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SIGMOID MODEL: APPLICATION TO HEAT TRANSFER IN VEGETABLE PRESERVES STERILIZED IN GLASS JARS

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***Abstract*— A sigmoid model is proposed for the simulation of food temperature evolution during the processing of preserves in batch low capacity sterilizers. Predicted results are compared against experimental data and a formula method (exponential) widely used in the simulation and control of industrial processes. The proposed model result to be simple and accurate for the prediction of thermal histories of foods of different shapes and sizes sterilized in glass jars of different sizes, and may be very useful for low volume processors. The exponential model did not provide accurate predictions for these processing conditions.**

***Keywords*— Modelling; Heat Transfer; Glass Containers; Particulate Foods; Sigmoid Model**

I. INTRODUCTION

During the last years there has been in Argentina a steady increase in the processing of low volumes of vegetable and fruit preserves at commercial level (home-made, organic, specialties, etc.), due to their much higher value (www.alimentosargentinos.gov.ar, 2006). All these products are filled into transparent glass containers which are hermetically sealed and submitted to a heat treatment to secure microbial innocuousness and to increase their shelf life (Wang *et al.*, 2003). In these cases, visual quality (appearance) of the products - normally whole or sliced fruits or vegetables - is the main quality index that costumers count on (Marra and Romano, 2001). The sterilizing effect of heat treatment is due mainly to protein denaturation, especially of those enzymes that regulate the metabolism of microbes. Nutritious components, like vitamins, are also affected by the heat treatment. All these changes are tightly related to the time-temperature history of the food during thermal processing. So, it is mandatory design process schedules that provoke the minimal changes in colour, shape and overall appearance, and nutrients content, compatible with the destruction of microrganisms. That is why it is necessary to count on simple and accurate methods to predict product temperature evolution during thermal treatment, so as to minimize the usual thermal abuse due to overpricessing. Besides, as processors work at an artisan level, dealing with small batches under poorly standardized conditions, it is usual that they change the size of the containers or that of the products sterilized. An additionnal complexity is that retort temperatures – in these low volume batches – generally are not constant but vary during processing, increasing up to an almost constant value.

Although sterilization is widely used for food preservation, only processing of foods packaged in cans or plastic containers and continuous aseptic processing (without containers) have been studied in depth from the heat transfer point of view. Almost no attention has been devoted to food processing in glass containers (Maroulis and Saravacos, 2003).

Few references to this subject can be found in literature. Bimbenet and Michiels (1974) presented an initial theory for heat transfer in these systems (particulate foods in a liquid medium packaged in glass containers). Some later papers that dealt with the simulation of particular cases can be found (Akterian and Fikiin, 1994; Akterian, 1995; Abril *et al.*, 1998; Márquez *et al.*, 1998, 2001, 2002, 2003).

In this work an easy-to-use approximate calculation method able to predict heat penetration in particulate foods of different shapes and sizes, immersed in a liquid medium, and packaged in glass containers of diverse volumes is proposed.

The method is especially useful for heat treatments with time variable process conditions (come-up period) and enables to relate the variation of heating medium temperature to food temperature and to link it to microbe destruction and loss of quality kinetics.

II. MATERIALS AND METHODS

A. Containers and Samples

To perform the tests three types of cylindrical glass containers were used (Table 1). The containers were filled with cylinders, cubes or spheres of 1.0, 1.5 and 2.0 cm of characteristic dimension CL (diameter, side and diameter, respectively). The length of cylinders was different according to the volume and height of the glass containers used, being 9.0, 11.0 and 10.0 cm for jars of 360, 660* y 660** cm^3, respectively. These shapes and sizes were selected according to those of products and containers found in the markets.

As the objective was to simulate the pasteurization and sterilization of fruits and vegetables, a test material of thermal properties similar to those of fruits and vegetables was used for the samples, in this case high-density polyethylene. The amount of test material filled

Table 1: External Dimensions of Glass Jars

Volume of jars (cm^3)	Diameter (cm)	Height (cm)
360	7.32	11.95
660 *	8.72	15.05
660 **	8.99	13.63

to each container was calculated considering 45% of porosity. As covering liquid a 4% solution of NaCl was added, completing 90% of the total volume of the container.

