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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ

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NUMERICAL SIMULATION OF PROCESSES OF THERMAL FOOD STERILIZATION IN CYLINDRICAL CONTAINERS USING FINITE DIFFERENTIATION

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1. Introduction

One of the key issues in the area of food engineering are inactivate microorganisms in the products. The idea is, on the one hand, to prevent the potential contamination and to reduce the impact on public health, and, on the other hand, to increase the usefulness of the products by supplying the consumer healthy products of a high quality and minimizing the losses of nutritious and sensorial properties. The food's sterilization is a basic operation at industrial level, which consists of heating the solid or liquid food to a temperature higher than 100?C and during sufficient time for eliminating the microbial and enzymatic activity, thus, assuring the product's stability.

In this paper, we consider the process of sterilization in products packed at engineering's level as a thermal process. This process deals with a heater environment and the environment that is necessary to heat; besides, the different mechanisms of transfer of heat intervenes the process. These mechanisms add to the product's heterogeneity, resulting in a more complex process in case when one pretends to predict the behavior of the product.

In spite of the advance of the technology in the design, development, optimization and adaptation of technologies in the unitary operational area of food production, a significant backwardness exists for the case of the solid sterilization's products that are handled with steam water. In particular, one can point out at the irrational use of energy, the diminishing of the thermal efficiency of the process, at least in a number of cases. This decrease happens for there is regularly an excessive duration of the process (treatment's time), which is applied in order to assure the destruction of the microbial load, but, at the same time, often leading to the deterioration of the physical quality, organoleptic qualities, chemistry and sensorial of the product, and incurring in expensive costs of operation and of the maintenance of the equipment used in specific boilers.

The major objective of this paper is to use basic knowledge of the transfer of heat to perform a numeric simulation with respect to the thermodynamic kinetics of thermal inactivation of microorganisms. It is expected that the chosen approach would permit to create a theoretical model of the behavior of a process of thermal sterilization of solid products packed in cylindrical form. The theoretical model includes the construction of the curves of penetration of heat, times of prosecution, lethality of the process and value of sterilization of the thermal treatment.

In order to achieve the major objective of the present paper, the author defines his specific objectives as:

– to implement the technique of finite differentiation in cylindrical coordinated for predicting the curves of penetration of heat in packed food, and

– to determine the lethality, value of sterilization and effective time of the process of thermal sterilization.

2. Basic concepts of thermal sterilization of food

The food sterilization is a basic operation at industrial level where the solid or liquid food is heated to a temperature higher than 100 °C. The process lasts as long as is necessary to guarantee the elimination of the microbial and enzymatic activity for assuring the stability of the product.

As Fellows (2000) argues, the sterilization process in products packed at engineering level can be considered a process of thermal treatment of food; since there is a heater environment, the food and the container that contains it. In this process, the transfer of heat is applied to the conduction in the food and convection in the surface of the container. However, the transfer of heat adds to the heterogeneity of the product (food) and makes more difficult to predict its behavior because of a more complex process.

Although the principal objective is the destruction of the microorganisms, it is important to remember that there is also the side-effects like enzymatic destruction, softening of the fabrics, changes of the digestion, etc. that must be controlled for they don't produce excessive results. Besides, the following negative side-effects are also unavoidable: the destruction of nutritious components, the decrease in quality of organol?ptic features like color, aroma, etc.. Hence, the sterilization should be adjusted to such a model that to obtain desirable results and minimize the undesirable. In this model, it is likely that special conditions for finding the way that permits to obtain a satisfactory global result should be clearly defined (see Casp and April, 1999).

3. Quantification

3.1. Kinetics of the Microbial Inactivation. As well-known, the study of the microbial inactivation consists in the determination of characteristic variables of thermoresistance of a microorganism in question. In this paper, we devote a particular attention to the factor of decimal reduction, the key issue of microbial inactivation.

By the factor of decimal reduction (*D*), we understand the time necessary for the suspension of spores to a constant temperature *T*, with which it is possible to destroy the 90 % of the microorganisms present in the suspension (see Mafart,1994).

