Mathematical modeling of heat treatment processes conserving biological activity of plant bioresources

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Abstract. The aim of this study is to develop a mathematical model of the heat exchange process of LT-processing to estimate the dynamics of temperature field changes and optimize the regime parameters, due to the non-stationarity process, the physicochemical and thermophysical properties of food systems. The application of LT-processing, based on the use of low-temperature modes in thermal culinary processing of raw materials with preliminary vacuum packaging in a polymer heat-resistant film is a promising trend in the development of technics and technology in the catering field. LT-processing application of food raw materials guarantees the preservation of biologically active substances in food environments, which are characterized by a certain thermolability, as well as extend the shelf life and high consumer characteristics of food systems that are capillary-porous bodies. When performing the mathematical modeling of the LT-processing process, the packet of symbolic mathematics “Maple” was used, as well as the mathematical packet flexPDE that uses the finite element method for modeling objects with distributed parameters. The processing of experimental results was evaluated with the help of the developed software in the programming language Python 3.4. To calculate and optimize the parameters of the LT processing process of polycomponent food systems, the differential equation of non-stationary thermal conductivity was used, the solution of which makes it possible to identify the temperature change at any point of the solid at different moments. The present study specifies data on the thermophysical characteristics of the polycomponent food system based on plant raw materials, with the help of which the physico-mathematical model of the LT-processing process has been developed. The obtained mathematical model allows defining of the dynamics of the temperature field in different sections of the LT-processed polycomponent food systems on the basis of calculating the evolution profiles of temperature fields, which enable one to analyze the efficiency of the regime parameters of heat treatment.

1. Introduction

Sous-Vide or LT ("Low-Temperature") processing is one of the prospective lines of the food industry development as it uses sparing regimes for the thermal treatment of plant and animal raw materials.
with preliminary vacuum packaging in a polymer heat-resistant film [1, 2]. The use of LT-processing makes it possible to obtain a wide range of food products with improved consumer properties, high content of thermolabile biologically active substances, prolonged shelf life. However, the LT-processing process is non-stationary, characterized by a complex of thermochemical and biological transformations of food systems. Consequently, it is necessary to develop a mathematical model of the LT processing heat transfer process in order to evaluate the dynamics of temperature field changes and optimize the regime parameters, taking into account the non-stationarity of the process, the physicochemical and thermophysical properties of food systems.

2. Materials and methods

To calculate and optimize the regime parameters of the LT-processing process, a differential equation of non-stationary thermal conductivity was applied, which for Cartesian axes is written in the form:

$$\frac{\partial t}{\partial \tau} = k \left( \frac{\partial^2 t}{\partial x^2} + \frac{\partial^2 t}{\partial y^2} + \frac{\partial^2 t}{\partial z^2} \right),$$

(1)

where $t$ - temperature, °C; $\tau$ - time length, c; $k$ - temperature conductivity coefficient of the product, m²/s.

Adding (1) with initial and boundary conditions, solutions of the nonstationary heat conductivity problem in an analytical form for bodies of the simplest form could be obtained, for example, an unbounded plate, an unbounded cylinder, a ball, or numerical methods for bodies of arbitrary shape [3]. In the differential equation (1) of the parabolic type, it is assumed that the heat spreads to at an infinite velocity. The approach based on the finite velocity of heat propagation is considered in [4], which is typical for the majority of food products. This approach enabled the introduction of the "temperature front" term and the replacement of the derivative with temperature in time in the disturbed area by its average value, along the extent of the disturbed area, brought the partial differential coefficient equation for a one-dimensional region to an ordinary differential equation.

Such model approximation of the heat passage also allowed analyzing the problems appearing from the heat treatment of food products of the simplest geometric form in the analytical form. Nevertheless, both in the first and in the second case, to carry out specific calculations it is necessary to have reference data on the thermophysical properties of heat treated products.