B. Retort System

Tests were performed in a vertical batch retort built in stainless steel, with a holding capacity of 27 or 12 containers with 360 or 660 cm^3 of volume, respectively. This retort is furnished with an automatic security valve that opens at the pressure of 2 atmospheres, reaching and maintaining a final temperature of approximately 118 ºC. This type of retort and working temperature are typical to little-volume processors.

C. Data Acquisition

Temperatures within the retort and in the slowest heating place of the load in the containers (determined in exploratory runs) were measured, each 15 seconds, using Type T - copper-constantan - (Cu-CuNi) thermocouples. To this end, the metallic lids of the containers were drilled in the centre to let the passage of the thermocouple (Fig. 1). A high-temperature resistant seal was used to secure airtightness around the thermocouple in the lid. Thermal histories were measured and registered using a multi-channel data acquisition system KEITHLEY model AS-TC.

D. Thermal Processing

Thermal processing of the simulated preserves consisted of an initial heating stage of approximately 30 minutes, where retort temperature increases from the initial (ambient) temperature up to a final temperature of about 118 ºC, regulated by the security valve set to approximately two atmospheres. This stage is followed by a second period during which temperature maintains practically constant during 14 minutes.

In this work, only the heating stage is simulated, assuming that the stage of cooling is rapid enough to have little influence on microbe destruction or quality decay.

Experiments were performed by triplicate. The proposed calculation methods – described later - were adjusted to each thermal history, and the values of the regression parameters were averaged for each shape and size.

Figure 1: Containers and Samples, Showing the Insertion of Thermocouples through the Lids

E. Modelling of heat penetration

i) Heat penetration was modelled by means of a standard *Formula Method* (Ball, 1923; Ball and Olson , 1957; Holdsworth, 1997). This exponential model, widely used in industrial processing of preserves, is defined through two parameters: f_{he} and j_h,

$$T_c{}^d = \frac{T_r - T_c}{T_r - T_0} = j_h \cdot e^{-2.303 \cdot t / f_{he}} \tag{1}$$

being f_{he} the time the system needs to traverse a natural logarithm cycle in the semilogarithmic plot of Eq. (1) and depends on product thermal properties, shape and size and heat transfer conditions, meanwhile j_h is mainly related container and food shapes and sizes.

Their values were calculated by linear regression of the semilogarithmic plot of $T_c{}^d$ vs. time, being j_h and f_{he}, respectively, the intercept and the slope of the linear plot.

ii) After the study of the shapes of the experimental heating curves (see Figs. 2 and 3) a sigmoid model, defined by Eq. (2) and characterized by four parameters: A_1, A_2, t_o, and dt, is proposed:

$$T_c = \frac{(A_1 - A_2)}{1 + e^{(t - t_o)/dt}} + A_2 \cdot \tag{2}$$

To calculate the parameters, a nonlinear fitting of experimental data to Eq. (2) was done using the software Origin 7.0, prescribing parameter A_2 as the final retort temperature.

F. Calculation of Microbial Lethality

Accumulated lethalities were calculated in the usual way, by means of Eq. (3), as the integral of the lethal rate L along the processing time. Experimental thermal histories and those predicted by both models were used. As reference micrtorganisms *Clostridium pasteurianum* ($D_{120ºC}$ = 0.01min. and z_e = 10ºC), were used.

$$F = \int L dt = \int 10^{(Tc(t) - Tref)/z_e} dt \,. \tag{3}$$

Accumulated lethality values *F* were calculated by approximate integration of Eq. (3) with a second-order Newton-Cotes method, using Excel 7.0.

G. Validation of the Model

Both prediction methods were validated comparing simulated temperatures against experimental ones. To perform these comparisons average absolute percent residues, as defined in Eq. (4), were used:

$$R = \frac{1}{m} \sum_{i=1}^{m} \frac{|T_s - T_e|}{T_e} 100(\%) \cdot \tag{4}$$

Calculated values of accumulated lethality *F* were also compared, using the relative percent absolute difference DF:

