
Retort Processing Operations: Conduction-heated Foods in Oval-shaped Containers

Ricardo Simpson
Ivan Aris
J. Antonio Torres

WALTON COLLEGE LIBRARY
100 W. WALTON ST.
DEPT. OF CHEMISTRY
WALTON, IOWA 52758

Oregon Sea Grant
ORESU-T-89-002

AUTHORS

Ricardo Simpson is an assistant professor of food engineering in the Escuela de Alimentos, Universidad Catolica de Valparaiso, Valparaiso, Chile, and a visiting scientist in the Department of Food Science and Technology, Oregon State University. Ivan Aris is a student in the Escuela de Alimentos, Universidad Catolica de Valparaiso. J. Antonio Torres is an assistant professor in the Food Engineering Group, Department of Food Science and Technology, Oregon State University.

ACKNOWLEDGMENTS



This publication is the result of research sponsored by Oregon Sea Grant with funds from the National Oceanic and Atmospheric Administration, Office of Sea Grant, Department of Commerce, under grant no. NA85AA-D-SG95 (project no. E/ISG-6) and from appropriations made by the Oregon State Legislature. The U.S. Government is authorized to produce and distribute reprints for governmental purposes, notwithstanding any copyright notation that may appear hereon.

The computer program used in this paper was part of the B.S. (food engineering) thesis of one of the authors, Ivan Aris.

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ABBREVIATIONS AND SYMBOLS

$C(i,j,k)$	=	cell or quality factor concentration in volume element (i,j,k)
D	-	time for a decimal reduction of a thermally vulnerable factor (for example, microorganisms, nutrient, texture) at a temperature T (minutes)
D_r	-	time for a decimal reduction of a thermally vulnerable factor at a reference temperature T_r (minutes)
$E(i), F(j)$	=	proportionality factors
E_a	-	activation energy (Arrhenius model)
$E_{a,m}$	-	activation energy (microbial inactivation)
$E_{a,q}$	-	activation energy (destruction of a quality factor)
F_p	-	sterilization value of heating process
k	-	first-order rate constant
k_m	-	first-order rate constant for cell destruction
k_q	-	first-order rate constant for factor destruction
$k_{m,o}$ and $k_{q,o}$	=	constants
N	-	number of viable cells per unit volume
Q	-	concentration of quality factor (nutrient, color, and so on)
R	-	universal gas constant
$T(i,j,k)$	=	temperature in volume element (i,j,k)
T	-	temperature at any point at any time t
TR	-	retort temperature
T_r	-	reference temperature
TI	-	initial temperature
TC	-	cooling temperature
t	-	time
x	-	major axis direction
y	-	minor axis direction
z	-	vertical direction
Z	-	temperature increase required for a decimal reduction in the value of D for a given vulnerable factor
α	-	thermal diffusivity of food product
Δt	-	time increment

SUMMARY

Sterilization, one of the most important unit operations used in the seafood industry, provides a good example of the benefits that can be gained from mathematical modelling. First, all mathematical equations for the physical laws involved are well known. Moreover, experimentation with computer-supported models offers practical advantages over canning experiments, which are expensive and time consuming.

The model discussed in this publication can be used to evaluate retort operations for the processing of seafood in cylindrical or oval-shaped cans. Since several seafood products are processed overseas in oval-shaped containers, there was a need to develop a model to include this type of container. This is particularly important for U.S. companies that purchase or process seafood products overseas.

Several methods of modelling are available for sterilization calculations. Some evaluate the lethality at the slowest heating point while others, for example, the method chosen for this study, calculate a mass average lethality for the whole container. The advantage of using the latter methods is that food processors can easily incorporate estimates for nutrient retention (or any other quality factor) and energy consumption. This type of information is extremely necessary in today's highly competitive markets and could be included in a customized version of the program used in this publication. Other possible and rather simple modifications include process deviation considerations.

The mathematical model used by the computer program was based on a finite difference approximation of the differential equation for transient heat conduction in three dimensions. A large number of container locations were considered for average bacterial lethality and quality retention calculations. The reliability of the numerical method was evaluated by comparing computer predictions with published experimental data for the retention of thiamine, chlorophyll, and betanin in several food products.

The computer program was written in BASIC and can be used with any IBM-PCTM compatible computer. Computing time (IBM PC AT) was approximately 3 minutes per minute of real process time. Current research efforts are aimed at reducing computational time, although this might be less of a problem in the near future (for example, the use of an IBM Personal System/2 Model 70, 25 MHz clock, might reduce this time by about 80%).

INTRODUCTION

General Considerations

It is important to distinguish between mathematical modelling and mere computation. Although both require calculations, the purpose of mathematical modelling is to execute calculations that improve our understanding of an actual process. Sterilization, one of the most important unit operations used in the food industry, is a good example of the benefits of mathematical modelling. The mathematical equations for the physical laws involved are all well known and supported by a large volume of experimental data. Moreover, experimentation with mathematical models offers practical and economic advantages over the physical system which is often inconvenient to test (Clark, 1978).

The mathematical determination of a sterilization process requires temperature and kinetic information, that is, the rates of inactivation of microorganisms and destruction of various quality factors. Food temperature can be measured directly or predicted theoretically with extreme accuracy (Manson et al., 1974). Microbial lethality is mathematically approximated by the following equation (Charm, 1971):

$$D_r/D = 10^{(T - T_r)/z} \quad (1)$$

The quality factor degradation usually follows first-order reaction kinetics, and the temperature effect on the rate constant usually follows the Arrhenius model (Clark, 1978).