The vacuum-packed polycomponent food system, consisting of 16% weight percentage of carrots, 12.5% weight percentage of wheat germs flour [5], was represented as a geometric figure that can be approximated in the form of an intersection of a rectangular parallelepiped whose length and width are equal to $a = 140$ mm and $b = 105$ mm, respectively, with an ellipsoid of revolution whose semiaxes are equal to, $a$, $b$, and $c = 3.5$ mm. The corners of a rectangular parallelepiped are rounded by radius $R = 15$ mm. A schematic representation of the research object is shown in Figure 1.

![Figure 1. A schematic representation of the investigated vacuum-packed polycomponent food system.](image)

3. The study of the structure of the modified lead-tin-base bronze
To calculate the thermophysical characteristics of a polycomponent food system, it was assumed that the volume of the food system is equal to the sum of the volumes of its constituent components, then the mixture density can be calculated as follows [6]:

\[
\frac{1}{\rho} = \sum_{i=1}^{n} \frac{x_i}{\rho_i}
\]  

(2)

where \( \rho \) - food system density, kg / m³; \( x_i \) - weight percentage of the i – component, having density \( \rho_i \); \( n \) - number of components in the food system.

Specific thermal capacity of the food system is calculated from the following correspondence:

\[
c = \frac{1}{\rho} \sum_{i=1}^{n} \frac{\lambda_i}{k_i} \varphi_i
\]

(3)

where \( \lambda_i, k_i \) - thermal conductivity, W/(mK) and thermal diffusivity, m²/s, i –th component of the food system; \( \varphi_i \) - the volume ratio of the i - component of the food system, which is determined as:

\[
\varphi_i = \frac{x_i}{\rho_i} \cdot \frac{1}{\sum_{i=1}^{n} \frac{x_i}{\rho_i}}
\]

(4)

The extreme values of the thermal conductivity of the food system consisting of n components, with the use of the electroanalogy method, can be found from the following hypothesis:

- if all components of the food system are located in the direction of the heat flow, the maximum value of the thermal conductivity of the system will determine as:

\[
\lambda_{\text{max}} = \sum_{i=1}^{n} \lambda_i \varphi_i
\]

(5)

- the minimum value of the thermal conductivity of the food system corresponds to the case when individual particles have an arrangement perpendicular to the direction of heat passage (temperature gradient), which leads to application of the following relation:

\[
\frac{1}{\lambda_{\text{min}}} = \sum_{i=1}^{n} \frac{\varphi_i}{\lambda_i}
\]

(6)

For thermophysical calculations, the thermal conductivity of the food system is defined as arithmetic mean of the found extremum values:

\[
\lambda_{\text{min}} = \frac{\lambda_{\text{max}} + \lambda_{\text{min}}}{2}
\]

(7)

The thermal diffusivity of the food system in equation (1) is calculated by the formula:

\[
k = \frac{\lambda}{\rho c}
\]

(8)

The results of calculations of the thermophysical characteristics of a polycomponent food system subjected to LT-processing are presented in Table 1.
The dynamics of the temperature field in the food system, calculated using equation (1), is largely determined by the boundary conditions. Taking into account the fact that the heat treatment of the samples was carried out by hot air with a temperature of \( t_\infty = 95 ^\circ C \), for which the heat transfer coefficients are sufficiently small, boundary conditions of the 3\textsuperscript{rd} kind were determined by the equation:

\[
-\lambda \left( \frac{\partial t}{\partial n} \right)_{\text{sur}} = \alpha \cdot (t_\infty - t)
\]  

(9)

where \( \lambda \) - thermal conductivity of the product W/(m×K), \( n \) - sample surface normal, \( \alpha \) - heat-exchange coefficient from the air to the surface of the material, W/(m\(^2\)×K).

Since the test sample is contained inside the polymer container, it is necessary to evaluate its thermal resistance. Packing films have thickness of about 100 \( \mu \)m, and according to the available data [7] its thermal diffusivity has approximately the same value as the studied food system - \((11\div15)\times10^{-8}\) m\(^2\)/s; therefore its effect on the temperature field inside the product can be ignored.

