Katholieke Universiteit Leuven
Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen

DISSERTATIONES DE AGRICULTURA

Doctoraatsproefschrift Nr. 302 aan de Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen van de K.U.Leuven

Improved Procedures for Designing, Evaluating and Optimising In-Pack Thermal Processing of Foods

Proefschrift voorgedragen tot het behalen van de graad van Doctor in de Toegepaste Biologische Wetenschappen door

João Freire de Noronha

APRIL 1996

Doctoraatsproefschrift Nr. 302 aan de Faculteit Landbouwkundige en
Toegepaste Biologische Wetenschappen van de K.U. Leuven

Katholieke Universiteit Leuven
Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen

DISSERTATIONES DE AGRICULTURA

Doctoraatsproefschrift Nr. 302 aan de Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen van de K.U.Leuven

Improved Procedures for Designing, Evaluating and Optimising In-Pack Thermal Processing of Foods

Promotor:
Prof. M. Hendrickx, Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen, K.U.Leuven

Leden van de examencommissie:
Prof. P. Tobback, Vice-Decaan Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen, K.U.Leuven, Voorzitter
Prof. J. De Baerdemaeker, Faculteit Landbouwkundige en Toegepaste Biologische Wetenschappen, K.U.Leuven
Prof. W. Dutré, Faculteit Toegepaste Wetenschappen, K.U.Leuven
Prof. J. Oliveira, Escola Superior de Biotecnologia, Universidade Católica Portuguesa.

Proefschrift voorgedragen tot het behalen van de graad van Doctor in de Toegepaste Biologische Wetenschappen door

João Freire de Noronha

Acknowledgements

I would like to express my thanks:

To Prof. Marc Hendrickx for all the scientific and personal support, for the fruitful discussions we had in the field of thermal processing and in many other areas, for the help and suggestions in the preparation of the present thesis, for the care put in the revisions of the text, for all the help in the arrangement of all the practical details, for everything.

To Prof. Tobback for accepting my as a PhD student in his laboratory, for all the help and support during my stay in Leuven.

To all my colleagues in the Laboratory of Food preservation: Ann Kettler, Ann Van Loey, Geert Maesmans, Jorge Saraiva, Nick Stoforos, Philip Willockx and Suzy DeCordt for your friendship, the permanent interchange of ideas and profitable discussions.

To all the technical personal of the Laboratory of Food Technology I had the privilege to work with.

To the students I had the privilege of work with and that had a major contribution for the completion of the present work: Jo, Joris, Kathy, Johan, Siegfried, and Pieter.

To all my friends in Leuven that made the years spent in Leuven a very enriching experience. I will not try to list all of you because you were so many.

To my colleagues at Campden.

To my new colleagues in Portugal.

To the members of the jury.

To my family in Portugal that during my stay abroad never fail to give me their support.

To the Junta Nacional de Investigação Científica e Tecnológica (JNICT) for financial support from October 1991 to December 1994 in the framework of Programa CIENCIA.

João Noronha

Abstract

Sterilisation by heat is a critical step in the production of a large portion of foods for human consumption. In this thesis several issues in relation to the limitations of currently used approaches in the design, evaluation and optimisation of thermal processes are addressed.

In a first part, a new method for the design and evaluation of thermal processes, that combines the flexibility of finite-differences with the empirical description of heat penetration curves, is developed and validated against theoretical and experimental case studies. This includes process deviations consisting of drops on the heating medium temperature. The method is proven to provide a good prediction of product temperature evolution for conduction and/or convection heating products and thus constitutes a valuable tool for design and evaluation of thermal processes including evaluation of process deviations. The method has been extended to handle products that show a broken-heating behaviour as well as to the evaluation of process deviations consisting of drops of rotational speed during end over end batch rotary sterilisation. Again the method is able to closely predict experimentally obtained time-temperature data.

In a second part, the use of Variable Retort Temperature (VRT) control for the maximisation of quality factors at the product surface during in-pack thermal processing is investigated. Using a simulation approach it is shown that considerable increases in surface quality retention can be achieved using optimum VRT-profiles when compared with the retentions achieved using optimum constant retort temperature (CRT) profiles. It is shown that by using VRT profiles it is possible to substantially reduce processing times still achieving surface retentions as high as the retentions obtainable using optimum CRT-profiles. A four parameter empirical equation able to describe accurately optimum VRT-profiles is presented. Objective functions for the simultaneous optimisation of several quality optimisation factors are proposed and VRT-profiles are shown to be a valuable policy when several surface quality factors are to be considered at the same time. Optimum processing conditions, calculated for a number of case studies have been validated at a pilot scale level. The possibilities and limitations of the implementation of the calculated VRT-profiles as compared to CRT-profiles are discussed in detail.

General Introduction

In-pack sterilisation constitutes one of the most important technologies in food preservation. The aim of sterilisation processes is the reduction of the number of micro-organisms (vegetative cells and spores) to acceptable levels and the inactivation of enzymes that otherwise will cause food poisoning or spoilage and that could, if present, reduce the quality of the food.

From a safety point of view (minimum process requirements) sterilisation processes are designed in order to prevent the occurrence of botulism out-breaks. Botulism, a fatal condition, is caused by toxins produced by several strains of *Clostridium botulinum,* a heat-resistant micro-organism, that can grow under anaerobic, low acid (pH>4.5) conditions. The target organism during the sterilisation of low-acid canned foods is thus *Clostridium botulinum*.

There are two main groups of methods available for the design and evaluation of thermal processes: General Methods, the original being proposed by Bigelow *et al*. in 1920 and Formula Methods, the first one dating back to 1923 (Ball 1923) and still extensively used at present. General Methods can be considered the most accurate since they rely on experimentally determined time-temperature data to assess the impact of the process on the target organisms. However they lack predictive power as they do not provide means for product temperature prediction. Formula methods solve this problem by considering models to describe the temperature evolution in the product as a function of time. Formula methods combine kinetic models for microbial destruction by heat with empirical or theoretical heat transfer models. The first proposed Formula Methods used empirical formulas based on heat transfer models for conduction and were restricted to a limited range of boundary conditions, namely, constant heating and cooling temperature and initial homogeneous temperature distribution. The use of analytical and numerical solutions of the conduction equation broadened the scope of application of the methods to a wider range of boundary conditions.

During a sterilisation process a concomitant decrease in heat-labile quality attributes of the food is observed. If not taken into account this can lead to substantial losses in nutrients (e.g. vitamins) or to the rejection of the product by the consumer (e.g.

degradation of colour, texture). Due to differences in the temperature dependence between spore inactivation and degradation of quality factors there is room for optimisation. While high-temperature-short time processes can be used successfully for the sterilisation of foods with high rates of heat penetration (liquid foods) their use is not appropriate for the sterilisation of solid foods and solid liquid mixtures. In conventional heating techniques high temperatures will cause severe thermal degradation of the food near the surface before the food at the centre of the container has risen significantly in temperature. An optimum heating temperature profile can be calculated that minimises the degradation of the quality factors still providing the necessary microbial destruction. Optimum constant retort temperature profiles have been used for the minimisation of quality degradation during thermal processing of solid foods. The use of variable retort temperature policies as a mean to improve the overall (integrated) quality has been extensively reported but no significant increases in the quality when compared with the simpler use of optimal constant retort temperature profiles could be achieved. Recent studies show that when considering the optimisation of surface quality attributes (e.g. colour, texture) the use of variable retort temperature profiles can lead to substantial increase in quality or decrease in the process time when compared with the optimal constant retort temperature processes. In spite of the large amount of work published on optimisation of quality during thermal processes there are no available studies on the simultaneous optimisation of two or more quality factors.

In the present thesis, the first goal was the development of methods that allow the evaluation of deviations on the scheduled heating medium temperature during the sterilisation of foods heating via mechanisms other than conduction. The developed methods aim to combine the empirical description of a heat penetration curve (fh an jh values) with the flexibility of numerical solutions of the heat conduction equation. Applications of the methods include evaluation of process deviations and broken-heating curves.

A second goal of the present work was the investigation of the possibilities of variable retort temperature as a means for maximising surface quality retention or reduction of the thermal processing time during the sterilisation of packaged foods. The possibilities of generalising the obtained optimum variable retort profiles was investigated. Another purpose was the investigation of the possibilities of simultaneous optimisation of two or more surface quality attributes. The development of appropriate objective functions in order to pursue this task was investigated. Finally, the possibilities of the implementation of the optimum variable retort temperature profiles for single and multi-component surface quality retention was investigated. A schematic overview of the present thesis is given in Fig. 1.

The first part of the thesis on evaluation of process deviations is built up as follows. In Chapter 1, the principles of thermal processing are reviewed. The two main fields of knowledge necessary for a proper design and evaluation of thermal processing operations; the kinetics of destruction of micro-organisms, their spores, and quality factors and the principles that govern heat propagation inside foodstuff, are reviewed. A review on the available methods for the design and evaluation of thermal processes is given. The limitations of the currently available methodologies are also discussed there. In Chapter 2, new methods for the design and evaluation of thermal processes are presented. In Chapter 3, methods for the determination of the empirical parameters necessary for the proper use of the empirical methods presented in Chapter 2 are discussed. The methods are evaluated on their ability to handle process deviations consisting of drops in the retort temperature. In Chapter 4, the method is extended in order to handle products presenting broken-heating curves; the determination of the appropriate empirical parameters to be used in this special case is discussed. The use of the method for the evaluation of process deviations, consisting of drops in the rotational speed in rotary sterilisers, is proposed.

The second part of the thesis deals with the optimisation of surface quality during in-pack thermal processing of foods. In Chapter 5, the use of variable retort temperature control to decrease the degradation of quality factors at the surface of the product was tested. Quality retention and processing times for variable retort policies are compared with optimal constant temperature profiles. The similarities observed in the calculated optimum variable retort temperature profiles for different processing conditions, allows the development of an empirical function for the description of optimum variable retort temperature profiles. The use of this empirical equation together with an appropriate optimisation routine allowed for a substantial reduction in the computational effort necessary for the determination of optimal retort control policies.