The estimation of proper heat processes is based on the calculation of a sterilizing value, F_p , which can be computed as follows (Charm, 1971):

$$F_p = \int 10^{(T - T_r)/z} dt \quad (2)$$

Several methods have been reported for sterilization calculations and can be classified as shown in figures 1 and 2 (Hayakawa, 1978). Group I procedures are based on the evaluation of the lethality at the slowest heating point while those in group II are based on the evaluation of a mass average lethality for the whole container. The latter have the advantage of allowing the easy incorporation of estimates for nutrient retention (or any other quality factor); they can also include energy consumption calculations. This type of information is extremely necessary in today's highly competitive markets. Other possible and rather simple modifications include process deviation considerations.

Group I (figure 1) procedures can be divided into general methods and formula methods. General methods usually do not provide a means of predicting the food time-temperature relation. On the other hand, formula methods have built-in means for this prediction.

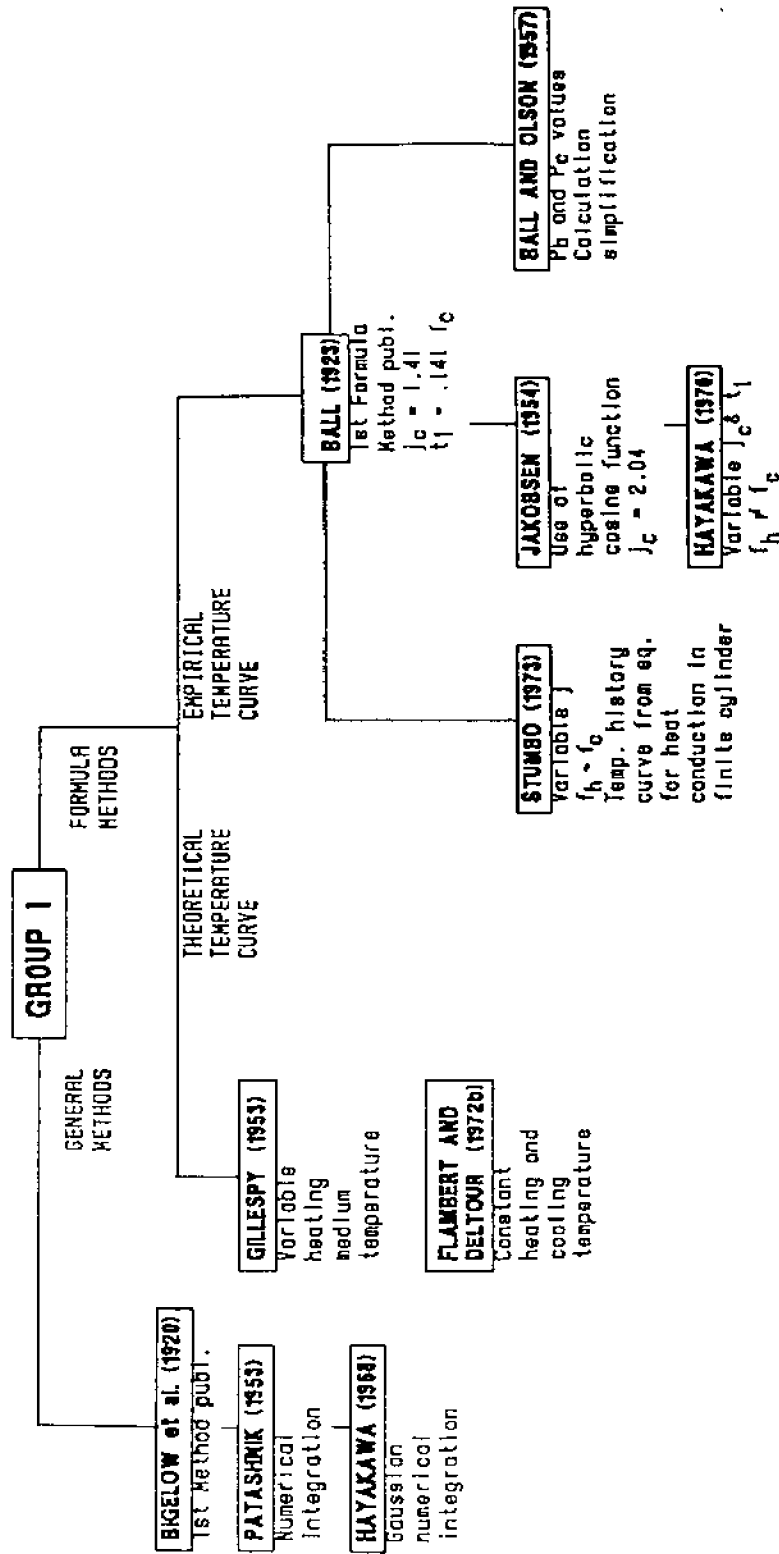


Figure 1. Methods of evaluation for the estimation of lethality at the slowest heating point (adapted from Hayakawa, 1978).