The upper surface of the sample has a small curvature, so the calculation of the heat-exchange coefficient in (9) will be carried out according to the criterion equations as in the case of a flow of a flat surface by a heating agent [6]. To select the calculation formula, one should calculate the Reynold’s number:

\[
Re = \frac{ud\rho}{\mu}
\]

(10)

where \( u \) - air velocity, m/s, \( \mu \) – dynamic air viscosity, Pa\( \times \)s, \( \rho \) – air density, kg/m\(^3\), \( d \) – length of the flow path along the heat exchange surface, m.

Since the position of the sample towards to the air movement direction can be arbitrary, and the sample has no complete symmetry, calculation will be carried out for two specific directions - along the major axis of the ellipsoid of revolution and in the transverse direction.

The length of the ellipse arc, obtained when the sample, crossed by a vertical plane passing through its major axis is determined by the formula [8]:

\[
l_1 = a \int_{t_1}^{t_2} \sqrt{1 - e_1^2 \cos^2 \theta} \, dt
\]

(11)

where \( e_1 \) - ellipse eccentricity, defined by the formula:

\[
e_1 = \sqrt{1 - \frac{b^2}{a^2}}, \quad e \in [0,1).
\]

(12)

For the accepted geometry of the sample, \( t_1 = \pi/3 \), but \( t_2 = 2\pi/3 \).

After substituting the accepted values, \( a=140 \) mm, \( b=105 \) mm in the ratios (11) and (12) and using the packet of symbolic mathematics «Maple» to take the elliptic integral in (11), let us get value \( l_1 = 145 \) mm as a result.
For the transverse direction, the calculated formulas take the form:

\[ l_2 = b \int_{t_1}^{t_2} \sqrt{1 - e_2^2 \cos t} \, dt \tag{13} \]

where

\[ e_2 = \sqrt{1 - \frac{c^2}{b^2}} \tag{14} \]

\[ a \, t_1 = \pi/3, \quad a \, t_2 = 2\pi/3. \]

For value \( c = 3.5 \) mm, the arc length of the ellipse, equal to \( l_2 = 109 \) mm, was obtained.

If one considers moist air as a binary mixture of dry air and water vapor, then its density can be calculated from the ratio [9, 10]:

\[ \rho = \frac{\rho_s (1 + x)}{(x + M_s / M_{da})} \tag{15} \]

where \( P \) - molar masses of water vapor and dry air, equal respectively to \( M_s=18.016 \) kg/kmol and \( M_{da}=28.96 \) kg/kmol; \( \rho_s \) - water vapor density, kg/m³, \( x \) - moisture content of steam-air mixture.

The density of water vapor is determined from the equation of state:

\[ \rho_{li} = \frac{M_s p}{R T} \tag{16} \]

where \( R = 8314 \) $J/(\text{kmol} \times \text{K})$ - universal gas constant; \( p \) - pressure that is assumed to be equal to atmospheric, Pa; \( T \) - absolute temperature, K.

The moisture content of air at its known relative humidity is found from the ratio [9, 10]:

\[ x = \frac{\varphi M_s}{M_{da} \left( \frac{p}{p_t} \right) t^4 \exp \left[ -B \left( 1 - t^4 \right) + C \left( 1 - t \right) \right] - \varphi \} \tag{17} \]

where \( p_t = 610.8 \) Pa - pressure of saturated water vapor at \( T_0 = 273.15 \) K; \( t = T / T_t \) - relative temperature, \( A, B, C \) - coefficients, the numerical values of which [9, 10] are equal to:

\[ A = 9.248; \quad B = 27.098; \quad C = 2.005. \]

The dynamic viscosity of moist air, depending on its moisture content, can be found using the Willkie’s formula [9, 10]:

\[ \mu = \frac{\mu_s x}{x + \Phi_{1,2} M_s / M_{da}} + \frac{\mu_{da}}{1 + \Phi_{2,1} x M_{da} / M_s} \tag{18} \]