The factor of decimal reduction is determined from the curve of surviving number of the reference microorganism to the temperature *T*, with respect to *t*. It is similar to the inverse of the slope. The value *D* is reference with respect to the temperature in which it was determinate (see Fig. 1).

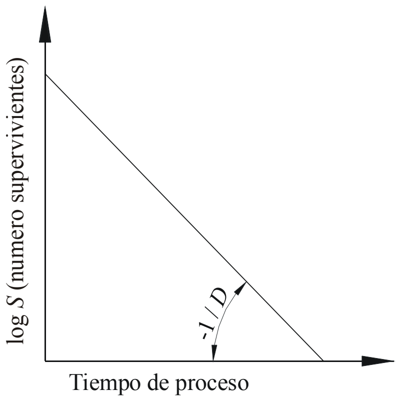

Figure 1. Curve of «surviving».

In addition, we introduce value *Z*, which defines the thermoresistance characteristic of each of the species of microorganisms in the environment of defined composition. As argued by Mafart (1994), when the temperature rises in z degrees, the time required for obtaining the same thermal destruction is 10 times minor.

The value *Z* is determined from the curve time of the process with respect to the temperature. Clearly, it is the same as to the inverse of the slope. The value *Z* is the reference to the respective lethality with which it was determined (see Fig. 2).

3.2 Lethality of the process or biological destruction. The lethality is the relation between two thermal treatments of 1 minute, one carried out on the reference temperature (*T**) and other to some temperature (*T*), for microorganism whose thermoresistance has value *Z* (°C).

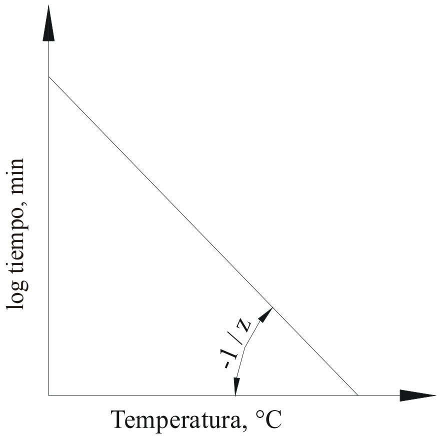

Figure 2. Curve of influence of the temperature on the time of thermal treatment.

Pham (1987), Casp and April (1999) and Ibarz, and Barbosa, (2003) described the determination of the lethality in the following way:

$$L_T = \frac{D^*}{D} = 10^{\frac{T-T^*}{z}}. \tag{1}$$

3.3. Value of sterilization of the process. If the lethality process is extended during the period of time *t* and it has a constant temperature, (1) is going to change to:

$$F_T = L_T \cdot t = t \cdot 10^{\frac{T-T^*}{z}}. \tag{2}$$

The [2] implicates that the heating and the cooling is instantaneous. However, this is not possible in practice, since during the process, there is a variation of the temperature with respect to the time of the process for that the lethality value obtained different values. Hence, (2) can be expressed as:

$$F_T = \sum L_{Ti} \cdot \Delta t_i. \tag{3}$$

For processes with a continuous variation of temperature (3) can be presented as:

$$F = \int_0^t 10^{\frac{T-T^*}{z}} dt. \tag{4}$$

We argue that to calculate the thermoresistance it is a good idea to examine the microorganism , which has a bigger thermal resistance to the destruction. For the case of sterilization the chosen microorganism is the Clostridium botulinum, which parameter *z* has a value of 10 °C (see Casp and April, 1999)

4. Curves of penetration of heat

The curves of penetration of heat are the record of the variation of the temperature in the time, for some point inside the product. Furthermore, these curves should be determined at some critical point, at which it is possible to find the biggest thermal resistance to the microorganism destruction. This is the point of the localization inside the product that would have the lowest probability of increasing its temperature.