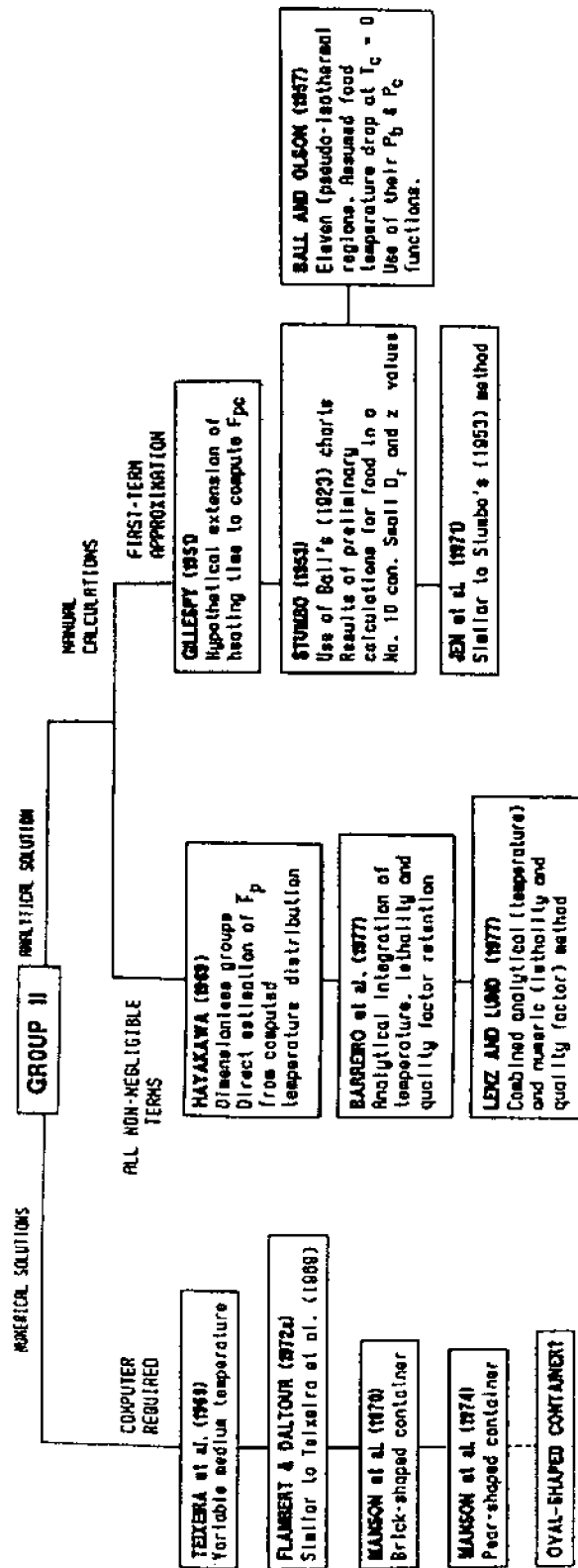


Figure 2. Methods of evaluation for the estimation of the mass average lethality (adapted from Hayakawa, 1978).

General methods are the most frequently used procedures for estimating the lethality of a process. Experimental heat penetration data are used directly in lethality calculations without any assumptions about the time-temperature relation. Moreover, a proper choice of the lethality calculation method can reduce the number of experimental time-temperature data points to only six (Hayakawa 1968, 1978).

Formula methods may be subdivided into two subgroups depending upon the nature of the formulas used for predicting the temperature history curve of a food undergoing a heat process. The two groups are those based on the use of empirical formulas and those based on the use of theoretical formulas. In empirical methods, food temperatures collected during heat processing are usually plotted on semi-log paper, on which a log scale represents temperature differences between food and the surrounding heating or cooling medium while a linear scale represents heating or cooling time. The first empirical method was developed by Ball (1923) and is still widely used by many workers. Several modifications have been published that have increased its flexibility and accuracy (see figure 1).

Several researchers have developed theoretical formulas to predict the heat transfer process in a can. Most of these methods are applicable only to cylindrical cans of solid food (that is, foods heated only by conduction). The first methods developed assumed that the food was initially at a uniform temperature, that the thermophysical properties of the food were independent of location and temperature, that the surface temperature of the food was identical to the temperature of the surrounding medium at any time during the process, and that there was no can headspace (Hayakawa, 1978). Later methods (for example, Hayakawa and Ball, 1971) have removed some of these restrictions.

Group II methods (figure 2) are based on mass average lethality (\bar{F}_p) and have the advantage that they can be adapted to include the prediction of nutrient retention. All published procedures have used solutions of a heat-conduction equation to estimate transient-state temperature distributions.

Oval-shaped Containers

Average lethality procedures have been used to model cylindrical (Teixeira et al., 1969), rectangular (Manson et al., 1970), and pear-shaped (Manson et al., 1974) containers. No published procedures were found for oval-shaped containers, although several conduction-heated food products, mostly seafood, are processed in oval-shaped containers and represent a significant percentage of the canning operation. These commercial operations would benefit from a simulation model to estimate thermal processes for this type of container and to predict the resulting food quality. Although analytical solutions for many heat conduction problems exist for most regular geometrical shapes (Carslaw and Jaeger, 1959; Kirkpatrick and Stokey, 1959), an approach based on numerical methods which are more flexible, was chosen for this study. In many sterilization processes the retort temperature may not be constant and the initial temperature distribution of the food in the can may not be uniform. Either one of these situations would invalidate many analytical solutions. A more useful approach suggested by Dusenberre (1959) would be a numerical method which uses a direct finite difference solution of the heat transfer

equation. This is the approach used in this paper because it allows the computer program to be customized to include

- 1) variable retort temperature;
- 2) nonuniform initial conditions of the temperature, bacterial load, and distribution of the quality factor;
- 3) a nonisotropic medium;
- 4) temperature-dependent thermophysical properties; and
- 5) headspace effects.