$$DF = \frac{|F_s - F_e|}{F_e} 100(\%) \cdot \tag{5}$$

III. RESULTS AND DISCUSSION

Figure 2 shows the thermal histories of cubes of CL=1,5 cm and for the three jar sizes, during thermal processing with variable external medium temperature. Respect to retort temperature, it shows two characteristic periods: one initial with continuous increase (firstly steady up to approximately 80ºC, later with lower slope) and a second period of constant temperature, regulated by internal pressure in the retort. Temperature histories within the autoclave were similar for both types of 660 cm^3 jars, but differed from those of the cases of 360 cm^3 jars, This difference is very clear up to autoclave temperatures near to 80 ºC, which could mean that it depends of the fraction of sterilizer volume filled with the jars. When using 360 cm^3 jars the free volume is smaller, because these containers allow a more compact stacking than 660 cm^3 jars. This, in turn, means a lower air volume with less resistance to heat transfer to the jars. When sterilizer temperatures are higher, from about 80ºC on, thermal histories of retorts tend to superimpose. This is probably due to saturation of air with water vapour, which facilitates heat transfer to jars, so that heat transfer rate is independent of the volume occupied by flasks.

In Figs. 2 and 3 it can be easily seen an initial period during which food temperature maintains constant (called time delay or lag). This delay depends of food material properties (higher thermal diffusivity implies less lag), diameter of the container (higher diameter increases delay, see Fig. 2), thickness of the glass of the flask (lower thickness implies less resistance to heat transfer and less delay) and the size (LC) of the heated products (smaller LC means lower delay, see Fig. 3). This behaviour has already been described by Márquez *et al.*, (2003).

Figure 4 shows the experimental and simulated – by both methods – thermal history for cylinders with 2.0 cm of diameter in a jar of 660** cm^3. As can be seen, the exponential model only works satisfactorily at long processing times (when retort temperature T_r is constant), but at short process times deviations are considerable. This model could be useful for low acidity foods (vegetables), were process times are long and the initial error in predicted temperature has no weight on overall calculated lethality.

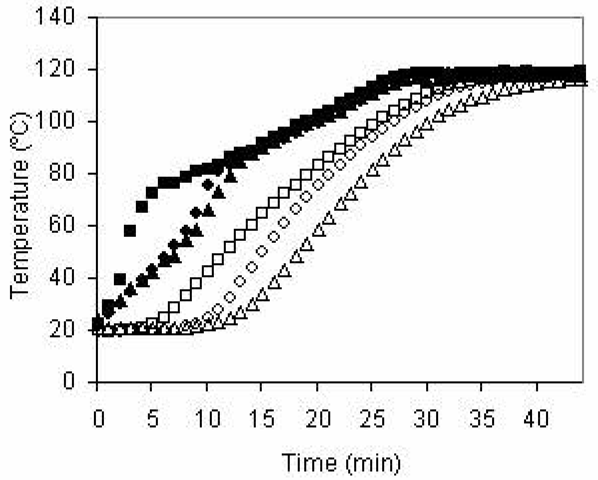

Figure 2: Experimental Thermal History of Retort Temperature and of a Cube of 1.5 cm of Side in the Slowest Heating Point. 360 cm^3: (□) cube, (■) retort; 660* cm^3: (○) cube, (●) retort; 660** cm^3: (Δ) cube, (▲) retort.

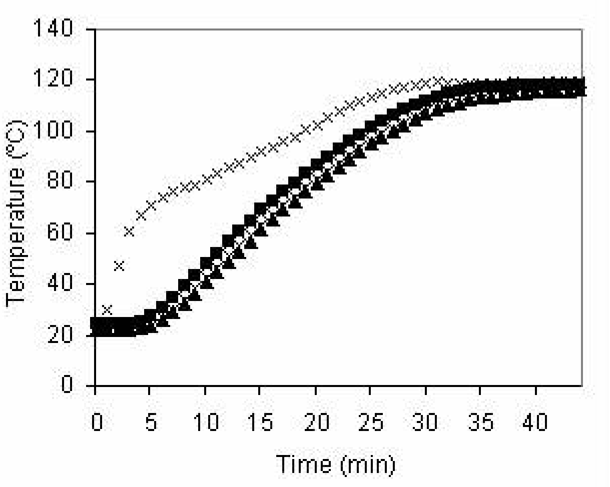

Figure 3: Experimental Thermal History of Spheres in Jars of 360 cm^3. (x) retort; (■) 1.0 cm; (○) 1.5 cm; (▲) 2.0 cm.