Here \( \mu_s, \mu_{da} \) - dynamic viscosity of steam and dry air, Pa:s:

\[ \Phi_{1,2} = \frac{\left[ 1 + \left( M_s / M_{da} \right)^{-1/4} \left( \mu_s / \mu_{da} \right)^{1/2} \right]^2}{2 \sqrt{2} \left( 1 + M_s / M_{da} \right)} \tag{19} \]

\[ \Phi_{2,1} = \frac{\left[ 1 + \left( M_{da} / M_s \right)^{-1/4} \left( \mu_{da} / \mu_s \right)^{1/2} \right]^2}{2 \sqrt{2} \left( 1 + M_{da} / M_s \right)} \tag{20} \]
If one uses nondimensional temperature  \( t = T / T_0 \), where \( T \) - temperature of the incoming air flow, K, then:

\[
\begin{align*}
\mu_s &= 2.91 \cdot 10^{-5} t^{3/2} / (t + 2.38) \quad (21) \\
\mu_{da} &= 2.41 \cdot 10^{-5} t^{3/2} / (t + 0.41) \quad (22)
\end{align*}
\]

At a heating air temperature of \( t_{\infty} = 100^\circ C \) and its relative humidity \( \varphi = 0.85 \) for a pressure of \( p = 101325 \) Pa, vapor density and the vapor content of the air were obtained equal to \( \rho_s = 0.588 \) kg/m\(^3\) and \( x = 3.577 \) respectively. Then, the density of moist air according to (15) will take value \( \rho = 0.642 \) kg/m\(^3\).

The dynamic viscosity of water vapor and dry air according to equations (21) and (22) is \( \mu_s = 1.24 \times 10^{-5} \) Pa\(\cdot\)s and \( \mu_{da} = 2.17 \times 10^{-5} \) Pa\(\cdot\)s, respectively; the dynamic viscosity of moist air according to equation (18) is equal to \( \mu = 1.38 \times 10^{-5} \) Pa\(\cdot\)s.

At the airflow velocity of \( u = 1.2 \) m/s, the Reynold’s number over longitudinal flow past the upper surface of the sample will be:

\[
\text{Re}_1 = \frac{1.2 \cdot 0.145 \cdot 0.642}{1.38 \cdot 10^{-5}} = 8109.
\]

Omitting the curvature, the heat transfer from the upper surface of the sample at \( \text{Re} < 5 \times 10^5 \) will be calculated for a planar surface by the following formula [6]:

\[
\text{Nu}_1 = 0.664 \times \text{Re}_1^{1/2} \times \text{Pr}^{1/3}
\]

where \( \text{Pr} \) - Prandtl number for air at the temperature of the oncoming flow, which is calculated from the ratio:

\[
\text{Pr} = \frac{\nu}{\lambda} = \frac{\nu \rho c}{\lambda}
\]

where \( \nu \) - kinetic viscosity, m\(^2\)/s; \( \rho c \) - volumetric heat capacity, J/m\(^3\)\(\times\)K; \( \lambda \) - thermal conductivity, W/m\(\times\)K of moist air.

Since \( \nu = \mu / \rho \), taking into account the previously obtained results, \( v = 2.15 \times 10^{-5} \) m\(^2\)/s.

Volumetric heat capacity of the medium as an additive quantity is found from the formula [6]:

\[
\rho c = \frac{\rho_s c_s (x + c_{da} / c_s)}{(x + M_s / M_{da})}
\]

where \( c_s, c_{da} \) - specific isobaric heat capacities of water vapor and dry air, which according to [6] for the temperature range of 0 - 95 °C can be taken equal to:

\( c_s = 1873 \) J/kg\(\times\)K, \( c_{da} = 1006 \) J/kg\(\times\)K.

As a result of the calculation by (25), one will have \( \rho c = 1079 \) J/m\(^3\)\(\times\)K.