A typical curve of penetration of heat with its respective phases for products packed during a sterilization process can be seeing in Fig. 3. Here, the following factors should be taken into account:

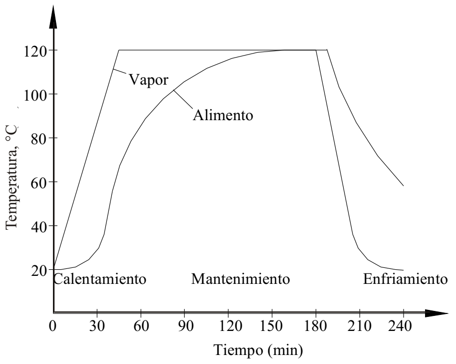

Figure 3. Curves of penetration of heat in packed food.

– Heating: During this stage, the change of temperature in the product is not appreciable.

– Maintenance: it is the longer stage of the sterilization, during which the product reaches the temperature of the fluid heater.

– Cooling: During this stage, the difference of temperatures between the enclosure and the critical point of the product is of crucial importance.

5. The importance at the level of industrial sterilization

The attention paid to this thermal treatment at the industrial level is the guarantee that the microbial and enzymatic activity elimination assures the product's stability that is possible to obtain through the treatment in question: The advantages are obvious:

– Longer conservation of the product delivered to the market. This reduces the industrial losses.

– The consumer's satisfaction with the product of high quality supported by a value of sterilization of 12 minutes that guarantees almost the total destruction of initial microorganisms.

– Comparative advantage of the product introduced to the market with the presence of similar characteristics.

– Maximization of the quantity of nutritious, good color and aroma characteristics of the product.

6. Numerical model

Thus far, we examined the process of thermal sterilization in solid isotropic and homogeneous products packed in cylindrical form and heated with steam water; the process that transfers the heat between heated environment and product. In the case with the steam water, it is presumed that the heat diffusion conductions into solid without circumferential dependence in cylindrical coordinates with convection of third class in the walls of container and that the camp temperature distribution depends on the time.

Besides, we despised the resistance of conduction for the container, just as it is the case with the industry use materials that are highly conductive.

We describe the distribution of temperature in cylindrical coordinate as follows:

$$\frac{1}{r}\frac{\partial}{\partial}\left(Kr\frac{\partial T}{\partial r}\right)+\frac{1}{r^2}\frac{\partial}{\partial \phi}\left(K\frac{\partial T}{\partial \phi}\right)+\frac{\partial}{\partial z}\left(K\frac{\partial T}{\partial z}\right)+\dot{q}=\rho C_P\frac{\partial T}{\partial t}, \tag{5}$$

where r – radial coordinate (m), z – axial coordinate (m), ϕ – angular coordinate (rad), K – thermal conductivity of the material (W/mK), ρ – density of the material (kg/m^3), C_P – heat specifies of the material (kJ/kg·K), $\dot{q}$ – energy generated by unit of volume (W/m^3), T – temperature (K), t – time (s).

For the process of sterilization, (5) is resolved based

– Initial temperature is uniform and constant in all

– Heat transfer in angular direction equals to zero,

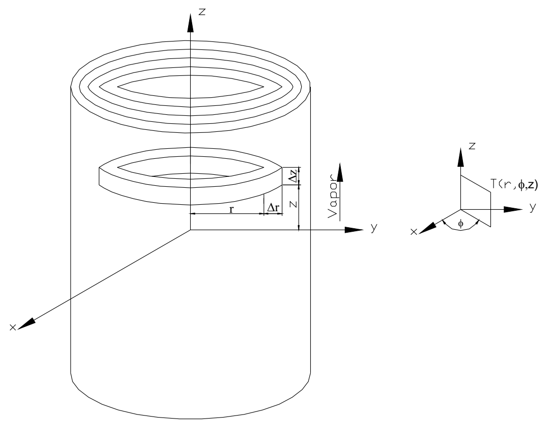

Figure 4. Outline of the process.

– Container resistance is presumed to be zero value, i.e. the external temperature of the product is similar to that of the container, resulting in that the fluid interacts directly with the product.