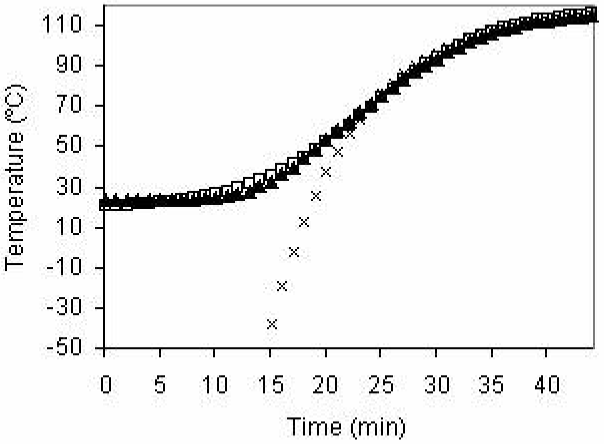

Figure 4: Experimental and Simulated Thermal History of a Cylinder of Diameter = 2.0 cm. (▲) Real; (x) Exponential Model and (□) Sigmoid Model.

Meanwhile, the sigmoid model predicts temperatures with high accuracy at short and large processing times, because it adequately considers the variation in T_r. This means that this model is also useful for short processing times, as in the case of high acidity foods (fruits).

The cited behaviours of the models were the same for the different shapes and sizes of containers and products.

Residues calculated according to Eq. (4), for all the predicted temperatures with the sigmoid model, were lower than 6 %, which verifies its high accuracy (Tables 2.a, 2.b and 2.c). Meanwhile, R for the exponential model were higher than 100% (results not shown).

Table 2.a: Calculated residues for the predicted temperatures for cylinders using the sigmoid model

Volume of Containers (cm^3)	CL (cm)		
	1.0	1.5	2.0
360	4.20	4.27	4.11
660*	3.47	4.78	4.67
660**	2.22	2.83	3.35

Table 2.b: Calculated residues for the predicted temperatures for cubes using the sigmoid model

Volume of Containers (cm^3)	CL (cm)		
	1.0	1.5	2.0
360	2.76	3.10	3.70
660*	4.62	4.47	4.95
660**	3.91	3.81	4.27

Table 2.c: Calculated residues for the predicted temperatures for spheres using the sigmoid model

Volume of Containers (cm^3)	CL (cm)		
	1.0	1.5	2.0
360	2.45	2.25	2.32
660*	5.26	3.77	4.04
660**	3.38	2.38	3.55

Accumulated lethalities *F* for the different container and product sizes are presented in Fig. 5.a, 5.b and 5.c, for cylinders, cubes and spheres, respectively. For the shapes of cubes and spheres it can be observed that *F* lowers when the characteristic dimension of the product increases. The same trend presents respect to the influence of jar diameter. The only exception is for one of the 660 cm^3 jars for cylinders, where the 660* has lower *F* than for the jars 660** (with higher external diameter). This could be explained based in the higher length of the cylinders for the first case. This allows us to deduce that lethality values depend more markedly on product size than on jar size.

The range of the differences DF is between 0.03% and 49.18%, with an average of 19.30%, when considering all shapes and dimensions tested.

Based on the previously presented results, the advantage of the sigmoid model respect to the exponential one, lies in its ability to reproduce with very good accuracy the whole thermal history of the processed product. This is useful for the precise predicttion not only of microbial death but also of the variation of product quality indexes (colour, texture, nutrient losses, etc.), using kinetic models coupled to the predicted thermal history.

Parameters of the sigmoid model calculated from the respective thermal histories are presented in Tables 3.a; 3.b and 3.c. In the sigmoid model, parameter t_0 (min) is related to the delay of the system and is defined as the time that the slowest heating point in the system reaches a temperature $(A_1+A_2)/2$ ºC. This parameter increases with the CL and with the outer diameter of the container.