The thermal conductivity of moist air is also an additive quantity and can be found from the equation [9, 10]:

\[
\lambda = \frac{\lambda_s x + \lambda_{da} M_s}{M_{da}}
\]

Here \( \lambda_s, \lambda_{da} \) - thermal conductivities of water vapor and dry air, determined by equations:
\[
\lambda_s = \frac{0.0595 \cdot t^{0.5}}{1 + \frac{2.46}{t}}
\]
\[
\lambda_{da} = \frac{0.0347 \cdot t^{0.5}}{1 + \frac{0.454}{t}}
\]

As a result of calculations according to (26) - (28), let us have:
\[
\lambda_s = 0.0248 \text{ W/(m×K)}, \quad \lambda_{da} = 0.0304 \text{ W/(m×K)}, \quad \lambda = 0.0257 \text{ W/(m×K)}.
\]
Thus, the Prandtl number by (24) will be equal to:
\[
\text{Pr} = 0.902.
\]

Nu number for the upper surface of the sample with its longitudinal air flow is \(\text{Nu}_1 = 57.8\).

Over the sample’s cross flow, when \(d = l_2 = 0.109 \text{ m}\), the Reynold’s number is \(\text{Re}_1 = 6096\), and Nu number is \(\text{Nu}_2 = 50.1\). Heat transfer coefficients can be found as:
\[
\alpha = \frac{\text{Nu} \lambda}{d}
\]

It gives the following results:
\[
\alpha_1 = \frac{57.8 \cdot 0.0257}{0.145} = 10.2 \text{ W/(m²×K)},
\]
\[
\alpha_2 = \frac{50.1 \cdot 0.0257}{0.109} = 11.8 \text{ W/(m²×K)}.
\]

The average value of the heat transfer coefficient over the upper surface of the sample will be
\[
\alpha = \frac{\alpha_1 + \alpha_2}{2} = 11.0 \text{ W/(m²×K)}.
\]

For the lower flat surface of a vacuum-packed product with longitudinal air flow, let us have \(d = 0.140 \text{ m}\), \(\text{Re}_1 = 7829\), \(\text{Nu}_1 = 56.8\), \(\alpha_1 = 10.4 \text{ W/(m²×K)}\).

For transverse air flow, when \(d = 0.105 \text{ m}\), let us have: \(\text{Re}_2 = 5872\), \(\text{Nu}_2 = 49.2\), \(\alpha_2 = 12.0 \text{ W/(m²×K)}\).

An average value of heat transfer coefficient is \(\alpha = 11.2 \text{ W/(m²×K)}\).

For the lateral surfaces, the heat transfer coefficient will be regarded on the upper surface.

To integrate numerically the equations of nonstationary heat conductivity (1) with boundary conditions of the 3\textsuperscript{rd} kind (2), let us reduce them to a dimensionless form. In this case it should be noted that the dimensions along the coordinate axes differ substantially for the tested object. As a result, the relaxation rates of temperature perturbations along these directions will also differ significantly. Consequently, the choice of the characteristic size of system \(l_0\), which determines the time scale for the investigated process, plays an important role.

\(l_0\) is defined as follows:
\[
l_0 = \frac{4V}{S}
\]

where \(V\) - body volume, m\(^3\); \(S\) - the area of its surface, m\(^2\).

Let us assume approximately that the vacuum-packed food system is a rectangular parallelepiped with sides \(a, b, c\). Then:
\[ l_0 = \frac{2abc}{ac + bc + ab} \]  

(30)

Let us denote \( c/a = \xi_1, c/b = \xi_2 \). Then (30):

\[ l_0 = \frac{2}{c(1 + \xi_1 + \xi_2)} \]  

(31)

Let the time scale be \( \tau_0 = t_0^2/k \). Then the dimensionless time will be \( \theta = \tau/\tau_0 = k\tau/l_0^2 \).

Let the dimensionless coordinates and temperature be defined by the expressions:

\( X = x/a; \quad Y = y/b; \quad Z = z/c; \quad T = (t_\infty - t)/(t_\infty - t_0) \),

where \( t_0 \) - the initial value of the body temperature, \( t_0 = 20^\circ C \).