The computer program was written in BASIC and implemented on a microcomputer (IBMTM PC AT). In its current version it can be used to evaluate mass-average bacterial lethality and the retention of any quality factor with known kinetics of destruction (vitamins, color, texture, and so on).

THEORETICAL CONSIDERATIONS

A general model for the sterilization process can be obtained by examining the following phenomena and their governing equations (Clark, 1978).

- (1) conduction heat transfer equation in rectangular coordinates, non-steady state and with thermophysical properties independent of temperature:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \quad (7)$$

- (2) kinetics of cell destruction:

$$\frac{dN}{dt} = -k_m N \quad (8)$$

- (3) kinetics of destruction of a quality factor:

$$\frac{dQ}{dt} = -k_q Q \quad (9)$$

where k_m and k_q are functions of temperature usually modelled with Arrhenius equations:

$$k_m = k_{m,o} \exp(-E_{a,m}/RT) \quad (10)$$

and

$$k_q = k_{q,o} \exp(-E_{a,q}/RT) \quad (11)$$

The energy required for the thermal destruction of cells and food quality factors is extremely small. Therefore, the heat transfer equations can be solved separately from the kinetic equations (Clark, 1978).

Computer Implementation

Figure 3 shows a schematic flow diagram of the computer program used to implement the model developed on the basis of the unsteady state heat transfer equation in rectangular coordinates (equation 7). It can be tested using literature data for the destruction of various quality factors in cylindrical cans by choosing oval cans with equal major and minor radius. Experimental data on foods processed in oval-shaped cans were not available in the literature.

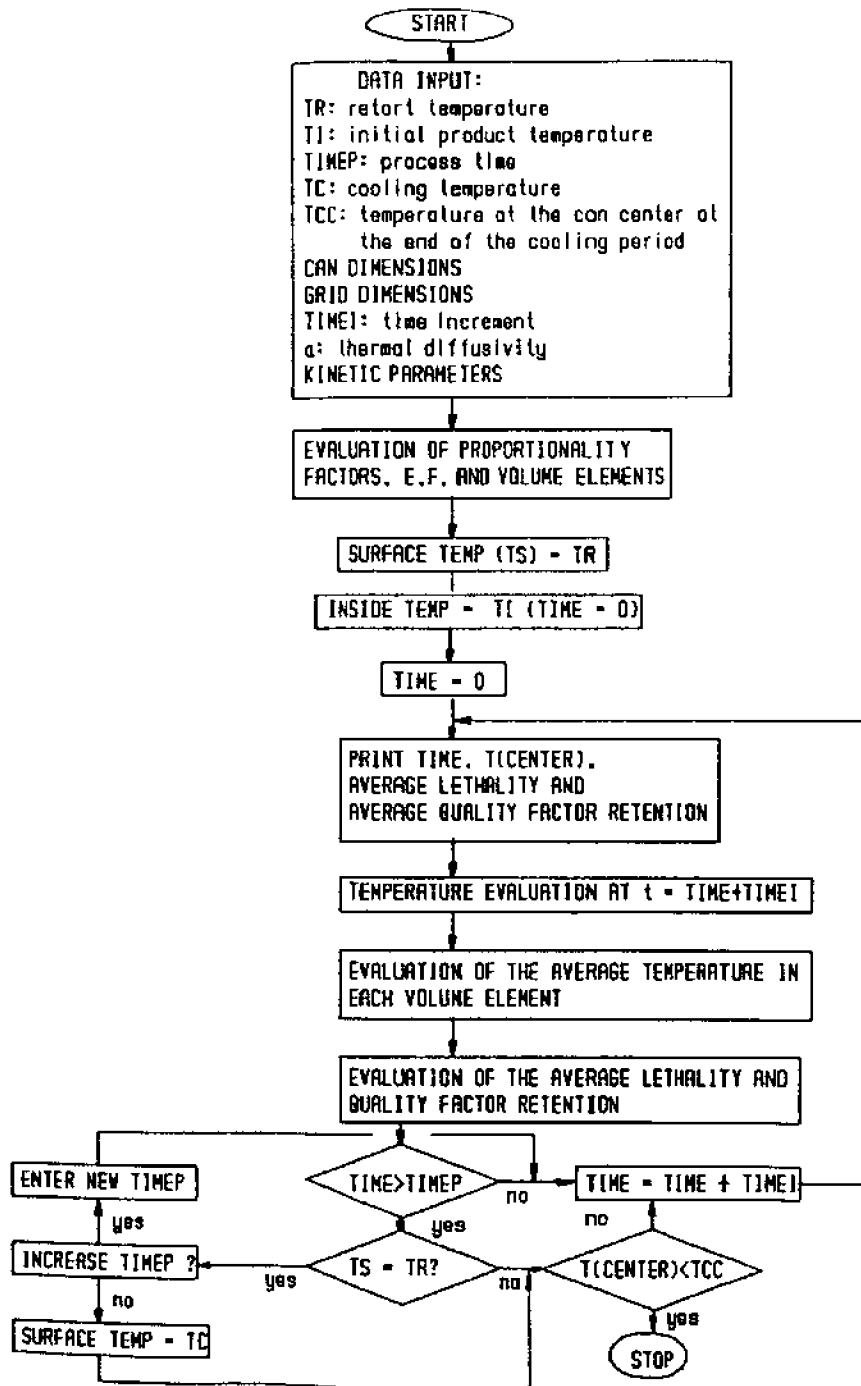


Figure 3. Schematic flow sheet of the computer program for an oval-shaped can.

