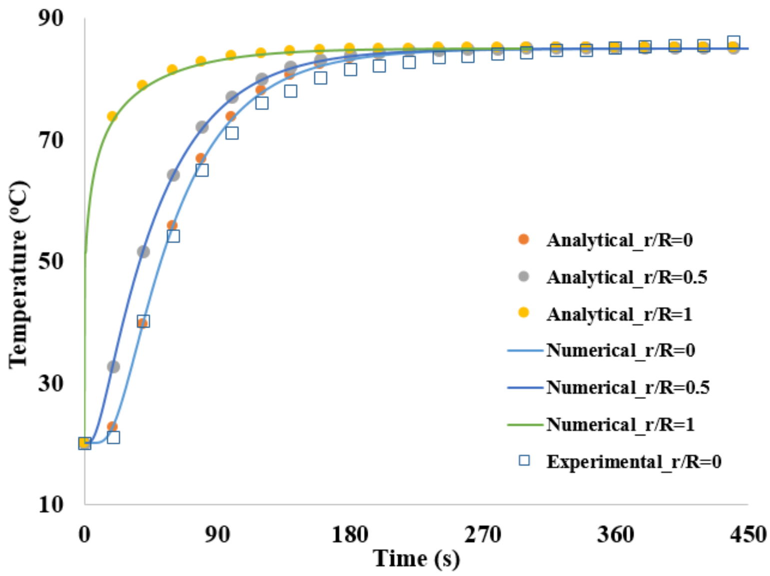

Fig. 2 Comparison of temperature determined by experimentation and prediction using analytical and numerical models

Analytical model

In order to verify the model, the results of the numerical modeling (finite difference method) were compared with the results of the analytical solution for spherical coordinates [18]. The Figure 2 shows the comparison between the results of the numerical model (finite difference) and the analytical model. As can be seen from the Figure 2, there is a complete agreement between the two models, so that for three points (center (r/R=0), middle (r/R=0.5) and surface (r/R=1)), the error estimated by MSE was equal to 0.182, 0.049 and 0.157, respectively, and the determination coefficient (R2) for all three points was determined to be above 99%. In order to validate the model, a comparison between the experimental results and the model data was used. As it is clear from the figure, there is an acceptable agreement between the temperature measured in the center of the sample and the temperature measured by the numerical model, so that the mean square error between the experimental data and the model data is equal to 1.8 and the coefficient of determination was 99%.

Analytical model

In order to facilitate the application of the model, a diagram showing the rate of heat transfer in an unstable state to the center of a sphere is given in the Figure 3. On one axis, the incomplete temperature change $((T_a-T)/(T_a-T_o))$ and on the other axis, the Fourier number $(\alpha t/r^2)$ are located when the time coordinate is considered. The curve is shown for different values of the Biot number. By using the graph, the temperature of the material can be predicted for any point and at any moment, for this purpose, we first determine the Fourier number using the radius of the sphere, and in the next step, we determine the Biot number. Finally, according to the Biot number and the Fourier number, the temperature of the fruit can be predicted [13].