Taking into account the agreed notation and ratio (31), equation (1) takes the form:

\[ \frac{\partial T}{\partial \theta} = \frac{4}{(1 + \xi_1 + \xi_2)^2} \left( \xi_1^2 \frac{\partial^2 T}{\partial X^2} + \xi_2^2 \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \right), \]  

(32)

Initial conditions are:

\[ T(X, Y, Z, 0) = 1. \]  

(33)

Boundary conditions are:

\[ \frac{\partial T(-1/2, Y, Z, \theta)}{\partial X} = -Bi_X T(-1/2, Y, Z, \theta) \]  

(34)

\[ \frac{\partial T(1/2, Y, Z, \theta)}{\partial X} = Bi_X T(1/2, Y, Z, \theta) \]  

(35)

\[ \frac{\partial T(X, -1/2, Z, \theta)}{\partial Y} = -Bi_Y T(X, -1/2, Z, \theta) \]  

(36)

\[ \frac{\partial T(X, 1/2, Z, \theta)}{\partial Y} = Bi_Y T(X, 1/2, Z, \theta) \]  

(37)

\[ \frac{\partial T(X, Y, -1/2, \theta)}{\partial Z} = -Bi_Z T(X, Y, -1/2, \theta) \]  

(38)

\[ \frac{\partial T(X, Y, Z^*, \theta)}{\partial Z} = Bi_{Z^*} T(X, Y, Z^*, \theta) \]  

(39)

Here \( Bi_X = \frac{\alpha_e \cdot a}{\lambda_t}, \quad Bi_Y = \frac{\alpha_e \cdot b}{\lambda_t}, \quad Bi_Z = \frac{\alpha_e \cdot h}{\lambda_t}, \quad h \sim \) the height of the rectangular parallelepiped, equivalent in volume to the sample, for which the upper edge is an ellipsoid of revolution (see equation (40)) and the lower edge is a plane.

If the equation of a triaxial ellipsoid of revolution, forming the upper edge of the sample, is:

\[ \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1 \]  

(40)

then the volume of the upper half will be:

\[ V_s = 4c \int_0^{1/2} \int_0^{b/2} \int_0^{a/2} dxdydz. \]  

(41)
Since the volume of the lower half is:

\[ V_l = ab \times c, \]  

then the total volume of the sample is:

\[ V = V_t + V_l, \]  

and the height of the equal rectangular parallelepiped is:

\[ h = V / (ab). \]  

Let us note that equation (32) under \( \xi_1 \to 0 \) and \( \xi_2 \to 0 \) becomes one-dimensional:

\[ \frac{\partial T}{\partial \theta} = 4 \frac{\partial^2 T}{\partial Z^2}. \]

thus, it corresponds to the case of heating (cooling) of an unbounded plate.

Computations, according to (44) in view of (41) - (43), carried out using the «Maple» symbol mathematics packet, gave the following result - \( h = 6.688 \) mm. The found value of the equivalent height of the rectangular parallelepiped made it possible to specify the characteristic size of investigated object \( l_0 \) by replacing value \( c \) by \( h/2 \) in (30).

When solving the system of partial differential equations (32) - (39), flexPDE mathematical package was applied, using the finite element method for modeling objects with distributed parameters. The spatial grid with the number of nodes \( n = 20000 \) was used in the calculations, the accuracy of the calculations is \( 1 \times 10^{-4} \). The analysis of calculations was processed using the developed software Python 3.4.

The simulation results, showing the evolution of the temperature fields in the \( Z = 0 \) plane and on the upper surface of the sample, having the shape of the ellipsoid of revolution are shown in Figure 2.
The validity check of the model approximations has shown that the maximum deviation of the calculation results from the experimental data on the LT-system is not more than 7.2%.

4. Conclusion
The developed mathematical model allows analyzing and optimizing the LT-processing regimes of a wide range of food raw materials, of various geometric shapes and sizes, having various physicochemical and thermophysical properties, taking into account their non-stationarity under thermal influence.

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