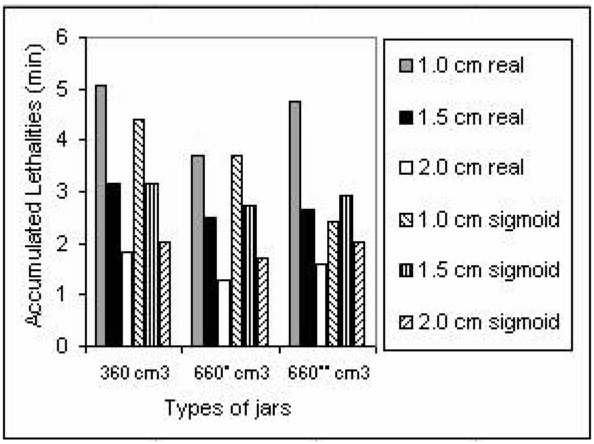

Figure 5.a. Calculated Accumulated Lethalities for Cylinders

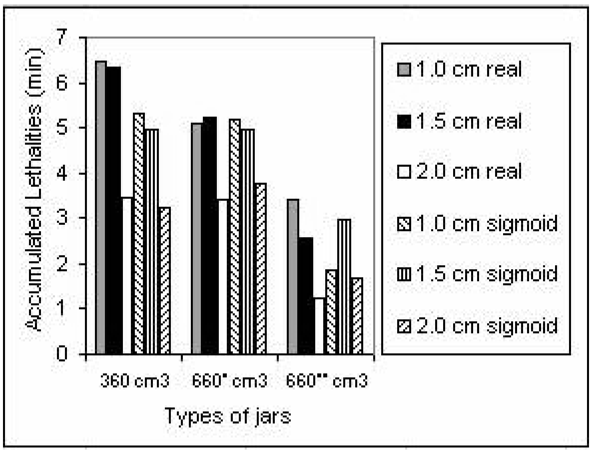

Figure 5.b. Calculated Accumulated Lethalities for Cubes

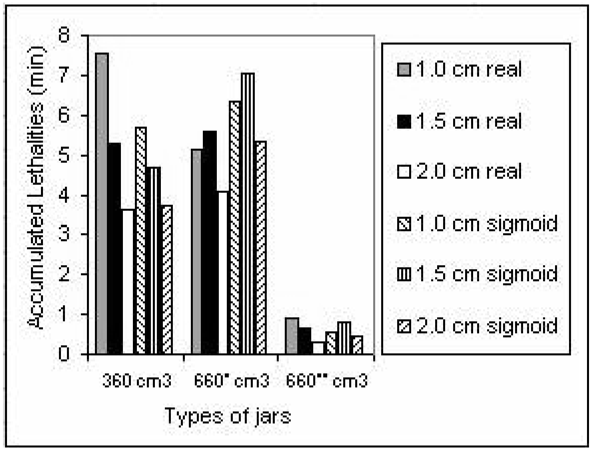

Figure 5.c. Calculated Accumulated Lethalities for Spheres

Table 3.a: Parameters of the Sigmoid Model for Cylinders.

Volume of jars (cm^3)	CL (cm)	A_1 (°C)	A_2 (°C)	t_o (min)	*dt* (min)
360	1.0	16.18	118.05	18.71	5.28
	1.5	14.87	118.05	19.18	5.90
	2.0	13.88	118.05	20.01	6.56
660*	1.0	19.96	118.22	21.82	4.87
	1.5	18.02	118.22	22.39	5.29
	2.0	18.49	118.22	24.19	5.56
660**	1.0	20.90	118.22	21.07	4.49
	1.5	20.13	118.22	22.98	5.00
	2.0	19.31	118.22	23.82	5.40

Table 3.b: Parameters of the Sigmoid Model for Cubes.

Volume of jars (cm^3)	CL (cm)	A_1 (°C)	A_2 (°C)	t_o (min)	*dt* (min)
360	1.0	4.07	118.44	13.90	6.26
	1.5	6.28	118.44	14.91	6.20
	2.0	2.63	118.44	15.51	7.01
660*	1.0	13.2	117.96	18.30	4.86
	1.5	13.2	117.96	18.51	4.93
	2.0	11.44	117.96	18.82	5.49
660**	1.0	15.38	117.88	20.83	4.94
	1.5	16.36	117.88	22.20	5.01
	2.0	16.03	117.88	23.90	5.51

Table 3.c: Parameters of the Sigmoid Model for Spheres.

Volume of jars (cm^3)	CL (cm)	A_1 (°C)	A_2 (°C)	t_o (min)	dt (min)
360	1.0	11.05	118.52	14.35	6.10
	1.5	9.20	118.52	14.90	6.44
	2.0	8.61	118.52	15.95	6.68
660*	1.0	14.10	118.37	17.26	4.88
	1.5	17.60	118.37	17.70	4.48
	2.0	15.11	118.37	18.49	5.02
660**	1.0	20.79	117.37	27.84	4.61
	1.5	21.11	117.37	29.25	4.59
	2.0	21.07	117.37	30.03	4.95

Meanwhile, *dt* (min) increases with CL, being related to the increase of process time with product size (higher CL means lower heating rate). Contrarily to t_0, this parameter lowers with higher container external diameters.