– Process is symmetric in relation to axis «x», «r» and «ϕ», and, therefore, the process is studied with a eighth of the cylinder, composed for fourth of ring showed in Fig. 5, where the internal limits are adiabatic.

* There is no generation of heat into the container

* There is no heat interchange for radiation in the container surface

* There is no transference of mass nor process of change of phase

In addition, we presume the following conditions to solve (5):

– Interior limits are adiabatic.

– External limits are at the same temperature as the heat fluid.

– Heat transfer in the external limits is only aimed only at convection.

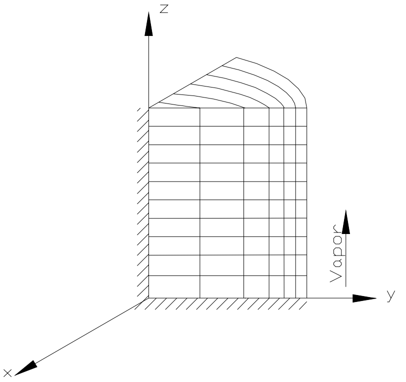

Figure 5. Isothermal ring.

6.1 Numeric solution. (5) is a partial differential equation of parabolic nature. To simulate the phenomenon of the transport wrapped in the process of thermal sterilization, we used the approximation method of solution of control volumes. We apply the energy analysis to control volumes for each node (control volumes) using the finite differentiation technique methods of implicit solution. This method was selected since there are no restrictions of stability originated for the value of the increment for the selected variable time (Δt). However, the increment in the variable time (Δt) must be reasonably small in order to obtain results that are near the real solution of the partial differential equation.

The finite difference is applied to determinate variable only in discreet point and, because of that, the following steps are necessary:

1. Subdivide the cylinder in number of small divisions.
2. Assign to each region a point of reference at the center (i.e. the nodal point or node).

Settlement of point is known as nodal red, mesh or grille. The Fig. 6 showed the mesh for the conductive bi-dimensional environment in the solution of (5).

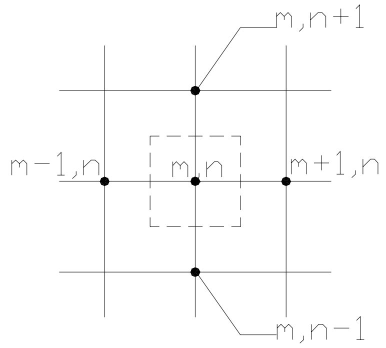

Figure 6. Conductive Environment.

Temperature of any node in the time (t+Δt) is calculated with the new temperature of the adjacent nodes. However, for the determination of the temperature of nodal ignorance in (t+Δt), the corresponding nodal equation should be considered simultaneously. With the implicit method, we come up with equation for each node that has been resolved simultaneously.

6.2. Form of the red nodal. Figure 7 shows a typical distribution nodal use for performing the analysis of energy control volume, where M is total number of nodes in axial direction and N is total number of nodes in radial direction, where the respective energy balance was applied to each Node. The axis of coordinate for Z=0 y R=0 is considered symmetry axes.

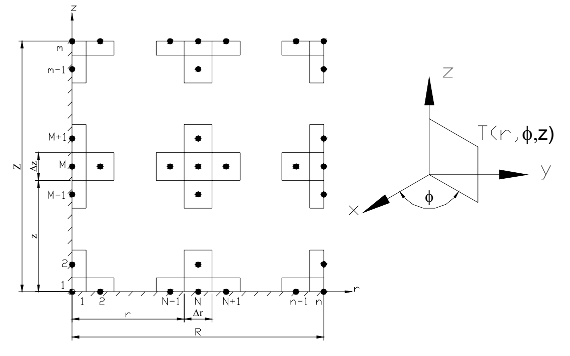

Figure 7. Red nodal.

For each node and depending on the coordinate, the heat transfer for conduction was defined with respect to the law of Fourier as follows:

$$q_{\text{cond}} = KA\frac{\Delta T}{\Delta L}, \tag{6}$$

where K – thermal conductivity of the material (W/mK), A – area of heat transfer perpendicular to the flow of heat (m^2), ΔT – difference of temperature between the node m, n and their contiguous one (K), ΔL – distances among the node m, n and their contiguous one parallel to the flow of heat (m).