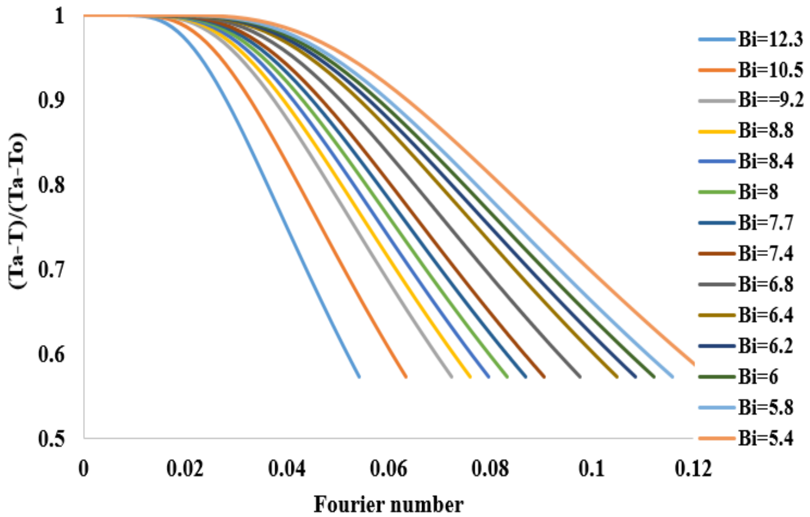

Fig. 3. Temperature at the geometric center of a sphere

Numerical model

As explained in the Materials and Methods section, the finite difference method was used to predict the temperature of the sample during the thermal process. Figure 4 shows the temperature profile obtained by the numerical method, in different layers of the sample during the thermal process. As expected, the slope of temperature changes in the geometric center (r/R=0) is lower than other layers, and with increasing distance from the thermal center of the sample, the slope of temperature changes increases so that the surface point (r/R=1) is the highest. This shows the rate of temperature change in the sample. By using this model, it is possible to easily determine the temperature changes at any point of the material at any time [3].

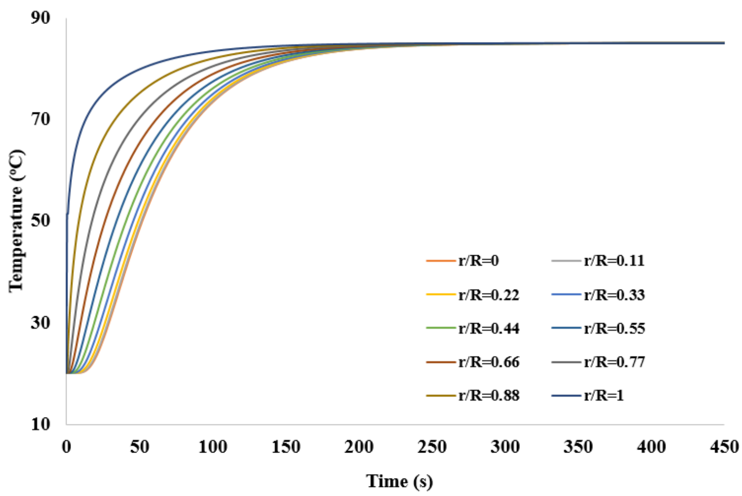

Fig. 4 Results obtained from numerical model in predicting temperature as a function of time and distance from the center

Sensitivity analysis

The sensitivity analysis was used to determine the most effective variable on the model. The analysis was performed with a 10% change in each of the variables (initial temperature, ambient temperature, sample diameter and heat transfer coefficient on the surface) and the effects were compared [19]. Figure 5 shows the effect of temperature changes on these variables. As shown, the two variables of ambient temperature and sample dimensions (diameter), respectively, show the greatest effect on the product temperature, and the initial temperature of the food item and the heat transfer coefficient have the least effect. Based on the results of the sensitivity analysis, it can be concluded that to control the process, the highest precision should be focused on these two parameters.

Validated model

Figure 6 shows the three-dimensional distribution (contour) of the temperature obtained from the numerical model in the thermal process with an ambient temperature of 85 °C over a time span of 0-120 seconds. The surface of the fruit whose temperature increases rapidly is exposed to hot water, and its temperature reaches about 40-50 °C after a few seconds. The cold point of the fruit is located at the geometric center of the fruit and the temperature changes in it very slowly. In addition, after about 100 seconds of the thermal process, the temperature changes at different points of the whole fruit show the same trend, i.e., increasing the duration of the process from this time on does not affect the temperature changes at different points of the sample. Similar results were reported by Cuesta et al. (2017) [5]. Such a diagram provides the possibility to easily determine the temperature value of each point of the sample as a function of the process time. This study is one of the few that did heat transfer modeling in olive fruit, which is important for understanding the effects of thermal processing on its quality and safety. Other studies have focused on different aspects of thermal processing of olives, such as the effect of heat treatment and ultrasound on the microbial and qualitative properties of green olives [2], the thermal processing of canned olives in brine in metal cans using computational fluid dynamics [4], and the development and validation of a computational fluid dynamics model for predicting the temperature profile during pasteurization of different fruits [21].