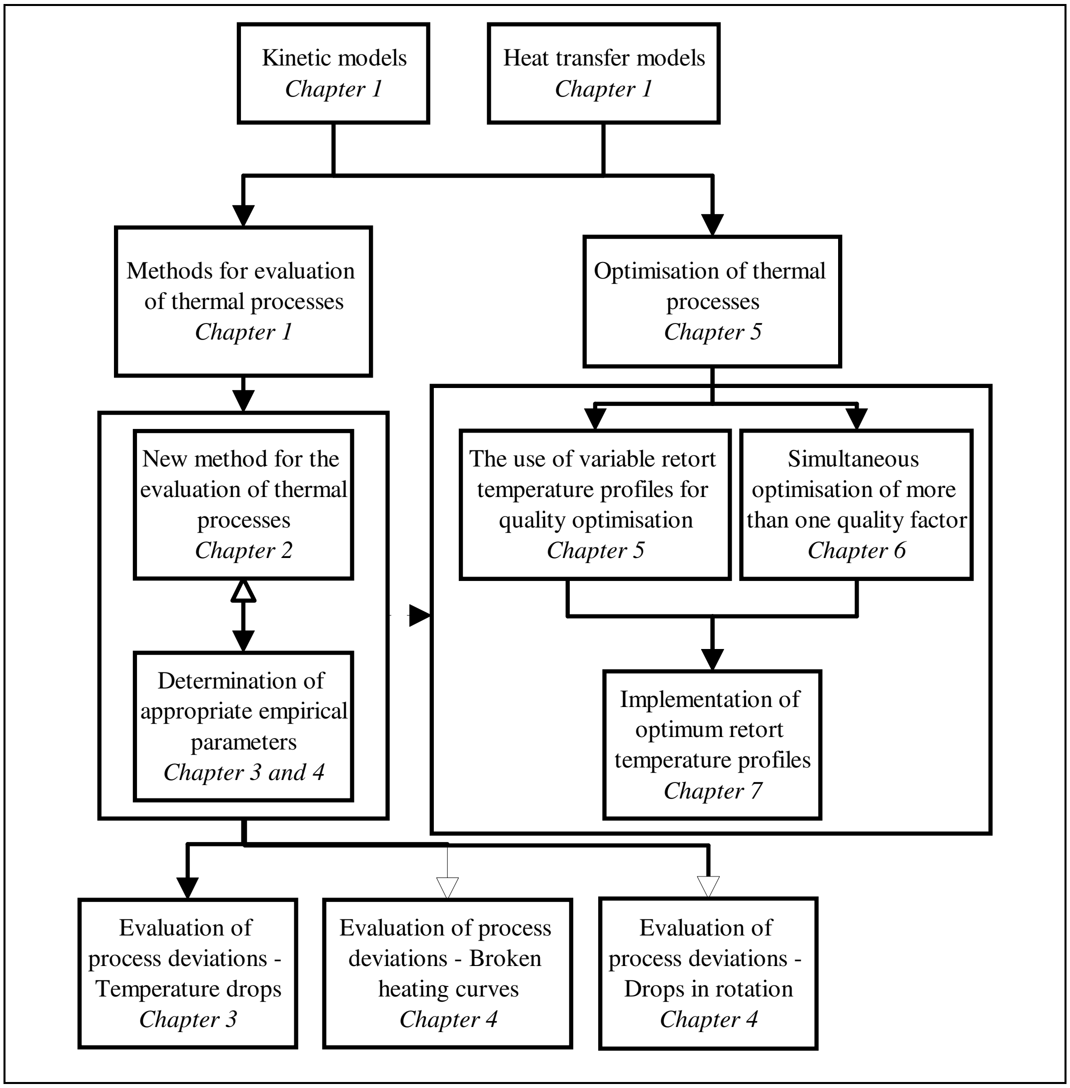

FIGURE 1 Outline of the structure of the present thesis showing the relationship between the subjects treated in the different chapters on the thesis.

In Chapter 6, the theoretical calculation of the optimum retort temperature profiles for the simultaneous optimisation of several surface quality factors is discussed. Special attention is given to the formulation of appropriate objective functions. Finally, in Chapter 7, the results of the practical implementation of optimum retort temperature profiles in a pilot plant retort are presented. The possibilities and limitations of the practical implementation of this type of profiles are discussed.

Table of contents

List of symbols

A	surface area available for heat transfer (m²)
a	slope of a linear temperature change in Eq. 1.15 (ºC/min)
a_0, a_1, a_2 and a_3	parameters used in Eqs. 5.10 and 5.11
Bi	Biot number
C_p	specific heat (J/(kg.K))
C	cook value (min)
D/Dt	substantial derivative $=\partial/\partial t+\nabla\bar{v}$
D_T	time at a constant temperature (T) required to achieve a decimal reduction on the concentration of a heat labile substance (min or s)
E_a	activation energy (J/mol)
F	processing value. Time at a constant temperature required to destroy a given percentage of micro-organisms (min)
f	time required to change the difference between heating medium and product temperature by a factor of 10 (min)
F_0	F at 121.1°C and for a z value of 10°C (min)
F_s	volume integrated process value (min)
g	acceleration due to gravity (m/s²)
h	surface heat transfer coefficient (W/(m². K))
j	coefficient determined as $(T_1-T_0')/(T_1-T_0)$, where T_0' is an extrapolated initial product temperature determined by assuming a exponential heating
j_{hb}	j-value with 42% correction for the retort come-up time
k_T	(first order) Reaction rate constant (s^{-1} or min^{-1})
L	length (m) or Lethal rate (Eq. 1.30)
m	mass of product (kg)
n	real parameter (Eq. 3.2)
N	concentration of a heat labile substance (number of micro-organisms/ml, g/ml or any other appropriate unit)
p	fluid pressure (Pa)
r	radial coordinate (m)
R	radius of cylinder or sphere (m)

R_g	universal gas constant (8.314 J/(mol.K))
R^2	coefficient of determination.
r	radial position (m)
T	temperature (°C or °K)
t	time (s)
U_0	overall heat transfer coefficient (W/(m².k))
U	F value calculated using retort temperature as reference (min), used also as a dimensionless temperature.
$\bar{v}$	mass average velocity vector (m/s)
V	volume (m³)
x, y and z	cartesian coordinates.
W_1, W_2, w_i	weight factors
X_b	break point time (min)
z	temperature rise necessary to achieve a decimal reduction of the D_T value (°C)
∇	Nabla operator = $\partial/\partial x+\partial/\partial y+\partial/\partial z$
∇^2	operator = $\partial^2/\partial x^2+\partial^2/\partial y^2+\partial^2/\partial z^2$

Greek Letters

α	thermal diffusivity (m²/s)
β_n	see notes on Tables 1.1 and 1.2
η	dynamic viscosity of Newtonian liquid (Pa.s)
λ	thermal conductivity (W/m/K)
λn	see notes on Table 1.1
ρ	density (kg/m³)
τ	a time constant defined by Eq. 1.17

Subscripts/ Superscripts

0	initial condition
1	heating medium
c	associated with the cooling cycle of the process (product related)
ce	centre
cp	centipoise (viscosity unit)
cw	cooling medium or associated with the cooling phase.
exp	experimenal
h	associated with the heating cycle of the process (product related) also holding (heating medium related).
g	associated with the end of the heating cycle (product related)
m	microbial
min	minimum.
opt	optimum
p	total process
pred	predicted
q	quality factor
R	retort.
ref	reference value
surf	surface
T	total
t	target value

Abbreviations

APNS	Apparent position numerical solution method (see Chapter 2)
ASDT	Analytical solution with Duhamel's Theorem (see Chapter 2)
ATNS	Apparent time numerical position (see Chapter 2)
BIM	Bimbenet and Michael's method (see Chapter 2)
CMC	Carboxymethylcellulose
CRT	Constant retort temperature
CUT	come-up time
FD	Finite-difference method
HYK	Hayakawa's method
PDE	Partial differential equation
PNSU	Probability of a non-sterile unit
RETS	Surface retention
r.p.m	Rotations per minute.
TDT	Thermal death time
TTI	Time-temperature integrators
VRT	Variable retort temperature

Chapter 1. Principles of thermal processing

1.1. Introduction

Preservation techniques rely on both inhibition and destruction of pathogenic and non-pathogenic micro-organisms. The general principle can be written as (Maesmans *et al.* 1990),

SAFETY = INTEGRAL(rate, time)

This equation indicates that the microbial load of a food product at the moment of consumption will depend on the initial microbial load and the rate of change of the microbial population as a function of time. This rate of change can be positive if the microbial population is growing (growth rate) or negative when the microbial population is decreasing (inactivation or destruction rate).

These rate constants are function of both intrinsic (characteristics of the product, *e.g.,* pH, a_w) and extrinsic factors (environmental conditions, *e.g.,* temperature, pressure). Their proper control, in order to deliver a shelf stable product, is the aim of food preservation. For acidified foods, in order to deliver a stable product, the intrinsic factor pH (pH<4.6) is combined with the extrinsic factor of temperature during the pasteurisation process, and the extrinsic factor of anaerobic conditions during storage at room temperature. For low-acid-canned-foods (4.6<pH) the extrinsic factors of a high processing temperature during sterilisation and anaerobic conditions of storage at room temperature are combined to deliver a safe product. For 'sous-vide' cooking the extrinsic factor of temperature at production level (60ºC-100ºC) is combined with the extrinsic factor of temperature (low temperature, <3ºC) during storage and distribution.

Thermal processing is one of the most important available technologies for the preservation of foods. The first goal of thermal processing is to extend the shelf-life of food products. Nicolas Appert described in 1810 the preservation of various meat and vegetables by heating them in closed containers in boiling water (Goldblith *et al.* 1961). He is considered as the founder of industrial scale food canning.

Thermal processing can be used as a single preservation step or it can be used as a step in conjunction with other preservation techniques (*e.g.,* blanching and pasteurisation). Depending on the intensity of the heat treatment and the objectives to be accomplished, different forms of heat processes can be identified (Lund 1975): (i) Cooking: a heating process, the primary objective of which is to produce more palatable food. Cooking is a preservation technique as cooked foods can be stored for longer periods than uncooked foods provided recontamination is minimised by proper storage. Cooking followed by proper refrigeration is a common household method of preservation. 'Sous vide' cooking (vacuum cooking) today is an industrial counterpart of home cooking. (ii) Blanching: a heat treatment applied to foods prior to freezing, drying, or canning. Blanching prior to freezing and drying has the principal objective to inactivate enzymes that otherwise would promote changes in properties such as colour, flavour and nutritive value. Prior to canning, blanching is used for the de-aeration of foods, to increase the initial product temperature, to cleanse foods, and to soften the tissues to facilitate packaging. (iii) Pasteurisation: a mild heat process designed for the reduction of the number of pathogenic and spoilage vegetative micro-organisms and used in conjunction with other hurdles (acidification, addition of preservatives, cooling, packaging,...) to distribute the food safely. (iv) Sterilisation or more properly 'commercial sterilisation': a severe heat treatment designed to reduce the number of heat resistant bacterial spores. The severity of the heat treatment necessary to achieve commercial sterilisation depends on many factors, including the nature of the food (*e.g.,* pH and water activity), the storage conditions following the thermal process, the heat resistance of micro-organisms and their spores, the heating characteristics of the food and the initial microbial burden.