As concern the superficial nodes or nodes located in the wall of the container, the heat transfer was defined in line with Newton's law of heating:

$$q_{\text{conv}} = hA\left(T_\infty - T_s\right), \tag{7}$$

where h – coefficient convection of steam water (W/(m^2·K)), A – area of heat transfer perpendicular to the flow of heat (m^2), T_∞ – temperature of the fluid (K), T_s – temperature of the surface (K).

As an illustration, node 6 in Fig. 8 has the energy balance as shown below:

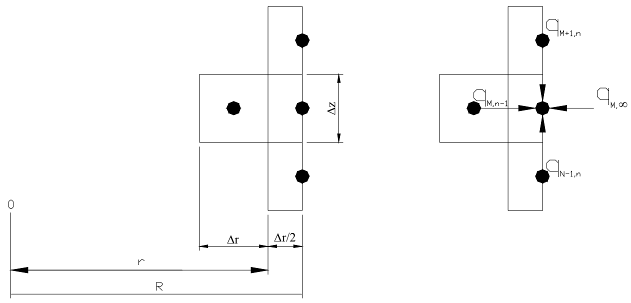

Figure 8. Node six.

$$q_{M,n-1} + q_{M,\infty} + q_{M-1,n} + q_{M+1,n} = V\rho C_P\frac{\partial T}{\partial t}. \tag{8}$$

From (6) and (7) we obtain:

$$q_{M,n-1}=\frac{KAdT}{L}=\frac{K2\pi\left(R-\Delta r/2\right)\Delta z\left(T_{M,n-1}^{i+1}-T_{M,n}^{i+1}\right)}{4\Delta r}=$$
$$=\frac{K\pi\left(2R-\Delta r\right)\Delta z\left(T_{M,n-1}^{i+1}-T_{M,n}^{i+1}\right)}{4\Delta r}; \qquad (9)$$

$$q_{M,\infty}=h_1AdT=\frac{2\pi R\Delta z h_1\left(T_\infty-T_{M,n}^{i+1}\right)}{4}=$$
$$=\frac{\pi R h_1\Delta z\left(T_\infty-T_{M,n}^{i+1}\right)}{2}; \qquad (10)$$

$$q_{M-1,n}=\frac{KAdT}{L}=$$
$$=\frac{K\pi\left(R^2-\left(R-\Delta r/2\right)^2\right)\left(T_{M-1,n}^{i+1}-T_{M,n}^{i+1}\right)}{4\Delta z}=$$
$$=\frac{K\pi\left(4R-\Delta r\right)\Delta r\left(T_{M-1,n}^{i+1}-T_{M,n}^{i+1}\right)}{16\Delta z}; \qquad (11)$$

$$q_{M+1,n}=\frac{KAdT}{L}=$$
$$=\frac{K\pi\left(R^2-\left(R-\Delta r/2\right)^2\right)\left(T_{M+1,n}^{i+1}-T_{M,n}^{i+1}\right)}{4\Delta z}=$$
$$=\frac{K\pi\left(4R-\Delta r\right)\Delta r\left(T_{M+1,n}^{i+1}-T_{M,n}^{i+1}\right)}{16\Delta z}. \qquad (12)$$

Volume differential:

$$V=\frac{\pi\left(R^2-\left(R-\Delta r/2\right)^2\right)\Delta z}{4}=\frac{\pi\left(4R-\Delta r\right)\Delta r\Delta z}{16}. \qquad (13)$$