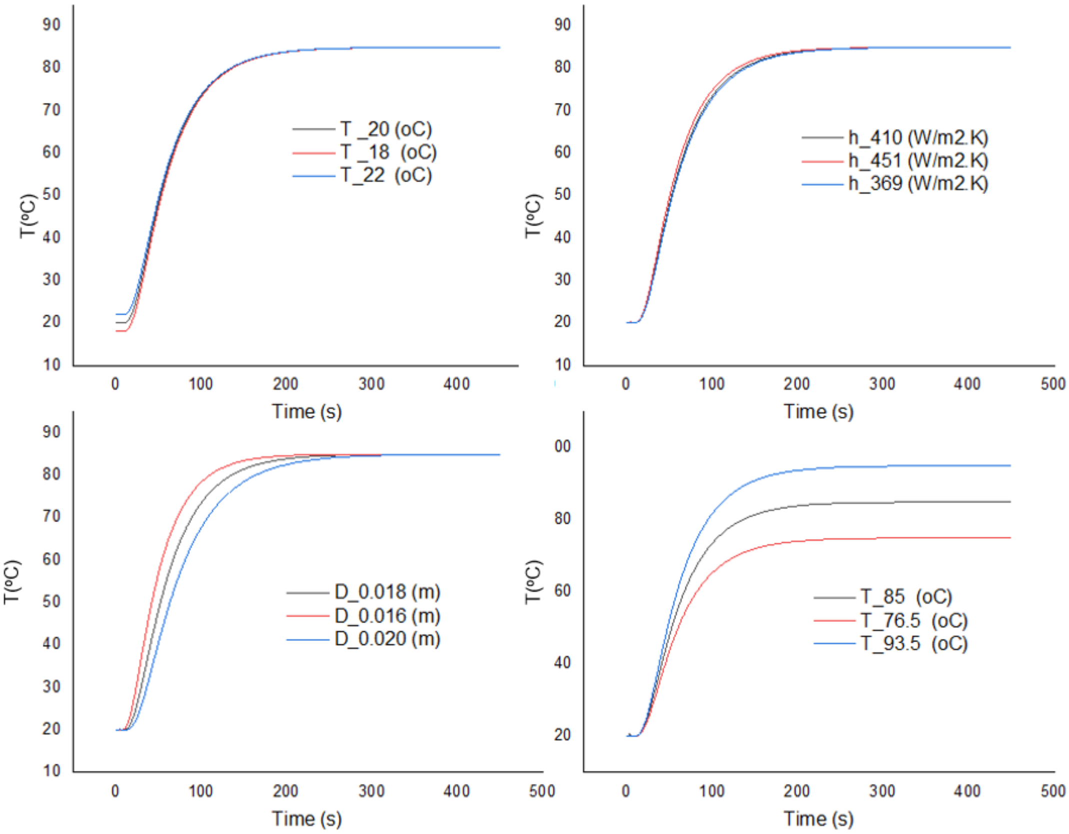

Fig. 5 The effect of sensitivity index on different variables of the model

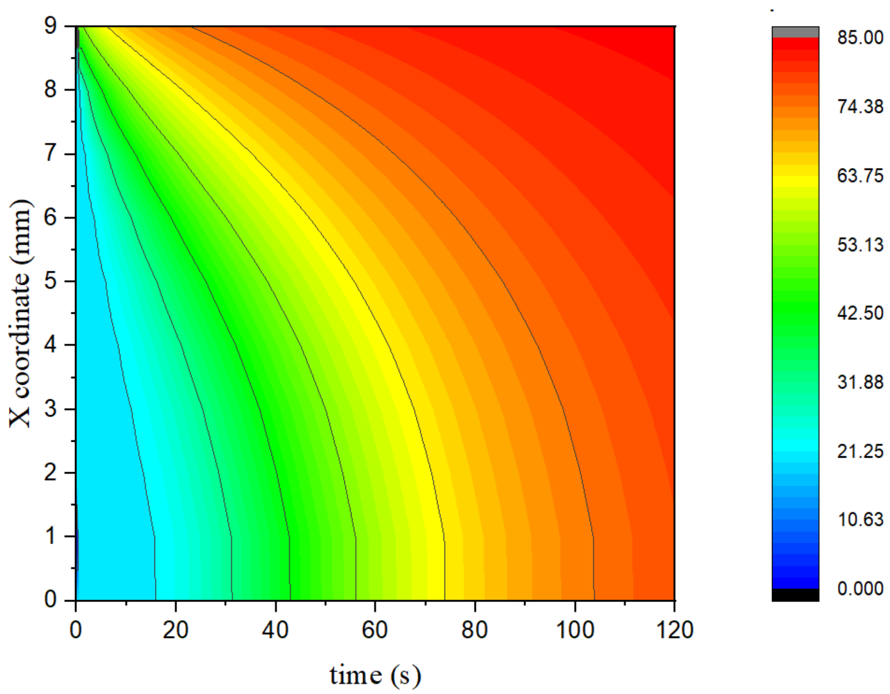

Fig. 6 Contour plot of the predicted temperature distribution during thermal processing

2. Conclusion

The heat transfer model was developed by numerically solving Fourier's second law for olive fruit during the thermal process. The model was verified by comparing the results of the analytical method with the results of the numerical method. The high correlation coefficient of 99% showed the validation of the developed data model. In the next step, the model was validated using experimental results. The mean squared error (MSE) between experimental data and model data was 1.8°C, which is within the acceptable range of ±2°C. The coefficient of determination (R^2) was 99%, indicating a high degree of fit between the model and the data. The high correlation between the predicted and measured temperature profiles showed that the developed model can well predict the temperature changes throughout the fruit. This model can be used for a better understanding of the heat transfer mechanism inside the product during the pasteurization process and validation of two-dimensional or three-dimensional heat transfer models. In the future step of this research, we will use the results of this model to optimize the pasteurization process of canned olives.