1.2. Thermal processing: End point definition

For one single unit of product, appropriate testing can be performed to check the presence of micro-organisms, and thus determine its sterility status. However, for large quantities, thousands or millions of units of product, the term 'sterile' does not apply since it is impossible to determine if each individual container is sterile. Due to death characteristics of microbial populations (see 1.4.1.) it is impossible to reach a zero contamination level. Instead of absolute sterility the term probability of survival or probability of non sterile unit (PNSU), expressed as the number of non sterile containers per 10^x containers, is used. In face of the impossibility of reaching a zero level contamination, processes are designed in order not to exceed certain PNSU levels. From a public health standpoint, safe from *C. botulinum*, a PNSU of 10^{-9} (one viable *C. botulinum* spore surviving in 1.000.000.000 containers of food) has been suggested (Pflug 1987c).

While the most important factor to be considered in the design of thermal processes is the production of microbiologically safe food, the thermal process design engineer should take into consideration the concomitant destruction of quality factors that should be minimised.

1.3. Available methods for the design and evaluation of thermal processes

The available procedures for the determination of proper heat sterilisation processes can be divided into three major groups: The *in situ* method, the methods using time temperature integrators (micro-organisms or chemical compounds for monitoring the lethal effect of heat processes), and the physical-mathematical methods.

1.3.1. The *in situ* method

In the *in situ* method the impact of a process on a certain attribute is determined by actually measuring the initial and final load of this attribute. This method constitutes the most accurate way of assessing the impact of a process on a certain attribute, as no assumptions regarding the mode of heat transfer, the kinetic parameters or their dependence on the temperature are made. Using this approach the impact of the thermal process on the parameter of interest is directly determined. The *in situ* method has been used in the evaluation of the nutritional quality (*e.g.,* vitamin loss, Mulley *et al.* 1975), changes in organoleptic properties (Hayakawa 1977b), changes in colour (Hayakawa and Timbers 1977) and textural properties (Van Loey *et al.* 1994a) of canned foods or enzymatic activity after blanching of fruits and vegetables (Whitaker 1991). Disadvantages associated with this methodology are that analysis of the parameter under consideration can be laborious, time consuming and expensive, which renders the method unfeasible for routine checks. In some cases the load of the parameter after processing is beyond the detection limit of available analytical methods or the sample size required for the analysis may be unacceptably large what makes this methodology impracticable (Maesmans 1993; Hendrickx *et al.* 1995). A typical example of the latter is the impossibility of *in situ* evaluation of food safety after sterilisation, because the residual concentration of micro-organisms is too low to be detected.

1.3.2. Time-temperature Integrators

Time-Temperature Integrators (TTI) are small, wireless, inexpensive devices showing a time-dependent, easily measurable and reversible change, that mimic the change of a well-defined target quality parameter of food undergoing the same variable temperature exposure (Taoukis and Labuza 1989; De Cordt *et al.* 1992). It has been shown (Hayakawa 1978; Hendrickx *et al.* 1992a) that the z value of the TTI (or the activation energy if the Arrhenius model is used) should be equal to that of the target quality attribute in order for the TTI to accurately mimic the changes of the target parameter. The decimal reduction time at reference temperature (D_{Tref}) of the TTI must be known in order to calculate the processing value, but does not need to be equal to that of the target quality attribute (Hayakawa 1978). However, the D_{Tref} value of the TTI must be conveniently high in the considered temperature range in order to give rise to measurable responses (De Cordt *et al.* 1992). In order to avoid the requirement on the equivalence on z values (or activation energy) between the TTI and the target quality attribute, a technique to relate the response of a series of TTI's characterised by a series of activation energies or z-values, with the response of the target quality, the equivalent point method, has been set forward (Swartzel 1982; Nunes and Swartzel 1990). However, the use of this approach for other than square-wave profiles or isothermal-like profiles can lead to serious errors (Maesmans 1993; Maesmans *et al*. 1993).

Microbiological systems (*e.g.,* inoculated packs, Yawger 1978), enzymic systems (Weng *et al.* 1991; Saraiva *et al.* 1993; De Cordt 1994), chemical systems (Wen Chin 1977; Pinheiro-Torres *et al.* 1994) and physical systems (Witonsky 1977) have been used as TTI's. A detailed discussion can be found in Hendrickx *et al.* (1995).

1.3.3. Physical-mathematical methods

Physical-mathematical methods combine information on the kinetics of destruction by heat of the relevant factor under consideration (microbial destruction when food safety is of concern or quality factor destruction when evaluation of quality retention is of concern) with the time-temperature evolution inside the product (Hayakawa 1977a). The microbial and engineering principles used for the determination of these data will be discussed in the subsequent sections. Because of the relevance for the present work this group of methods will be discussed in more detail in section 1.6.

1.4. Kinetics of thermal inactivation

In order to assess the impact of a thermal process, in terms of the decrease of the microbial load or a quality factor concentration (*e.g.,* process optimisation), there is a need of knowledge on the way these parameters respond to the heat treatment.

1.4.1. The first order model of thermal inactivation

In thermal process calculations thermal destruction of micro-organisms as well as of nutrients has been commonly described using first order reaction kinetics (Esty and Meyer 1922; Hayakawa 1978):

$$\frac{dN}{dt} = -k_T N \tag{1.1}$$

with N - concentration of a heat-labile substance (number of micro-organisms/ml, g/ml or other appropriate unit).

k_T - rate constant at temperature T (s^{-1}).

The decimal reduction time (D_T), the time at constant temperature to reduce the concentration by a factor of ten can, be written as,

$$D_T = \frac{\ln(10)}{k_T} \tag{1.2}$$

Eq. 1.1 can be written as,

$$\frac{d(\log N)}{dt} = -\frac{1}{D_T} \tag{1.3}$$

When a microbial population is exposed to a constant, lethal temperature, Eq. 1.3 implies that when the logarithm of the remaining concentration of micro-organisms is plotted as a function of the time (semi-logarithmic survivor curve) a straight line is obtained. From the slope of this line, the k_T or D_T values can be determined. In several cases the critical microbial population may yield a semi-logarithmic survivor curve that is not a straight line. In these cases an analysis procedure appropriate to the specific data must be used (Pflug 1987b). When the available data in literature is considered, microbial destruction curves of almost any shape are found. However in about 40% of the cases the data can be approximated using the straight-line, semi-logarithmic curve. For curves where the initial portion shows either a much lower or a much higher destruction rate (concave downward or upward respectively) followed by a straight-line destruction (which is observed in another 40% of the curves) appropriate adjusted parameters can be used in such a way that the adjusted straight-line model represents a worst-case condition (Pflug 1987b). Moats *et al.* (1971) based on experimental survivor curves for vegetative bacteria, disputed the validity of assuming the logarithmic behaviour of survivor curves. They advocated the direct measurement of times required for a given probability of kill at a given temperature (thermal death point or F values) for the comparison of survival at different temperatures or under different conditions, instead of the usual use of D values that become meaningless when the survivor curves are not truly logarithmic.

When the available alternatives for establishing the processing value of a low-acid canned food process, that extend from empirical and historical values to complex, multivariate models are considered, the straight line, semi-logarithmic microbial model is the only model that can be directly, and in a simple way, used for the engineering purpose of design and evaluation of thermal processes (Pflug 1987b). Moreover, the use of the straight-line model might be considered appropriate since the microbial destruction curves for *Clostridium botulinum* spores, the target for sterilisation, show a straight line behaviour in the sterilisation temperature range (Stumbo *et al.* 1950).

1.4.2. Temperature dependence of the rate constant

The dependence of the rate constant with temperature can be described both using the Arrhenius model and the Bigelow model (the TDT, thermal death time, model). In the Arrhenius model, Eq. 1.4 gives the dependence of the reaction rate constant on temperature.

$$k_T = k_{T_{ref}} \exp\left(\frac{-E_a}{R_g}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \tag{1.4}$$

with E_a - activation energy (J/mol).

R_g - universal gas constant (8.314 J/mol/K).

k_{Tref} - rate constant at reference temperature T_{ref} (s^{-1}).

In food sterilisation the empirical Bigelow model, Eq. 1.5 is often used to express the effect of temperature on the rate of microbial destruction (Ball and Olson 1957),

$$D_T = D_{T_{ref}} \, 10^{\left(T_{ref} - T\right)/z} \tag{1.5}$$

with z - number of degrees Celsius necessary to change the D value by a factor of ten (°C).

D_{Tref} - D value at reference temperature T_{ref} (min).

Both models are empirical in nature when used to express the temperature dependence of the rate of destruction of micro-organisms. In spite of the preference of certain authors for one of the models, there are no *a priori* scientific arguments to decide in favour of any of the models. For limited temperature ranges, the small differences between the predictions of the two models, allied with the errors associated with the experimental data, do not allow to choose between the models. Both models have been successfully used to express thermal destruction of micro-organism and quality factors (Manji and De Voort 1985).

1.4.3. The processing F-value

The impact of a thermal process on a heat-vulnerable factor can be evaluated by integration of Eq. 1.1 or Eq. 1.3. If the temperature during the process is constant (k_T and D_T are therefore constants) simple, exponential decay curves are obtained. When the temperature on the food varies during the sterilisation process, the dependence of the rate constant on temperature (Eq. 1.4 and Eq. 1.5) must be taken into account in integrating Eqs. 1.1 and 1.3.

Two approaches can be used to assess the impact (measured as the processing value), of a thermal process. The first one is based on calculating the impact at a single point. In the second approach a volume integrated processing value is calculated by appropriately integrating the effects of the heat treatment throughout the whole volume of the product.

The F-value (processing value) provides a mean for comparing different thermal processes. It can be defined as the time of a hypothetical process, at constant reference temperature, that would result in the same impact (microbial reduction or quality degradation) as the actual process.

An expression for the calculation of the sterilising value at a single point can be derived by proper integration of Eq. 1.1.

$$\int_{N_0}^{N} d(\log N) = -\frac{1}{D_{T_{ref}}} \int_0^{t_p} 10^{\frac{\left(T(t)-T_{ref}\right)}{z}} dt \qquad (1.6)$$

with N_0 - initial load of a heat-labile substance (number of micro-organisms, g/l,...).
N- final load of a heat-labile substance (number of micro-organisms, g/l,...).
t_p - total process time (s).

From this equation we obtain,

$$F_{T_{ref}}^{z} \equiv -D_{T_{ref}} (\log N - \log N_0) = \int_0^{t_p} 10^{\frac{(T(t)-T_{ref})}{z}} dt \qquad (1.7)$$

with, $F_{T_{ref}}^{z}$ - Time at a constant reference temperature (T_{ref}) required to destroy a given percentage of micro-organisms whose thermal resistance is characterised by z (min).