RESULTS AND DISCUSSION

Numerical Method Parameters: Grid Dimensions and Time Increment

The accuracy of the numerical method can be improved by reducing the size of the volume elements and the time increments at the expense of increasing computational time. Therefore, an increment size study was completed to identify the conditions for accurate solutions within a reasonable computation time. The numerical method published by Teixeira et al. (1969) was used to develop a computer program to calculate thiamine retention (307 x 409 cans; TR = 122.153°C; TI = 71.1°C) in green beans puree ($f_h = 60$ min) (Almonacid, 1988). Thiamine was chosen as the quality factor because of the high temperature dependence of its rate of destruction ($z = 25^\circ\text{C}$; $D_r = 188.7$ min at $T_r = 118.9^\circ\text{C}$). A rather severe thermal process (80 minutes) was chosen to facilitate the detection of discrepancies between both numerical methods. As shown in figure 4, a 7.5-second time increment and a 9 x 9 x 9 partition matrix of the major radius, minor radius and half-height, respectively, lead to acceptable accuracy. This set of numerical method parameters results in approximately 3 minutes of computational time (Compiled Advanced Basic, IBM PC AT) per minute of real process time. For the same time increment, this number of volume elements (729) is greater than the 100 elements used by Teixeira et al. (1969) to model a cylindrical container. Most likely, this is related to the use by these authors of cylindrical coordinates (figure 5). This approach results in elements close to the center (small radius r values) being smaller than those close to the surface. It should be noted that surface elements are overprocessed and do not significantly affect the values for average bacterial lethality and for the average retention of quality factors. The accuracy of the prediction depends greatly on the precision of values calculated for the can center. This suggests the need for future studies that use other strategies for the sizing of volume elements.

Model Validation: Prediction of Biological Changes

Experimental nutrient retention data obtained from the literature (Lenz and Lund, 1977) were used to compare with values calculated by the numerical method employed for oval-shaped cans (table 1). Table 1 also includes the prediction values obtained with the L-T method developed by the same authors. To make this comparison possible the computer program was run with equal major and minor radii to simulate cylindrical cans.

Table 1 shows that the oval-shaped can method predicts biological changes with acceptable accuracy and that estimates of retention of quality factors are well within experimental error (Lenz and Lund, 1977). The average experimental error between predicted and measured values was 6.3% for the oval-shaped can method and compares well with the reported error for the L-T method (5.9%; Lenz and Lund, 1977).

Thiamine retention values predicted by the oval-shaped can method were also compared with several other published prediction methods (Hayakawa, 1969; Teixeira et al., 1969; Jen et al., 1971; Lenz and Lund, 1977). Table 2 shows that the oval-shaped can method was as accurate as all other published methods and that again predictions were close to experimental values (Lenz and Lund, 1977).

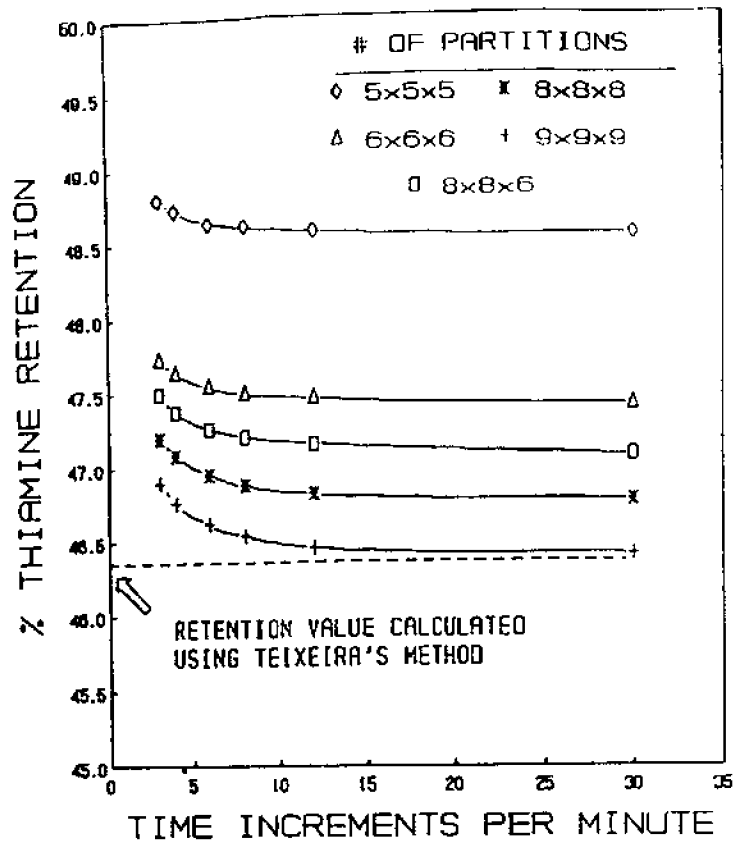


Figure 4. Effect of numerical method parameters on its prediction accuracy.