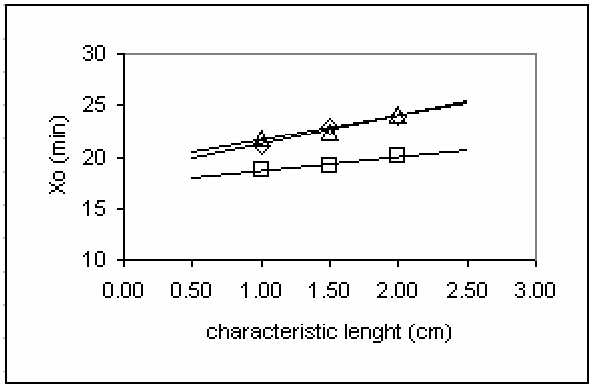

Figure 6.a: Variation of t_0 of Cylinders for the Different Jars. (□) 360 cm^3, (○) 660* cm^3, (Δ) 660** cm^3.

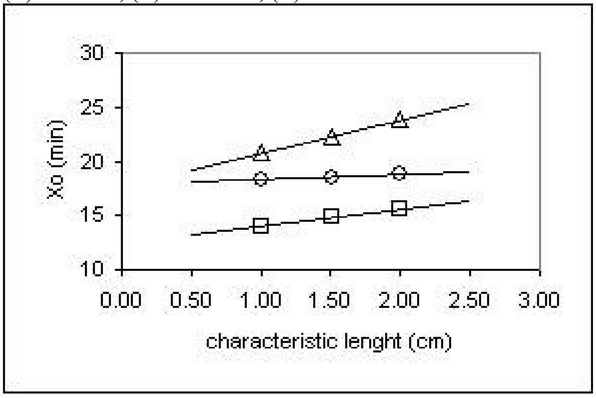

Figure 6.b: Variation of t_0 of Cubes for the Different Jars. (□) 360 cm^3, (○) 660* cm^3, (Δ) 660** cm^3.

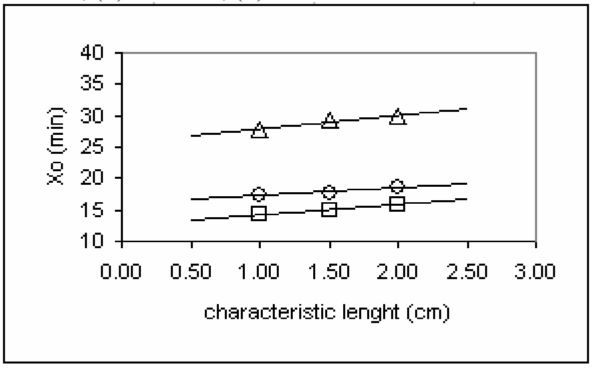

Figure 6.c: Variation of t_0 of Spheres for the Different Jars. (□) 360 cm^3, (○) 660* cm^3, (Δ) 660** cm^3.

The parameters of the sigmoid model (t_o and *dt*) obtained through the fitting of experimental thermal histories can be related to product size (CL) and to the dimensions of the glass jar, as previously expressed. Figures 6.a, 6.b and 6.c. show that t_0 increases in a linear way with CL for all shapes. Simultaneously, t_0 lowers with the increase of jar size.

With the aim of obtaining a relationship for *dt* independent of the initial and final temperatures (related to A_1 and A_2, respectively) a new parameter is defined as $(A_2\text{-}A_1)/(4\ dt)$ (ºC/min). This represents the first derivative of Tc respect to time, evaluated at t_0 and is directly related to the heating rate. For these systems it lowers linearly with the increase of food size, as shown in Fig. 7.a, 7.b and 7.c.

These figures allow to interpolate for calculating their values for intermediate sizes.

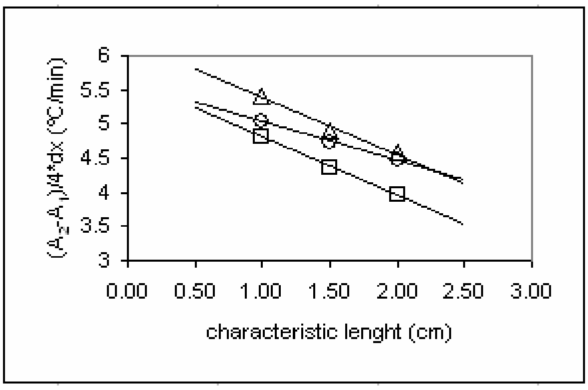

Figure 7.a: Variation of $(A_2\text{-}A_1)/4*dt$ of Cylinders for the Different jars. (□) 360 cm^3, (○) 660* cm^3, (Δ) 660** cm^3.