Eq. 1.7 provides two ways for the calculation of the processing, F, value. The first is based on the actual measurement of the initial and final loads of the heat-labile substance (N_0 and N, respectively) while the second is based on the complete knowledge of the temperature history (T(t)). For the evaluation of the impact of a sterilisation process in terms of the reduction of the number of spores of *Clostridium botulinum* a reference temperature of 121.1°C and a z value of 10°C are commonly used and the symbol F_0 is employed. For the evaluation of the impact of a thermal process in terms of changes in organoleptic properties or in quality factor contents a reference temperature of 100°C and z values typically in the range 20-40 °C are used and the symbol C (instead of F), representing 'cook value' is used.

Using the Arrhenius model, the F value can be written as,

$$F_{T_{ref}}^{E_a} \equiv -\frac{1}{k_{T_{ref}}}(\ln N - \ln N_0) = \int_0^{t_p} \exp\left(\frac{E_a}{R_g}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right)dt \qquad (1.8)$$

with $F_{T_{ref}}^{E_a}$ - Time at a constant reference temperature (Tref) required to destroy a given percentage of micro-organisms whose thermal resistance is characterised by E_a (min).

When the calculation of the effect of a thermal process in terms of the overall food volume is of concern, the impact of the process in each elemental food volume is needed (by applying Eqs. 1.7 or 1.8 to each elemental volume). A second integration is performed over the total volume to calculate the volume integrated, mass average, sterilising value. Considering the D-z model we obtain the following expression for the calculation of the mass average sterilisation value (Eq. 1.9)

$$F_s = D_{T_{ref}} \log\left(\frac{1}{V_T}\int_V 10^{-\frac{F(V)}{D_{T_{ref}}}} dV\right) \qquad (1.9)$$

with F(V) - Sterility value in the volume element dV (min).

F_s - Volume integrated sterility value (min).

Volume integrated, mass average, processing values, should be used to assess the impact of thermal processes both in terms of destruction of micro-organisms or reduction of the quality of the product. However the information necessary for the calculation of this volume integrated value, the time-temperature evolution in all points of the container, is seldom available. Due to this lack of information a single point sterilisation value is used. To assess the safety of a process the processing value at the cold spot, critical, or least lethality point is often used. The use of this approach relies on the fact that if this critical point becomes commercially sterile, then the rest of the product will also be commercially sterile. To evaluate the safety of the process, the microbial load is considered to be concentrated at the critical point and the process is evaluated at this single point. To estimate the impact of the process in terms of quality degradation the volume average processing value ('cook value') can be approximated by the surface value.

1.5. Modelling heat transfer during in-pack thermal processing of foods

The theoretical calculation of the temperature evolution in a food container can be a difficult task, because of the possible existence of coupled heat, mass and momentum transport. Only for simple initial and boundary conditions and for conventionally shaped bodies analytical equations can be found in the literature that describe accurately the heat transfer in the food. The solutions for these problems will be discussed as they provide guidelines for more complex cases, where no analytical or in some cases even no numerical solutions are available or feasible.

1.5.1. Analytical solutions

1.5.1.1. Conduction heating

The partial differential equations (PDE's) that describe the mechanism of heat transfer by conduction are well established (Carslaw and Jaeger 1959). Techniques to solve these PDE's, both analytical and numerically, for a variety of initial and boundary conditions are available (Carslaw and Jaeger 1959; Myers 1971).

The governing equations, for unsteady state heat transfer (Fourier 2nd law) into a three dimensional object in rectangular co-ordinates, can be written as (Carslaw and Jaeger 1959),

$$\rho C_p\left(\frac{\partial T}{\partial t}\right)=\frac{\partial}{\partial x}\left(\lambda_x\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_y\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda_z\frac{\partial T}{\partial z}\right) \qquad (1.10)$$

with ρ - density (Kg/m³).

λ_i - thermal conductivity in the i (x, y or z) direction (W/(m K)).

C_p - Specific heat (J/(Kg K)).

For constant thermal properties and for a finite cylinder, a two-dimensional heat conduction problem, the governing conduction equation in cylindrical co-ordinates, is given by,

$$\frac{1}{\alpha}\frac{\partial T}{\partial t}=\frac{1}{r}\frac{\partial T}{\partial r}+\frac{\partial^2 T}{\partial r^2}+\frac{\partial^2 T}{\partial x^2} \qquad (1.11)$$

with α - thermal diffusivity (m²/s).

r - radial co-ordinate (m).

For geometries showing one dimensional heat transfer (infinite cylinder, infinite slab and sphere) Fourier's second law is given by Eq. 1.12.

$$\frac{\partial T}{\partial t} = \frac{1}{r^{(\gamma-1)}} \frac{\partial}{\partial r}\left(\alpha r^{(\gamma-1)} \frac{\partial T}{\partial r} \right) \tag{1.12}$$

Where, γ takes the values 1, 2 and 3 for an infinite slab, an infinite cylinder and a sphere, respectively.

Analytical solutions for Eqs. 1.10, 1.11 and 1.12 for simple shaped bodies with constant thermal diffusivity considering the following boundary conditions:

1. Initial uniform temperature: t=0, $\forall_{x,y,z}$,T(x,y,z)=T_0.
2. Step change in the heating medium temperature: t>0, T_{surf}=T_1.
3. Surface temperature equal to heating medium temperature: T_{surf}=T_1.

are presented in Table 1.1.

When resistance to heat transfer at the surface is present, the third boundary condition is replaced by a convective boundary condition:

$$-\lambda \frac{\partial T}{\partial x} = h\left(T_{surf} - T_1\right) \quad (t>0)$$

with h - surface heat transfer coefficient (W/m²/K).

The analytical solutions for this type of boundary condition are given in Table 1.2.

TABLE 1.1 Analytical solutions of Fourier equation for several simple geometries considering infinite heat transfer coefficient at the surface.

Geometry	Analytical Solution
Infinite slab	$\frac{T(x,t)-T_0}{T_1-T_0}=1-\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\cos\left(\frac{(2n+1)\pi x}{2L}\right)\exp\left(\frac{-(2n+1)^2\pi^2\alpha t}{4L^2}\right)$
Infinite cylinder	$\frac{T(r,t)-T_0}{T_1-T_0}=1-2\sum_{n=1}^{\infty}\frac{J_0(\beta_n r/R)}{\beta_n J_1(\beta_n)}\exp\left(\frac{-\alpha t\beta_n^2}{R^2}\right)$ (*)
Sphere	$\frac{T(r,t)-T_0}{T_1-T_0}=\begin{cases}1+\frac{2R}{\pi r}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\sin\left(\frac{n\pi r}{R}\right)\exp\left(\frac{-n^2\pi^2\alpha t}{R^2}\right) & \text{for } 0<r<R\\ 1+2\sum_{n=1}^{\infty}(-1)^n\exp\left(\frac{-n^2\pi^2\alpha t}{R^2}\right) & \text{for } r=0\end{cases}$
Finite cylinder	$\frac{T(t,r,x)-T_0}{T_1-T_0}=1-4\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{(-1)^{m+1}}{\lambda_m}\cos\left(\lambda_m\frac{x}{L}\right)\frac{J_0(\beta_n r/R)}{\beta_n J_1(\beta_n)}\exp\left[-\left(\frac{\lambda_m^2}{L^2}+\frac{\beta_n^2}{R^2}\right)\alpha t\right]$ (#)

(*) βn are the positive roots of the equation $Jo(\beta n)=0$. $J_n(x)$ are the Bessel functions defined as

$$J_n(x)=\sum_{i=0}^{\infty}\frac{(-1)^i}{i!(i+n)!}\left(\frac{x}{2}\right)^{(n+2i)}$$

(#) $\lambda_m=(2m-1)\frac{\pi}{2}$

1.5.1.2. Convection heating

The modelling of heat transfer for convection heating foods (liquid foods) involves the simultaneous solution of the following three fundamental transport equations (Bird *et al.* 1960) :

1. Continuity: $\nabla\bar{v}=0$

2. Motion: $\rho\frac{D\bar{v}}{Dt}=\nabla p+\eta\nabla^2\bar{v}+\rho g$

3. Energy: $\rho C_p\frac{DT}{Dt}=\lambda\nabla^2 T$

TABLE 1.2 Analytical solutions of Fourier equation for several simple geometries considering finite heat transfer coefficient at the surface.

Geometry	Analytical Solution	
Infinite slab	$\frac{T-T_0}{T_1-T_0}=1-\sum_{n=1}^{\infty}\frac{2Bi\cos(\beta_n x/L)}{(\beta_n^2+Bi^2+Bi)\cos(\beta_n)}\exp\left(\frac{-\beta_n^2\alpha t}{L^2}\right)$	(*)
Infinite cylinder	$\frac{T-T_0}{T_1-T_0}=1-\sum_{n=1}^{\infty}\frac{2\,Bi\,J_0(\beta_n x/R)}{(\beta_n^2+Bi^2)\,J_0(\beta_n)}\exp\left(\frac{-\beta_n^2\alpha t}{R^2}\right)$	(+)
Sphere	$\frac{T-T_0}{T_1-T_0}=1-\frac{2BiR}{x}\sum_{n=1}^{\infty}\frac{\sin(\beta_n x/R)}{\left(\beta_n^2+Bi^2-Bi\right)\sin(\beta_n)}\exp\left(\frac{-\beta_n^2\alpha t}{R^2}\right)$	(#)

(*) β_n are the positive roots of the equation $\beta\tan(\beta)=Bi$.
(+) β_n are the positive roots of the equation $\beta J_1(\beta)-Bi\,J_0(\beta)=0$
(#) β_n are the positive roots of the equation $\beta\cot(\beta)+Bi-1=0$
Bi represents the Biot number, $Bi = h\,R/\lambda$, and expresses the ratio between the surface heat transfer resistance and the internal heat transfer resistance.

These equations are valid for pure liquids with constant density, viscosity, and thermal conductivity, and neglecting the viscous dissipation of energy within the fluid.

When heat transfer for mixed systems with liquid and particulates is considered, the above equations and equations that describe the heat transfer inside the particles must be solved simultaneously. This makes the modelling even more complex.