Replacing (9), (10), (11), (12) and (13) in (8) and simplifying one obtains:

$$T_{M,n}^{i+1}\left(\frac{4\left(2R-\Delta r\right)}{\Delta r^2\left(4R-\Delta r\right)}+\frac{8Rh_1}{K\left(4R-\Delta r\right)\Delta r}+\frac{2}{\Delta z^2}+\frac{\rho C_P}{K\Delta t}\right)-$$
$$-\frac{4\left(2R-\Delta r\right)T_{M,n-1}^{i+1}}{\Delta r^2\left(4R-\Delta r\right)}-\frac{T_{M-1,n}^{i+1}}{\Delta z^2}-\frac{T_{M+1,n}^{i+1}}{\Delta z^2}= \qquad (14)$$
$$=\frac{\rho C_P T_{M,n}^{i}}{K\Delta t}+\frac{8Rh_1T_\infty}{K\left(4R-\Delta r\right)\Delta r}.$$

Equally was worked the other nodes where: n – number of nodes in the radial direction; m – number of nodes in the axial direction; N – number of the node in the radial direction, their value oscillates among 2 y n–1; M – number of the node in the axial direction, their value oscillates among 2 y m–1; R – radial dimension of the recipient (m); Z – axial dimension of the recipient (m); Δr – dimension of the radial differential; Δz – dimension of the axial differential.

With the lineal equation of each node we obtain a mould system of the form:

$$\left[A\right]\left[T^{i+1}\right]=\left[T^{i}\right],$$

where the mould A is composed of element that depends of the geometric form of the container, food properties, number of nodes in the radial and axial direction, coefficient heat transfer for convection of fluid heater, coefficient heat transfer for conduction of the food, vector T^i, initial temperature that is uniform in all products.

7. Conclusions

We illustrate our theoretical approach with the results in the list below that were obtained using the above algorithm for two established geometries:

* Composition of water = 60.8 %
* Composition of Proteins = 18.7 %
* Composition of fat = 19.6 %
* Composition of carbohydrates = 0 %
* Composition of ashy = 0.9 %
* Container 1: Height = 0.073 m
* radiate = 0.027 m
* Container 2: Height = 0.2222 m
* radiate = 0.0786 m
* Temperature heater fluid (steam water) = 125 °C
* Temperature cooling fluid (Water) =25 °C
* Initial temperature of the food = 25 °C
* Temperature sterilization = 121 °C
* Coefficient of convection of the vapor = = 600 W/(m^2·K)
* Coefficient of convection of the water = = 200 W/(m^2·K)
* Numbers of nodes to which was applied the calculations = 1
* Delta of time = 120 s
* Time on dimension of the process = 30000 s
* CUT = 300 s

We argue that based on data from Table 1, one can easily observe that sterilization time for the smallest container size is less that the time for the biggest container size, the phenomena described before. This is because the biggest container needs more time for

Table 1

Time and sterilization of the process

Height, m	Radius, m	Nodes radial	Nodes axial	Time heating, min	Sterilization heating, min	Time cooling, min	Sterilization cooling, min
0.0730	0.02700	30	30	62	12.7864	4	$3{,}5\cdot10^{-5}$
0.2222	0.07860	30	30	356	11.8076	386	3.4839

catching up the necessary temperature for its sterilization. Also, from above data it is clear that in the cooling area the sterilization is extremely small with respect to the heating area. Hence, it is possible to depreciate this kind of sterilization, and appreciate in the lethality curves because the cooling time is significantly shorter.

Curves of heat penetration. Figures 9 and 10 show that the container of the biggest size requires more time in the fluid heater for catching up a temperature that guarantees the sterilization of the product Besides, one can see from these figures the heating and cooling areas of the product as well as thermal behavior of the environment heater.

Curves of Lethality. Figures 11 and 12 show that the biggest size container needs more time for catching up with the maximum lethality value, which guarantees the sterilization of the product. Cooling area has a low contribution to the lethality since the curves in this area have vertical behavior that indicates that the lethality in this stage is very low and have a short life time.