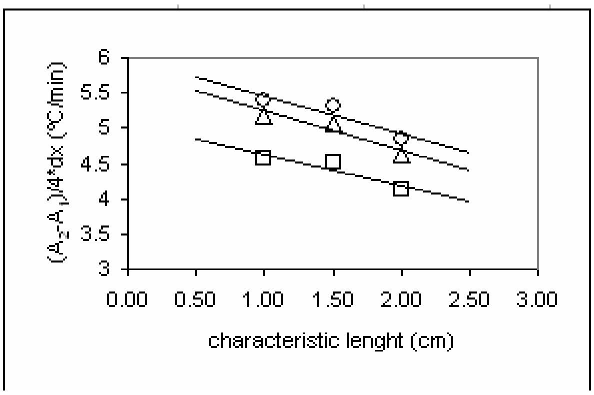

Figure 7.b: Variation of $(A_2\text{-}A_1)/4*dt$ of Cubes for the Different Jars. (□) 360 cm^3, (○) 660* cm^3, (Δ) 660** cm^3.

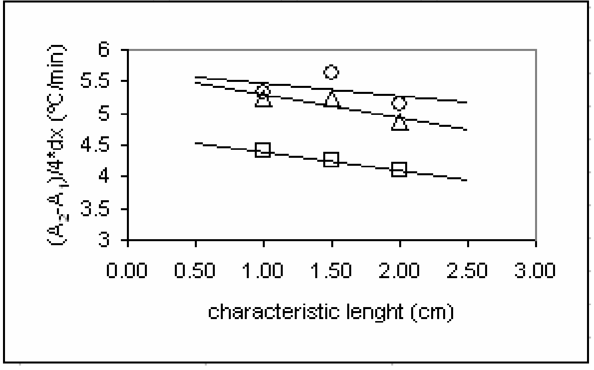

Figure 7.c: Variation of $(A_2\text{-}A_1)/4*dt$ of Spheres for the Different Jars. (□) 360 cm^3, (○) 660* cm^3, (Δ) 660** cm^3.

IV. CONCLUSIONS

A sigmoid model has been proposed for the prediction of thermal histories in particulate foods (of different shapes and sizes) packaged in glass containers, that can be very practical for calculation of low-volume productions. The also tested formula method (exponential) – normally very useful for industrial processing conditions where constant retort temperatures are reached almost instantaneously – does not provide accurate results for the initial variable retort temperature of the tested working conditions.

The proposed model predicted with good accuracy the thermal evolution of all the tested cases, with average relative absolute differences lower than 6%, fulfilling the usual technical requirements.

Besides, it was found that model parameters t_0 and $(A_2\text{-}A_1)/(4\ dt)$ can be easily related to food size for each shape and to the different jar sizes, which enables to use the model to simulate process conditions for food sizes different from the tested ones.

The model allows to calculate the sterilization time needed to secure microbial inactivation and – at the same time – assuring to minimize quality loss due to overprocessing.

NOTATION

A_1	Pseudo-initial temperature of the slowest heating point (ºC).
A_2	Final retort temperature (ºC).
D	Decimal reduction time (min).
DF	Relative percent absolute difference between calculated F using real and simulated temperatures (%).
dt	Constant in sigmoid model related to the first derivate ($\frac{dT_c}{dt} = \frac{A_1 - A_2}{4dt}$) evaluated at t_0 (min).
F	Accumulated lethality (min).
f_{he}	Time for dimensionless temperature to traverse a natural logarithm cycle (min).
j_h	Lag factor.
CL	Characteristic length (m).
m	Number of experimental temperatures compared.
R	Percent residue (%).
T	Temperature (ºC).
t	Time (min).
t_0	Time the slowest heating point needs to reach the temperature $(A_1+A_2)/2$ (min).
z_e	Thermal resistance factor (ºC).

Subscripts

c	thermal centre of the slowest heating product.
e	experimental.
h	heating phase.
o	initial.
r	retort.
ref	reference.
s	simulated.

Superscripts

d	dimensionless.

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