For homogeneous, perfectly mixed liquid canned foods simple mathematical models describing the temperature evolution inside the container can be derived.

$$U_0A(T_1-T)=mC_p\frac{dT}{dt} \tag{1.13}$$

with U_0 - overall heat transfer coefficient (W/m²/K)

A - area available for heat transfer (m²)

The solution of Eq. 1.13 for a product initially at temperature T_0 and suddenly immersed in a medium at temperature T_1 can be obtained by integrating this equation,

$$t=\frac{\ln(10)mC_p}{U_0A}\log\left(\frac{T_1-T_0}{T_1-T(t)}\right) \tag{1.14}$$

When the medium temperature changes linearly with time (Eq. 1.15), the analytical solution of Eq. 1.13 is given by Eq. 1.16 (Bimbenet and Michiels 1974).

$$T_1(t) = T_{1,0} + at \tag{1.15}$$

$$T(t) = T_{1,0} + a(t - \tau) + (T_0 - T_{1,0} + a\tau)\exp\left(-\frac{t}{\tau}\right) \tag{1.16}$$

where τ, a time constant, is defined as,

$$\tau = \frac{mC_p}{U_O\, A} \tag{1.17}$$

1.5.1.3. Duhamel´s Theorem

Duhamel's theorem (Carslaw and Jaeger 1959; Myers 1971) states that if ψ(x, t) is the response of a system of initial zero temperature to a single unit step surface temperature change, then the response of the system to the surface temperature history, $T_s(t)$, is given by Eq. 1.18.

$$T(x,t) = \int_0^t T_s(\tau)\frac{\partial\psi(x, t-\tau)}{\partial t}d\tau \tag{1.18}$$

Using Duhamel's theorem it is possible to derive analytical solutions for several cases of variable surface temperature. For cases where the surface temperature is a complex function of time or when it is given by a discrete set of values the use of Duhamel's theorem to derive analytical solutions becomes very tedious or even impossible, and numerical implementations of Duhamel theorem are preferable.

1.5.2. Numerical solutions

1.5.2.1. General aspects

The combination of digital computers and numerical methods has given rise to a very powerful and reliable tool for the solution of the heat transfer equations. Even for problems where analytical solutions are available, numerical methods have been used extensively, due to easiness of their implementation and their capabilities of handling variable boundary conditions (Clark 1978).

Finite-difference solutions have been widely used for the solution of linear partial differential equations (PDE's). While the explicit method is the most used finite-difference scheme for solution of PDE's due to the easiness of its implementation and its low requirements in terms of memory, several other finite-difference formulations presenting better convergence and stability properties are available (implicit method, Crank-Nicholson method, implicit alternating-direction method; Carnahan *et al.* 1969).

The use of a non-capacitance node (a node with no associated mass) allows to increase the time step and to use a coarser network in the finite-difference method without loosing the accuracy in the results (Chau and Gaffney 1990; Silva *et al.* 1993). For geometries where the heat transfer is one-dimensional (infinite slab, sphere and infinite cylinder) the finite-difference solution of Eq. 1.12, when a non-capacitance node at the surface is considered, is given on Table 1.3. The meshing of the geometry, the definition of the different nodes, the elemental volumes and the areas are presented in Fig. 1.1 for a generalised one-dimensional geometry. Definitions of areas and volumes will vary accordingly to the actual geometry.

The finite-difference approach is limited to cases where the body has or can be assumed to have a simple geometry (Naveh *et al.* 1983). Another numerical method, the finite-element method, is normally used for more complex cases. The finite-element denomination arises from the fact that in this method the region under study is divided into small elements. The different elements are connected at nodal points which are located at the corners and eventually along the sides of the elements.

Some of the advantages and disadvantages of the finite-element method compared with the finite-difference method have been reviewed (Singh and Segerlind 1974; Puri and Anantheswaran 1993). As advantages over the finite-difference method the finite-element method allows (i) an easier handling of spatial variation in the material properties, (ii) a greater accuracy in handling irregular boundaries, as curved boundaries can be used in this method, (iii) non-linear problems can be handled easier, (iv) the size of the elements can be varied, which allow the use of fine and coarse grids

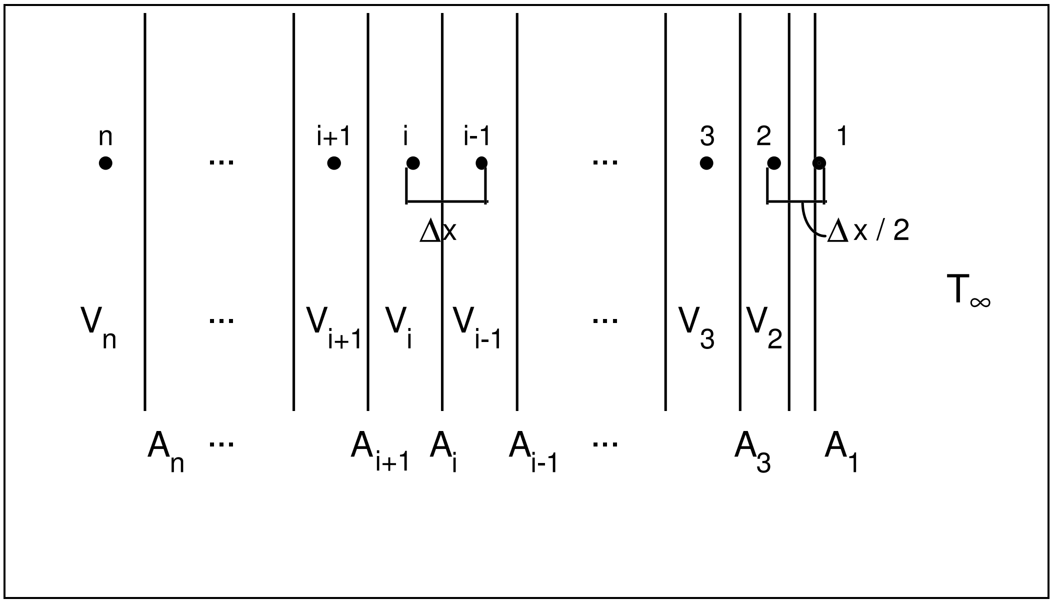

FIGURE 1.1 Finite-difference grid for a one-dimensional heat transfer problem, using a non-capacitance surface node (Silva *et al.* 1993).

TABLE 1.3 Finite-difference numerical solution for one-dimensional heat transfer problems considering a surface heat transfer boundary condition.

$$T_n^{t+\Delta t} = \frac{\Delta t \alpha A_n}{\Delta x V_n} T_{n-1}^t + \left(1 - \frac{\Delta t \alpha A_n}{\Delta x V_n}\right) T_{n-1}^t \text{ for the n}^{\text{th}} \text{ node.}$$

$$T_i^{t+\Delta t} = \frac{\Delta t \alpha A_i}{\Delta x V_i} T_{i-1}^t + \frac{\Delta t \alpha A_{i+1}}{\Delta x V_i} T_{i+1}^t + \left(1 - \frac{\Delta t \alpha A_i}{\Delta x V_i} - \frac{\Delta t \alpha A_{i+1}}{\Delta x V_i}\right) T_i^t \text{ for } 2<i<n$$

defining, $P_1 = \dfrac{h A_1 \Delta x}{\lambda A_2}$

$$T_2^{t+\Delta t} = \frac{\Delta t \alpha A_3}{\Delta x V_2} T_3^t + \frac{\Delta t \alpha A_2}{\Delta x V_2} \frac{P_1}{P_1 + 2} T_\infty^t + \left(1 - \frac{\Delta t \alpha A_3}{\Delta x V_2} - \frac{\Delta t \alpha A_2}{\Delta x / 2 \; V_2} \frac{P_1}{P_1 + 2}\right) T_2^t$$

$$T_1^{t+\Delta t} = \frac{P_1}{P_1 + 2} T_\infty^t + \frac{2}{P_1 + 2} T_2^{t+\Delta t}$$

in regions where high and low gradients of the desired parameters exist, (v) spatial interpolation is more meaningful than in the finite-difference method and (vi) mixed boundary value problems are easier to handle.

As disadvantages it was pointed out (Puri and Anantheswaran 1993) that the finite-element formulation is (i) mathematically more complex than the finite-difference method and (ii) uses more computational resources, both in terms of computation time and memory requirements.

1.5.2.2. Applications in modelling of in-pack sterilisation of foods

The finite-difference method has been used to model the conduction heat transfer with infinite heat transfer coefficient in cylindrical metal cans (Teixeira *et al*. 1969a and 1969b; Saguy and Karel 1979; Ohlsson 1980a; Teixeira and Manson 1982; Young *et al.* 1983; Gill *et al.* 1989), in rectangular containers (Manson *et al.* 1970), in oval-shaped containers (Simpson *et al.* 1989), in spherical fruits and vegetables (Bimbenet and Duquenoy 1974), in flexible pouches (Ohlsson 1980b; Kopelman *et al.* 1982; McGinnis 1986; Tandon and Bhowmik 1986; Bhowmik and Tandon 1987) and in cylindrical plastic cans (Shin and Bhowmik 1990). Finite-difference models with incorporation of surface heat transfer coefficients have been considered (Tucker and Clark 1990; Tucker and Holdsworth 1991; Silva *et al.* 1992a).

Several examples of the use of the finite-element method in solving food related conduction heat transfer problems can be found in literature. The finite-element method has been used for the calculation of heat transfer during the sterilisation of conductive heating foods in cylindrical container (De Baerdemaeker *et al.* 1977; Naveh *et al.* 1983 and 1984) and in glass jars (Naveh *et al.* 1983). Several examples of the use of the finite-element method to solve the heat transfer equations in irregular shaped bodies (cooling of fruits, De Baerdemaeker *et al.* 1977), bodies composed of diverse materials (heating of a chicken leg, De Baerdemaeker *et al.* 1977) or anisotropic and non-homogeneous conduction heating canned foods (Banga *et al.* 1993) can be found in literature. The flexibility of the finite element method allowed the simulation of the simultaneous solution of the heat and mass transfer equations during in-pack thermal processing (sterilisation of canned mushrooms, Sastry *et al.*

1985). The finite element method was also used to study the influence of random initial temperature and stochastic ambient temperature and surface heat transfer coefficient during thermal processing (Nicolaï and De Baerdemaeker 1992) and the influence of the variability of thermophysical properties on the transient temperature distribution (Nicolaï and De Baerdemaeker 1993, Nicolaï 1994).

Natural convection during thermal processing of foods has been studied by several authors. Due to the difficulties in building mathematical models to describe the problem several experimental studies were performed for the determination of the direction and distribution of the convection currents inside the container during processing. The addition of a methylene blue solution (Fagerson and Esselen 1950) or the use of the particle-streak method (Hiddink 1975) were some of the approaches used to visualise the flow patterns during heating in containers. Temperature distribution was measured by the insertion of thermocouples at different locations in the container (Hiddink 1975).