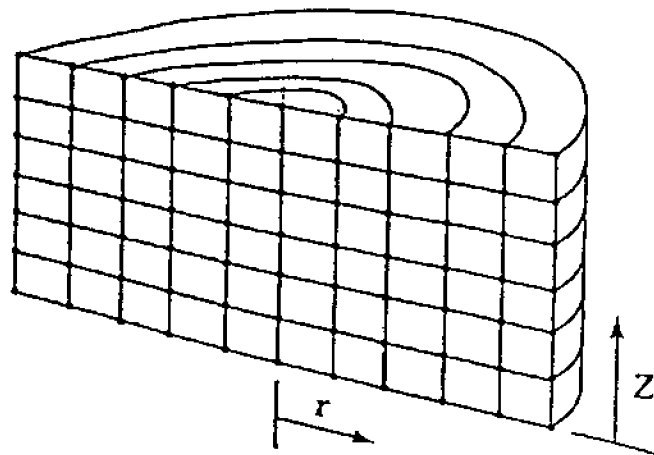


Figure 5. Schematic representation of a cylindrical container.

Table 1(a,a)

Comparison of predicted quality factor retention with values obtained by chemical analysis

Quality factor	Product	TR °F	TI °F	Heating time min	α cm ² /min	k_q min ⁻¹	$E_{a,q}$ Kcal/g-mole	Z Quality factor retention		
								Measured value (b)	Predicted values	
									L-T Method (c)	Oval-shape Method (d)
Thiamine	Pork puree	260	71	20	.1143	.0385	26	78.4	79.2	79.3
		260	71	30	.1143	.0385	26	58.2	60.5	61.0
		280	71	20	.1180	.084	26	53.3	53.4	62.6
	Pea puree	260	70	20	.0925	.021	24	80.0	89.5	89.2
		280	62	45	.0881	.0435	24	76.8	75.0	73.5
		280	62	30	.0881	.0435	24	76.8	75.0	73.5
Chlorophyll	Pea puree	240	70	20	.0918	.0145	22	81.4	80.9	81.5
		260	50	20	.0990	.033	22	77.7	82.8	82.5
		280	54	20	.1005	.063	22	89.7	70.7	71.5
Betanin	Beet puree	240	40	30	.1054	.0395	11	61.8	59.8	60.6
		267	40	31	.1096	.065	11	52.3	46.9	44.6

(a) Adapted from Lenz and Lund (1977)

(b) Average quality factor retention. Products processed in 202 x 314 cans except beet puree which was processed in 307 x 306 cans; TC = 54°F (pea and beet puree), TC = 52.5° F (pork puree). In all cases $T_r = TR$.

(c) Lenz and Lund (1977)

(d) Oval-shape can method simulating a cylindrical container

(e) TR = retort temperature; T_r = reference temperature; TI = initial temperature; TC = cooling temperature.

Table 2^(a)

Mass average retention of thiamine as predicted by
several computational methods

I THIAMINE RETENTION								
TR	TI	Heating time (minutes)	Measured	Predicted values				
			Value (b)	Hayakawa (c)	Jen (d)	Teixeira (e)	L-T Method (f)	Oval-shape Method
^o F	^o F							
240	40.0	30	94	91	94	92	91	91
250	66.5	30	87	84	88	86	83	86
250	55.5	60	66	60	61	61	56	61

(a) Adapted from Lenz and Lund (1977)

(b) Product: pea puree; quality factor: thiamine

(c) Process conditions:

202 x 314 cans, TC = 54^oF, E_a = 24 Kcal/g-mole, k₂₅₀ = .0144 min⁻¹ and
α = .1077 cm²/min (Hayakawa, 1969). In all cases T_r = TR.

(d) Jen et al. (1971)

(e) Teixeira et al. (1969)

(f) Lenz and Lund (1977)

Comparisons summarized in tables 1 and 2 show that the oval-shaped method is as accurate as other published methods for predicting the mass-average retention of a thermally vulnerable component. It is important to note that all comparisons were made against cylindrical container data because of the unavailability of experimental data for oval-shaped cans. The strength of the computer program lies in the ease with which it could be modified to incorporate unusual process conditions, including process deviations, nonuniform thermophysical properties, and non-uniform initial temperature conditions.

An Application Example: Optimization of Retort Temperature

Computer-supported sterilization models have many practical applications in the seafood industry. They include on-line process control, the prediction of product quality (color, texture, nutritive value, and so on), and the optimization of processing conditions.

An example of process optimization is shown in figure 6. Thiamine retention predictions as a function of retort temperature and equal lethality conditions suggest that a retort temperature of about 118°C would lead to optimum thiamine retention.