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مدلسازی ریاضی برای انتقال حرارت در میوه زیتون

محسن دلوی اصفهان

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چکیده

هدف از این مطالعه توسعه یک مدل عددی است که بتواند دمای میوه زیتون را در طی فرآیند حرارتی با شبیه‌سازی انتقال حرارت در مختصات کُروی را تخمین بزند. در گام اول، خواص ترموفیزیکی میوه زیتون اندازه‌گیری یا برآورد شد. معادله انتقال حرارت با استفاده از روش تفاضل محدود شبکه ثابت با شمای طرح صریح حل شد. میانگین قطر هندسی محصول برابر با ۱۸/۱۸ میلی متر، دانسیته توده ٥٥٦ کیلوگرم بر متر مکعب، تخلخل ٤۸٪ و گرمای ویژه زیتون برابر با ۳۱۸۰ کیلوژول بر کیلوگرم تخمین زده شد. هدایت حرارتی میوه زیتون با روش معکوس تعیین شد که مقدار آن برابر با ۰/٤٤ وات بر متر درجه سانتیگراد بود. مُدل با مقایسه مقادیر پیش‌بینی‌شده با پروفیل‌های دمای تجربی به‌دست‌آمده در طی فرایند حرارتی میوه (ضریب همبستگی بیشتر از ۰/۹۹ و میانگین مجذور خطا کمتر از ۱/۸ درجه سانتی‌گراد) تأیید شد. نتایج ضریب حساسیت نشان داد که در بین پارامترهای مختلف موثر بر انتقال حرارت محصول، مهمترین عوامل به ترتیب دمای محیط گرمایشی و قطر محصول می‌باشد. نتایج نشان داد که این مدل در شبیه سازی فرآوری حرارتی میوه زیتون موثر است. نتایج این تحقیق می‌تواند برای بهینه سازی فرایند پاستوریزاسیون میوه زیتون مورد استفاده قرار گیرد.