An empirical approach has been followed for the determination of the dependence of the heat transfer coefficients during the processing of food containers subjected to rotation. Correlation equations involving dimensionless parameters (Nu, Re, Pr) for the determination of the overall heat transfer coefficient have been developed for Newtonian fluids with various viscosities in several sizes of cylindrical containers under axial, end-over-end rotation and reciprocating axial mode (Javier *et al.* 1985), axially rotated cans filled with Newtonian liquids (Soulé and Merson 1985), Newtonian (Anantheswaran and Rao 1985a) and non-Newtonian (Anantheswaran and Rao 1985b) liquid foods in cans during end-over-end rotation, for Newtonian and non-Newtonian fluids in cans processed in a steritort (Rao *et al.* 1985 and 1988) and viscous materials in axially rotating cans (Rotstein *et al.* 1988). The use of an equivalent thermal diffusivity for the study of convection heating by analogy with conduction has been proposed (Bera *et al.* 1987). The magnitudes and evolution of this factor allow to assess the relative importance of conduction and convection during the heating process.

Finite-difference based models have been used for the prediction of the transient flow patterns and temperature profiles during the heating of a cylindrical can filled with water (Datta and Teixeira 1988). The simulation results were in closed agreement with the experimental results obtained by Hiddink (1975). Finite-element schemes for the simultaneous solution of the equations of mass, motion and energy conservation (see section 1.5.1.2.) have been used for the simulation of pasteurisation processes for fluids contained in bottles or cans (Engelman and Sani 1983) and the simulation of the natural convection heating of a thick viscous liquid food within a can during sterilisation (Kumar *et al.* 1990).

1.5.3. Empirical solutions

Due to difficulties encountered in developing theoretical models that allow for an accurate description of transient heat transfer during in-pack sterilisation of foods an empirical description is often preferred.

One advantage of empirical formulas is that no *a priori* assumptions are made with respect to the way the heat propagates inside the body (conduction /convection/ mixed mode), nor with respect to the geometry or to the presence or not of resistance to the heat transfer at the surface of the product. Empirical formulas for the description of the heat evolution are only valid for simple boundary conditions. Usually, empirical formulas are valid for a single or at most two consecutive step changes in the medium temperature. Furthermore, empirical description of the heat penetration does not allow an easy extrapolation to different processing conditions that might result in changes in the heat penetration parameters.

The empirical description of experimental heat penetration data using the simple log-linear model, set forward by Ball (1923), still constitutes the most used approach for the empirical description of heat transfer in canned foods and is still widely used in methods for the design of appropriate thermal processes. The empirical description advanced by Ball allows to describe the heat penetration curves with the aid of a reduced set of empirical parameters determined from the experimental heating and cooling curves (Fig. 1.2) that allow to extrapolate heat penetration data taken from a set of processing conditions to other conditions.

Ball's formula (Eq. 1.19) is based on the linear behaviour observed when the logarithm of the difference between the temperature at a given location in the food and the heating medium temperature is plotted against time (Fig. 1.2).For the characterisation of the linear relationship, two parameters, f and j, are used.

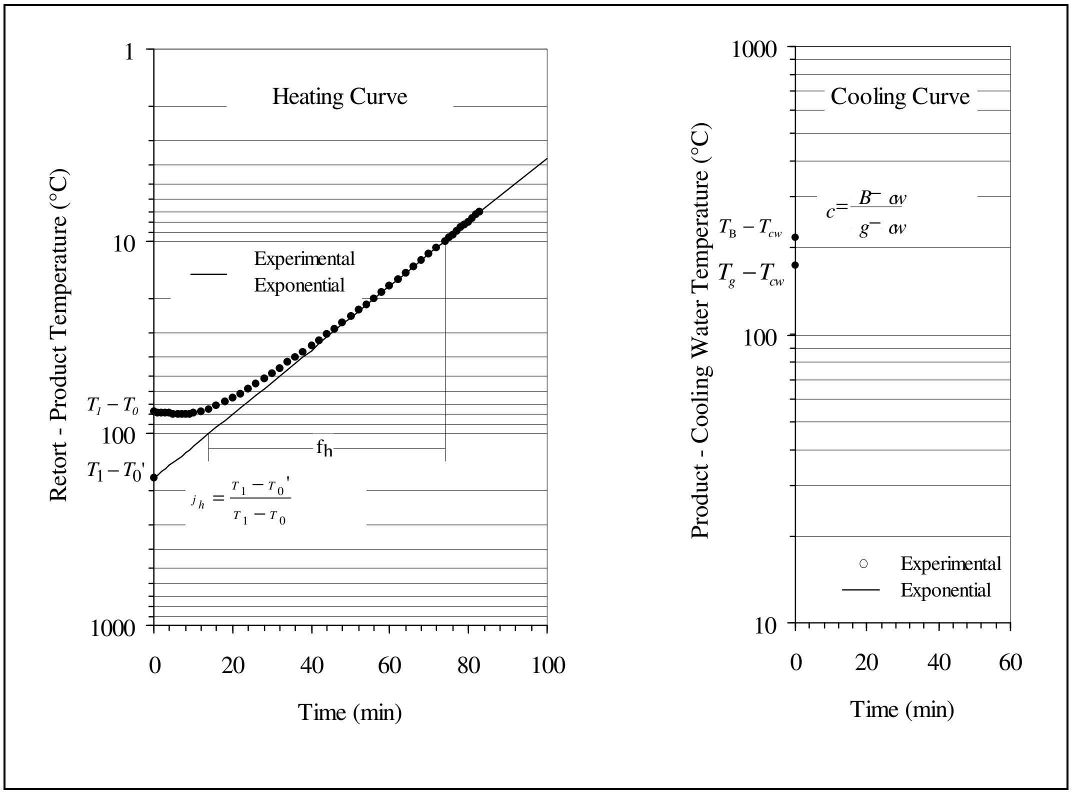

FIGURE 1.2 Heat penetration curve in log-linear co-ordinates. Definition of the heat penetration parameters.

$$t = f \log\left(j \frac{T_1 - T_0}{T_1 - T(t)} \right) \tag{1.19}$$

The equations used to describe the food temperature during the cooling cycle are more complicated than those used during the heating cycle. Ball (1928) made the assumption that the initial lag portion of the cooling curve could be approximated by a hyperbola (Eq. 1.20).

$$\frac{\left[T_g + 0.3\left(T_g - T_{cw}\right) - T(t)\right]^2}{\left[0.3\left(T_g - T_{cw}\right)\right]^2} - \frac{t^2}{\left(0.175 f_h\right)^2} = 1 \tag{1.20}$$

this initial cooling ends, according to Ball, at,

$$T(t) = T_g - 0.343\ (T_g - T_{cw}) \tag{1.21}$$

After this initial curvilinear portion the temperature follows the straight-line behaviour (in semi-log co-ordinates, see Fig. 1.2) (Eq. 1.22),

$$T = T_{cw} + j_c(T_g - T_{cw})10^{-t_c/f_c} \tag{1.22}$$

In order to derive Eq. 1.20 several assumptions about the exact shape and position of the hyperbola had to be made, the most important of them being the assumption of a fixed value for j_c (=1.41).

Modifications on the description of the cooling curves to allow for variations on the j_c and f_c -values were proposed (Ball and Olson 1957; Griffin *et al.* 1969 and 1971; Larkin and Berry 1991). Equations for the prediction of temperatures in the cooling phase for j_c-values larger (Eq. 1.23) and smaller (Eq. 1.24) than 1 respectively, were used.

$$T = T_{cw} + (T_g - T_{cw})\left[j_c 10^{-t/f_c} - (j_c - 1)10^{-j_c t/((j_c-1)f_c)}\right], \text{ for } j_c \geq 1 \tag{1.23}$$

$$T = T_{cw} + (T_g - T_{cw})\left[j_c 10^{-t/f_c} + (1 - j_c)10^{-j_c t/((1-j_c)f_c)}\right], \text{ for } j_c \leq 1 \tag{1.24}$$

Hayakawa (1970 and 1982) developed a set of experimental formulas (Table 1.4) for the description of the curvilinear portion of heat penetration curves with j-values from 0.001 to 6500. These formulas take into account the initial curved portion observed in heat penetration curves.

Datta (1990) presented theoretical justification for the use of the semi-logarithmic empirical description for conduction heating of arbitrary shapes. For the case of natural convection heating he concluded that a semi-logarithmic time-temperature relation is unlikely from physical as well as mathematical considerations, although, for practical purposes, both numerical solutions as well as experimental data for natural convection heating can be approximated to a semi-logarithmic form over small ranges of processing times.

Indeed, in spite of the extreme difference in the two heat transfer models discussed in sections 1.5.1.1. and 1.5.1.2., experimental heat penetration curves are often approximated as exponential functions of time at least after a short time. It is possible to derive theoretical expressions for the empirical heat penetration parameters for the case of perfect mixing and of conduction heating.

TABLE 1.4. Formulas proposed by Hayakawa to describe the curvilinear portion of heat penetration curves (Hayakawa 1982; Lekwauwa and Hayakawa 1986)

j- value range	Hayakawa's formulas
$0.001 \leq j \leq 0.4$	$\begin{cases} U(t) = 1 - 10^{-\eta\sqrt{\frac{t}{B}}} \\ \eta = \left((t_v / f) - \log_{10} j\right) / (t_v / f) \\ t_v = f\left(0.3913 - 0.3737 \log_{10} j\right) \\ B = t_v\left[(t_v / f) - \log_{10} j\right]^{\eta} \end{cases}$
$0.4 \leq j < 1$	$\begin{cases} U(t) = 1 - \Delta T_0^{\cot\left(Bt + (\pi/4)\right) - 1} \\ B = \dfrac{1}{t_v}\left\{\arctan\left[\dfrac{\log_{10}(\Delta T_0)}{\log_{10}(j\Delta T_0) - (t_v / f)}\right] - \dfrac{\pi}{4}\right\} \\ t_v = 0.9 f (1 - j) \end{cases}$
$1 < j \leq 5.8$	$\begin{cases} U(t) = 1 - \Delta T_0^{\cos(Bt) - 1} \\ B = \dfrac{1}{t_v}\arccos\left[\dfrac{\log_{10}(j\Delta T_0 - t_v / f)}{\log_{10}\Delta T_0}\right] \\ t_v = 0.7 f (j - 1) \end{cases}$
$5.8 < j \leq 6500$	$\begin{cases} U(t) = 1 - \Delta T_0^{\cos(Bt) - 1} \\ B = \dfrac{1}{t_v}\arccos\left[\dfrac{\log_{10}(j\Delta T_0 - t_v / f)}{\log_{10}\Delta T_0}\right] \\ t_v = 1.54 f \log_{10}(j / 1.8) \end{cases}$

By comparing Eq. 1.14 with Eq. 1.19 we can derive expression for the theoretical expected values for the empirical parameters f and j for perfectly mixed liquids (Merson *et al.* 1978) subjected to a constant heating or cooling medium temperature (Eq. 1.25 and Eq. 1.26).

$$j = 1 \tag{1.25}$$

$$f = \frac{\ln(10) m C_p}{U_0 A} \tag{1.26}$$

For conduction heating bodies it is possible to relate the empirical parameters, f and j, in Eq. 1.19, with the geometry and thermal properties of the object. Considering the analytical solution for the temperature evolution at the centre of a finite cylinder with infinite heat transfer coefficient (Table 1.1) and considering sufficiently high values of time, so that all the terms in the series with the exception of the first vanish, the equation reduces to,

$$\frac{T(t,r,x)-T_0}{T_1-T_0}=1-\frac{8}{\pi}\frac{J_0(0)}{\beta_1 J_1(\beta_1)}\exp\left(-\left(\frac{\left(\frac{\pi}{2}\right)^2}{L^2}+\frac{\beta_1^2}{R^2}\right)\alpha t\right) \tag{1.27}$$

Comparing Eq. 1.19 and Eq. 1.27 we find, that for this case,

$$j = 2.03970 \tag{1.28}$$

$$f=\frac{\ln(10)}{\left(\frac{\left(\frac{\pi}{2}\right)^2}{L^2}+\frac{\beta_1^2}{R^2}\right)}=\frac{0.398}{\left(\frac{0.427}{L^2}+\frac{1}{R^2}\right)} \tag{1.29}$$

Using a similar reasoning theoretical expressions for the empirical parameters can be derived for other geometries considering an infinite (Table 1.5) or finite (Table 1.6) surface heat transfer coefficient.