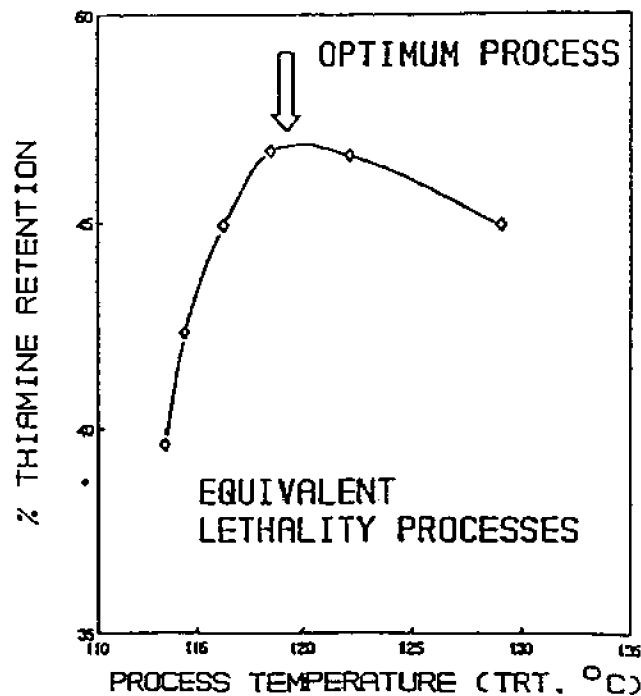


Figure 6. An example of process optimization: determination of retort temperature for maximum nutrient retention. Processing conditions: lethality = 5 decimal reductions; TR = 250° F; TI = 160° F; can size = 307 x 409; $\mu = 1.696 \times 10^{-7} \text{ m}^2/\text{s}$; microorganism with $D_r = 3 \text{ min}$, $z = 10^\circ \text{ C}$, $T_r = 121^\circ \text{ C}$; quality factor (thiamine) with $D_r = 188.7 \text{ min}$, $z = 25^\circ \text{ C}$, $T_r = 118.9^\circ \text{ C}$.

CONCLUSIONS

Validation experiments show that the oval-shaped can method of mathematical modelling predicts time-temperature data and biological changes with accuracy well within experimental error. The numerical approach is flexible, and the developed computer program could easily be modified to accept variable retort temperature, nonuniform initial temperature conditions, changing kinetic parameters, and heterogeneous medium conditions. The program could also be used to optimize processing conditions that would lead to optimum quality retention.

Although the mathematical model was developed for first-order kinetics for estimations of microbial lethality and degradation of a single quality factor, this program could be modified to consider several quality factors, each one with its own kinetic model. In its current form the computer program is rather slow for the desired level of accuracy. Several strategies are currently being explored to solve this difficulty. Computational speed is particularly important for on-line correction of process deviations (Teixeira and Manson, 1982; Datta et al., 1986).

APPENDIX: DEVELOPMENT OF MODEL

Under the assumption of pure conduction heat transfer in an isotropic and homogeneous medium, the unsteady state equation in rectangular coordinates (equation 7) can be used as the basis for the sterilization model for an oval-shaped can. The isometric view of the oval container indicates that for symmetrical boundary and initial temperature conditions the model needs to consider only one-eighth of the total volume (figure 7a). Figures 7b and 7c show a closer view of the grid used by the finite difference method to solve equation (7). The x-y plane view (figure 7b) illustrates the need to introduce the proportionality factors E(i) and F(j) (having values between 0 and 1) for grid points located on the curved boundary (Ozisik, 1968; Kreith, 1976). The following equations can then be derived:

$$\frac{\partial^2 T(i,j,k)}{\partial x^2} = \left[\frac{T(i+1,j,k) - T(i,j,k)}{(1 + E(i))} + \frac{T(i-1,j,k) - T(i,j,k)}{(1 + E(i))E(i)} \right] \frac{2}{(\Delta x)^2} \quad (12)$$

$$\frac{\partial^2 T(i,j,k)}{\partial y^2} = \left[\frac{T(i,j+1,k) - T(i,j,k)}{(1 + F(j))} + \frac{T(i,j-1,k) - T(i,j,k)}{(1 + F(j))F(j)} \right] \frac{2}{(\Delta y)^2} \quad (13)$$

$$\frac{\partial^2 T(i,j,k)}{\partial z^2} = \left[\frac{\{T(i,j,k+1) - T(i,j,k)\} + \{T(i,j,k-1) - T(i,j,k)\}}{(\Delta z)^2} \right] \quad (14)$$

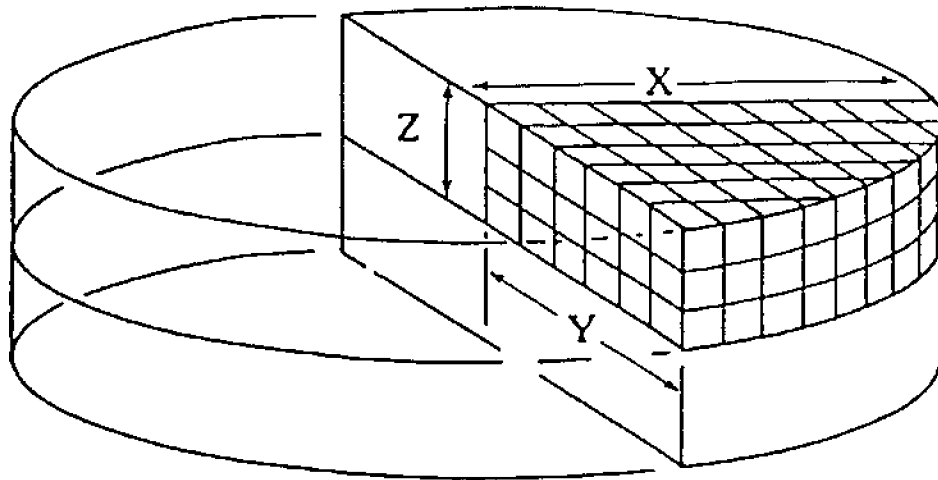
$$\frac{\partial T(i,j,k)}{\partial t} = \left[\frac{T(i,j,k)^{t+1} - T(i,j,k)^t}{\Delta t} \right] \quad (15)$$