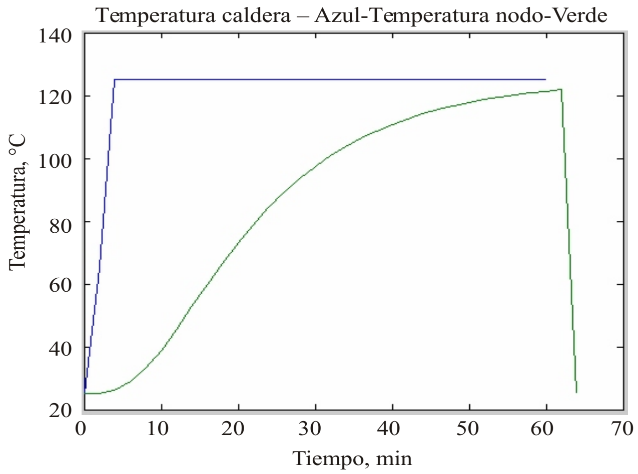

Figure 9. Behavior of the temperature in time for the container 1.

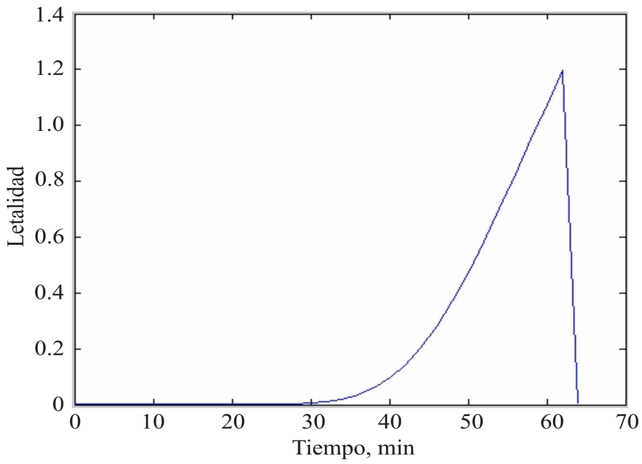

Figure 11. Behavior of the lethality in time for the container 1.

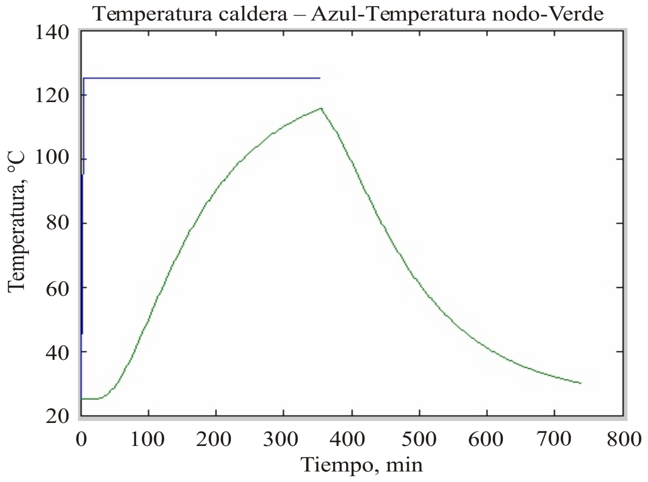

Figure 10. Behavior of the temperature in time for the container 2.

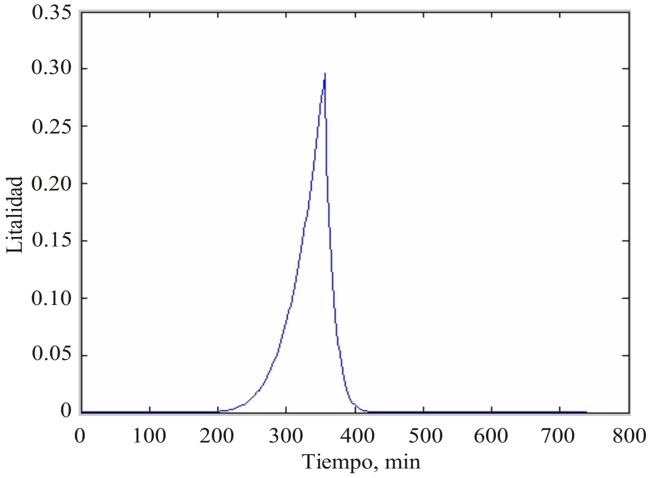

Figure 12. Behavior of the lethality in the time for the container 2.

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