1.6. Physical-mathematical methods for the design and evaluation of thermal processes

The available physical-mathematical methods for thermal process calculations can be divided into two major classes, the general methods and the formula methods. The former methods do not usually provide means for predicting the time-temperature relationship of food during the processing, the latter have built-in means for this prediction.

TABLE 1.5 Theoretical values of f and j-values for various geometries when the initial temperature distribution is uniform and Bi is infinite (adapted from Ball and Olson 1957).

Geometry	f value	j (centre)	j at any point in the object
Infinite Slab	$0.933\,\dfrac{L^2}{\alpha}$	1.27324	$1.27324\cos\left(\dfrac{\pi y}{2L}\right)$
Infinite Cylinder	$0.398\dfrac{R^2}{\alpha}$	1.60218	$1.60218\,J_0\left(\dfrac{\beta_1 r}{R}\right)$
Sphere	$0.233\dfrac{R^2}{\alpha}$	2.000	$0.63662\dfrac{R}{r}\sin\left(\dfrac{\pi r}{R}\right)$
Finite Cylinder	$\dfrac{0.398}{\left(\dfrac{0.427}{L^2}+\dfrac{1}{R^2}\right)\alpha}$	2.03970	$2.03970\,J_0\left(\dfrac{\beta_1 r}{R}\right)\cos\left(\dfrac{\pi y}{2L}\right)$
Brick	$\dfrac{0.933}{\left(\dfrac{1}{a^2}+\dfrac{1}{b^2}+\dfrac{1}{c^2}\right)\alpha}$	2.06410	$2.06410\cos\left(\dfrac{\pi x}{2a}\right)\cos\left(\dfrac{\pi y}{2b}\right)\cos\left(\dfrac{\pi z}{2c}\right)$

1.6.1. General methods

General methods are the most accurate mathematical procedures for the estimation of the sterilisation value of a thermal process, since food temperatures experimentally determined are directly used for the computation of the sterilising value without any assumptions on the time-temperature relationship of the food during the course of the sterilisation process. They strongly rely on the assumption of first order kinetics of destruction discussed in section 1.4.1. Errors are associated with measuring errors on time and temperature and on the kinetic model used (including errors on the parameters).

TABLE 1.6 Theoretical values of f and j-values for various geometries when the initial temperature distribution is uniform and Bi is finite (adapted from Ball and Olson 1957).

Geometry	f value	j (centre)	
Sphere	$\frac{2.303R^2}{\alpha\beta_1^2}$	$\frac{2Bi\beta_1}{\sin(\beta_1)*\left(\beta_1^2+Bi^2-Bi\right)}$	(*)
Infinite Cylinder	$\frac{2.303R^2}{\alpha\beta_1^2}$	$\frac{2Bi}{\left(\beta_1^2+Bi^2\right)J_0(\beta_1)}$	(+)
Infinite Slab	$\frac{2.303L^2}{\alpha\beta_1^2}$	$\frac{2Bi}{(\beta_1^2+Bi^2+Bi)\cos(\beta_1)}$	(#)

(*) β_1 is the first positive root of the equation $\beta \cot(\beta)+ Bi-1=0$

(#) β_1 is the first positive root of the equation $\beta \tan(\beta)= Bi$.

(+) β_1 is the first positive root of the equation $\beta J_1(\beta)-Bi J_0(\beta)=0$

Bi represents the Biot number, $Bi = h R/\lambda$, and expresses the ratio between the surface heat transfer resistance to the internal heat transfer resistance.

The first mathematical method proposed for the calculation of processing values for canned foods has been introduced by Bigelow *et al.* (1920). This method allows to co-ordinate the information relating the death of micro-organisms at different temperatures (from TDT curves) with the heat penetration curves observed for the product under evaluation. The method, as originally presented, did not make any assumption with regard to any mathematical model relating the thermal death time with temperature. The method consists in allocating to each time-temperature pair observed during the heating and cooling curves a lethal rate value, plot the calculated lethalities as a function of time and calculate the overall processing value by graphically integrating the obtained lethality curve. The lethal rate value for each point was originally calculated as the inverse of the time necessary to destroy all the micro-organisms (spores) at the temperature represented by the point, the thermal death time. Ball (Ball 1928; Ball and Olson 1957) made several improvements on the General method. The major assumption that was introduced is the linear character of the thermal death-time curve. Another important improvement consisted of calculating the lethal rate using Eq. 1.30, with T_{ref} = 121.1°C (250°F).

$$L = 10^{\frac{T - T_{ref}}{z}} \quad (1.30)$$

Contributions such as the development of special co-ordinate paper (Schultz and Olson 1940; Cass 1947; Hayakawa 1973; Leonhardt 1978) or numerical integration schemes (trapezoidal rule: Patashnik 1953; Simpson's rule: Anonymous 1967; Gaussian integration: Hayakawa 1968) were introduced to make the General method less laborious. Formulas for converting heat-penetration data obtained for one condition of initial and retort temperatures to corresponding data for different retort and initial temperatures were proposed to increase the applicability of the General method (Schultz and Olson 1940), however these formulas were developed based on pure conduction or perfect mixing models and must be used with caution for intermediate modes of heat transfer.

Even though General methods have been developed for the evaluation of experimental time-temperature data, 'General method schemes' have been widely used for the integration of time-temperature data from constructive computation (*e.g.,* Teixeira 1969a).

General methods are the most accurate and suited method of process evaluation for a given experimental time-temperature curve. However, as they do not provide a model for temperature prediction General methods have no predictive power. For a different set of processing conditions it is necessary to obtain a new experimental time-temperature curve in order to evaluate the process.

1.6.2. Formula methods

Formula methods combine the knowledge on the kinetics of destruction of micro-organisms with methods for the prediction of the temperature evolution in the food during processing. As they provide means for the prediction of the temperature evolution, they allow the extrapolation between different processing conditions which improves their applicability when compared to the group of methods previously described. On the other hand, due to the assumptions made on temperature prediction their applicability is limited to cases where these assumptions are valid (*e.g.,* the methods for the determination of the mass average sterilising value to be discussed in section (1.6.2.2.) are only valid for conduction heating foods as in the development of these methods the assumption on conduction heating was made).

Two different groups of formula methods can be found in literature. In the first group the aim is to calculate the sterilising value at the slowest heating point of the container, the cold spot, the point least affected by the heat treatment in terms of microbial destruction. The second group of procedures calculates a volume integrated processing value by appropriately integrating the effect of the heat treatment throughout the volume of the product.

1.6.2.1. Evaluation of critical point lethality

In most formula methods, empirical formulas for estimating temperature history curves of food are applied (see 1.5.3.). These formulas were obtained without any assumptions on the type of food, size and shape of the container, or method of heat transfer. Therefore, formula methods are applicable to almost any heat process (Hayakawa 1978).

The first formula method reported in the literature dates from 1923 (Ball 1923) and in spite of its limitations is still extensively used today. Ball's formula method was derived to reduce the time necessary to obtain results, as the only method available at that time, the General Method of Bigelow *et al.* (1920), is very cumbersome in use, and does not allow extrapolation from one set to another set of processing conditions. Ball's method provides a way of co-ordinating the various factors that enter the calculation of the time necessary to process canned foods (Ball 1923).

Ball's formula method is used when the heat penetration curve (Fig. 1.2) can be represented by one or two straight lines on semi-logarithmic paper. The formula permits evaluating processes for retort and initial temperature conditions differing from those for which the heat penetration data were obtained.

In the development of the method empirical equations able to describe the internal temperature evolution in the can were used (Eqs. 1.19 to 1.22). These equations were substituted into Eq. 1.7 and integration was performed for the calculation of the F_0, process, value. As the resulting integral could not be solved analytically the integration was performed graphically and the results of the integration were presented in tabular or graphical form as f_h/U vs. log g relationships, with U being the sterilising values in terms of minutes at retort temperature and g being the number of degrees below retort temperature at the beginning of cooling.

For the calculation of the processing value, F_0, for straight-line heating curves (for broken-heating curves see Ball and Olson 1957; Lopez 1987), the following procedure is used,

(1) Calculate log g from Eq. 1.31,

$$\log g = \log jI - \frac{B_B}{f_h} \tag{1.31}$$

with I - Retort minus initial product temperature, T_1-T_0 (°C).

B_B-Process time according to Ball. Time from the beginning of process to the beginning of the cooling phase (min).

(2) Find f_h/U from graphs of f_h/U vs. log g presented by Ball.

(3) Calculate F_0 from Eq. 1.32,

$$F_0 = \frac{f_h}{(f_h / U)F_i} \tag{1.32}$$

where F_i is defined as,

$$F_i = 10^{\frac{T_{ref} - T_1}{z}} \tag{1.33}$$

To determine the heating time necessary at a given retort temperature to achieve a certain processing value the reverse procedure is used. That is,

(1) Calculate f_h/U from Eq. 1.34,

$$f_h / U = \frac{f_h}{F_0 F_i} \tag{1.34}$$

(2) Find log g from f_h/U vs. log g graphs.

(3) Calculate B_B from Eq. 1.35.

$$B_B = f_h(\log jI - \log g) \tag{1.35}$$

To avoid the cumbersome use of tables and graphs associated with the Formula method nomograms to carry out the calculations involved were constructed (Olson and Stevens 1939). Regression equations, substituting table or graph readings allowing for the implementation of Ball's method in a programmable calculator were proposed by Vinters *et al.*(1975).