Substituting equations (12-15) in equation 7 leads to the following expression:

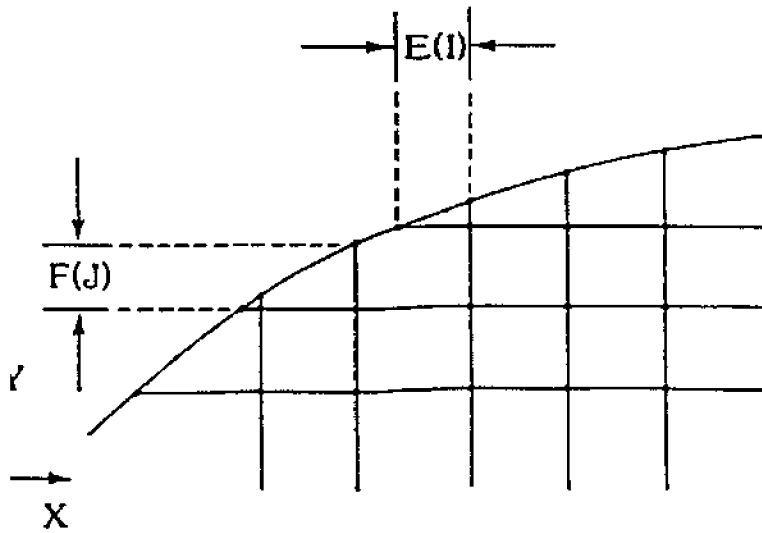
$$\begin{aligned} T(i,j,k)^{t+1} = & T(i,j,k)^t + \\ & \alpha \Delta t \left\{ \left[\frac{\{T(i-1,j,k) - T(i,j,k)\}^{t+1}}{(1 + E(i))E(i)} + \frac{\{T(i+1,j,k) - T(i,j,k)\}^t}{(1 + E(i))} \right] \frac{2}{(\Delta x)^2} \right. \\ & + \left[\frac{\{T(i,j-1,k) - T(i,j,k)\}^{t+1}}{(1 + F(j))F(j)} + \frac{\{T(i,j+1,k) - T(i,j,k)\}^t}{(1 + F(j))} \right] \frac{2}{(\Delta y)^2} \\ & \left. + [\{T(i,j,k-1) - T(i,j,k)\}^{t+1} + \{T(i,j,k+1) - T(i,j,k)\}^t] \frac{1}{(\Delta z)^2} \right\} \quad (16) \end{aligned}$$

Equation (16) can be rearranged to obtain an expression for $T(i,j,k)^{t+1}$. In the case of retort operations it is possible to assume that the food surface is always equal to the retort temperature (Biot number >40; Kreith,

A. ISOMETRIC VIEW (1/8 of volume)



B. X - Y PLANE



C. X - Z PLANE

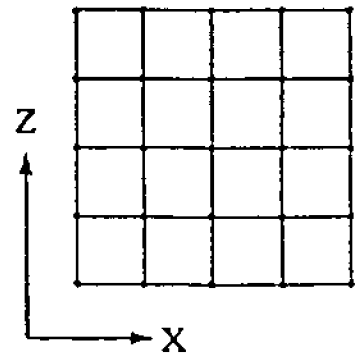


Figure 7. Schematic representation of the oval container.

1976). To simplify model development and model testing, we assumed that the initial can temperature was uniform (= T_I). Finally, the alternating direction explicit procedure (ADEP) was then used to solve this equation. As noted by Allada and Quon (1966), although equation (16) is an implicit equation, a proper choice of the initial point conditions generates explicit calculations. In addition, the method combines the stability of implicit methods with the computational ease of explicit methods (Larkin, 1964; Allada and Quon, 1966).

Microbial Lethality and Retention of a Quality Factor

The general expression for a first-order model is

$$\frac{dC(i,j,k)}{dt} = -k C(i,j,k) \quad (17)$$

where

$C(i,j,k)$ = cell or quality factor concentration in volume element (i,j,k)
 k = rate constant = $f(\text{temperature})$

Equation (17) can be integrated using an average temperature ($\bar{T}(i,j,k)$) for the volume element (i,j,k) between time t and $t + \Delta t$. $\bar{T}(i,j,k)$ was defined as the average temperature for its vertices at time t and those temperatures at time $t + \Delta t$. This allows k for the volume element (i,j,k) to be approximated as a constant during time Δt . The accuracy of this approximation depends upon the size of the volume element and the time increment.

$$k(i,j,k) = k_0 \exp(-E_a/\bar{RT}(i,j,k)) \quad (18)$$

Substitution in equation (17) and integration between time t and $t + \Delta t$ leads to

$$\int_{C^t}^{C^{t+\Delta t}} \frac{dC(i,j,k)}{C(i,j,k)} = -k_0 \exp(E_a/RT(i,j,k)) \int_t^{t+\Delta t} dt \quad (19)$$

Therefore

$$C(i,j,k)^{t+\Delta t} = C(i,j,k)^t \exp\{-k_0 \exp(-E_a/RT(i,j,k)) \Delta t\} \quad (20)$$

Equation (20) can be used to predict the microbial lethality and the retention of the quality factor of a thermal process using the temperature values calculated with equation (16).

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