In the development of the graphs and tables several assumptions were made that restrict the application of Ball's formula method. It was assumed, sometimes erroneously, that: (i) the cooling lag factor is constant ($j_c = 1.41$); (ii) the portion of the cooling curve immediately following 'steam-off' satisfies the equation of a hyperbola. (iii) the deviation of the curved portion of the heating curve (low temperatures) from the extrapolated straight portion does not seriously affect the sterilising value of the process and (v) the heating medium is suddenly raised to process temperature (i.e., no coming-up-time).

The fact that the original formula method was developed considering a fixed value for j_c lead to the development of new formula methods where this restriction was abandoned.

Stumbo and Longley (1966) observed that values of j_c other than the fixed value of 1.41 should be used to accurately estimate the sterilising value of the cooling part of a heat process. By graphical integration of lethality curves, calculated from heat penetration curves manually drawn, they calculated new tables of f_h/U:g to account for different values of j_c. All the values reported on the tables presented were calculated by considering that the difference between the processing and cooling temperature was 180 °F (100 °C) since, as they reported, a 10 °F variation on this value only causes about 1% variation on the calculated processing values. The f_c-values was assumed to be equal to f_h. As they indicated for experimental values of f_c 20% larger than f_h the method fails to predict accurately the processing value.

A new set of tables for thermal process calculations based on modified empirical equations (Eqs. 1.23 and 1.24) during the cooling cycle, were proposed (Herndon *et al.* 1968; Griffin *et al.* 1969 and 1971). These new tables allowed to consider j_c-values other than the fixed value of 1.41 on Ball's formula method. Later a method based on the same empirical formulas for the description of the cooling cycle, but where the

TABLE 1.7 Formula methods reported in the literature considering critical point lethality.

Reference	Notes	*modus operandi*
Ball (1923, 1928)	log-linear heating, $f_c = f_h$, $j_c = 1.41$, initial hyperbolic cooling	Tables
Olson and Stevens (1939)	same as Ball (1923)	Nomograms
Herndon *et al.* (1968) Griffin *et al.*(1969, 1971)	heating portion as in Ball's method. Initial portion of cooling approximated by a different empirical formula. $f_c \neq f_h$, $j_c \neq 1.41$	Tables
Steele and Board (1979)	sterilising ratios instead of temperature differences.	Tables and Regression Equations.
Vinters *et al.* (1979)	uses regression equations, $f_h/U : g$, from Ball's tables	computerised
Stumbo and Longley (1966)	$f_c = f_h$, $j_c \neq 1.41$, m + g = 180 °F (100 °C), heating curves drawn manually.	Tables
Jen *et al.* (1971)	extension of the tables of Stumbo and Longley (1971). Uses heat conduction model.	Tables
Purohit and Stumbo (1973); Stumbo (1973)	refinement of the tables of Jen *et al.* (1971)	Tables
Tung and Garland (1978)	Interpolation on the tables of Stumbo (1973)	computerised
Pham 1987	$f_c = f_h$.	empirical formulas
Pham 1990	$f_c \neq f_h$.	empirical formulas
Hayakawa (1970)	Experimental formulas for prediction of transient temperatures at initial heating and cooling stages.	Tables
Kao *et al.* (1981)	regression equations f_h/U (g, j_c, z) Hayakawa's (1970) functions used to describe cooling. $f_c = f_h$.	computerised
Gillespy (1951)	Conduction heating.	Tables
Gillespy (1953)	Allow for variable heating medium temperature.	Tables
Jakobsen (1954)	heating and cooling curves approximated by a hyperbolic secant. Conduction heating	Tables
Flambert and Deltour (1972)	Conduction heating	Tables
Lenz and Lund (1977a)	Conduction heating. Arrhenius dependence	Charts

number of tables was greatly reduced by the use of sterilising ratios, was presented (Steele and Board 1979).

Hayakawa (1970), using a set of experimental formulas for estimating the entire portion of transient temperature history curve for an extended range of j_c (Table 1.4), presented a new formula method for the evaluation of thermal processes. Regression equations for the calculation of the f_h/U ratio for different g, z and j_c values, based on Hayakawa's equations were presented later(Kao *et al.* 1981).

Several formula methods were developed using to some extent the heat conduction model discussed in section 1.5.1.1. This group of methods should be used with caution if the mode of heat transfer is not purely conduction.

Gillespy (1951) estimated that for conductive heating products in cylindrical cans the lethality achieved during the cooling phase would be equivalent to the lethality achieved by considering a hypothetical cooling curve where the can contents are initially (at the start of the cooling) at a homogeneous temperature, equal to the temperature that would be achieved at the centre of the can if the heating phase were extended for a further $0.03 \cdot f_h$ minutes, and the can is suddenly subjected to a medium at cooling temperature. This simplification does not allow the actual calculation of the central temperatures achieved during the cooling phase but provides a simple way of calculating the contribution of the cooling phase to the total achieved lethality. It is clear that the accuracy will depend on the appropriateness of the $0.03 \cdot f_h$ factor.

Stumbo and co-workers (Jen *et al.* 1971; Purohit and Stumbo 1973; Stumbo 1973) recalculated the tables presented previously by the same group (Stumbo and Longley 1966) by using time-temperature curves, theoretically predicted based on the equations of heat conduction in a finite cylinder, as in their original method the tables were calculated for f_c values equal to f_h and no provision to account for f_c different f_h was made. In order to calculate curves for different j_c-values the time-temperature curves at different radial positions in a finite cylinder were considered. A modified version of this method, where the effects of initial product temperature and cooling water temperature and where variations between f_h and f_c were considered, was later presented (Pham 1987 and 1990).

A set of tables for the exact calculation of the lethality at the centre of conduction heating foods, assuming that the temperatures of the heating and cooling medium are constant throughout the respective phases of the process was presented (Flambert and Deltour 1972). Later a similar method, the lethality Fourier number method, where the main difference consisted in using the activation energy rather than the traditional z value to describe the temperature dependence of reaction rates was proposed (Lenz and Lund 1977a). In Table 1.7 a summary of the published formula methods for the evaluation of critical point lethality is presented.

A method using the numerical solution of the heat conduction equation was proposed for the evaluation of thermal processes for products showing any j-value. In order that j-values other than the theoretically expected value for a finite cylinder (2.04, see Table 1.5) could be handled the use of a time-shift was proposed (Teixeira *et al.* 1992; Bichier and Teixeira 1993).

A large amount of work is published where analytical (Tables 1.1 and 1.2) or numerical solutions (*e.g.,* Table 1.3) of the heat conduction equation (Eqs. 1.10 to 1.12) were used for the determination of the critical point lethality. In theses studies, the processing value is calculated by evaluation of the integral in Eq. 1.7 after calculating the time-temperature history using the appropriate solutions (analytical or numerical) of the heat conduction equation. As examples of this kind of studies we can cite the following: Thompson 1919, Schultz and Olson 1938, Hayakawa and Ball 1971, Teixeira *et al.* 1969b, Manson *et al.* 1970, Bhowmik and Tandon 1987, Chau and Gaffney 1990, Shin and Bhowmik 1990, Tucker and Holdsworth 1991 and Tucker 1991.

1.6.2.2. Evaluation of average lethality

As it was referred in section (1.4.3.), to evaluate the volume integrated (mass average) lethality through evaluation of Eq. 1.9 it is necessary to know the time-temperature evolution in all points of the container. In order to develop methods for the evaluation of the volume integrated lethality, solutions of the heat conduction equation have been used (Hayakawa 1977b) as these solutions provide means of calculating the temperature evolution in all the points of the container. The applicability of the available methods for the calculation of the volume integrated lethality is then restricted to foods heating by conduction.

Gillespy (1951) presented one of the first methods for the calculation of the mass average sterilising value. The container was divided in iso-lethality surfaces, the retention at each surface calculated and the mass average concentration determined by integrating the retention over the total volume of the container. Stumbo (1953), using a similar reasoning, developed a simple formula for the evaluation of the volume integrated processing value throughout cylindrical containers filled with conduction heated foods. For the development of the formula the integration of the lethal value over a series of iso-lethality surfaces was considered. In the final format the formula was presented (Eq. 1.36), it suffices to calculate the processing value at the centre of the container and at a point in the container presenting a j-value equal to half of the value at the geometrical centre. Ball's formula method (Ball 1923 and 1928) has been suggested in order to carry out the calculations. In application, the procedure employs the same process parameters as used for the evaluation of the lethal effect at a single point in a container.

$$F_s = F_c + D_{Tref}\left(1.084 + \log\frac{F_\lambda - F_c}{D_{Tref}}\right) \qquad (1.36)$$

with F_c - lethality at the centre. (min)

F_λ - lethality at a point in the container where, $j = 0.5\ j_c$. (min)

Ball and Olson (1957) developed a method for calculating mass average sterilisation values by considering the division of the can volume into elemental volumes delimited by 11 iso-j surfaces. The microbial reduction achieved at each region was calculated and the total and the overall retention calculated as a weighted average of the retention achieved at each of the elemental regions. Jen *et al.* (1971) developed a new equation similar, to the one presented by Stumbo (1953) that extends the applicability of Stumbo's method for the calculation of the retention of quality factors. Downes and Hayakawa (1977) proposed the combined use of Jen *et al.* (1971) equation and Hayakawa's (1970) tables to take into account the effect of the initial curvilinear portion of the heating curve and the effect of different experimental values for the slopes of the heating and cooling curves. Barreiro *et al.* (1984) using an

TABLE 1.8 Formula methods reported in the literature considering mass average lethality.

Reference	Notes
Gillespy (1951)	Integration over iso lethality components
Stumbo (1953)	Integration over iso-F surfaces. Cylindrical containers
Ball and Olson (1957)	Integration of lethality over 11 iso-j surfaces in cylindrical containers.
Jen *et al.* (1971)	As Stumbo (1953). Extended for the validation average degradation of quality factors.
Barreiro *et al.* (1984)	Similar to Stumbo (1953). Brick-shaped containers.
Hayakawa (1969)	Solution of the conduction equation. Dimensional analysis for the selection of relevant dimensionless parameters.
Lenz and Lund (1977b)	Correlation equations based on numerical solution of the conduction equation. (Lenz and Lund 1977a)
Thijssen *et al.* (1978)	Analytical Solution of the conduction equation. Numerical integration of the volume average lethality. Uses Arrhenius equation.
Thijssen and Kochen (1980)	Extension of the previous method for variable retort temperatures. Numerical solutions of the conduction equation.

approach similar to Stumbo (1953) developed a formula for the calculation of the mass average retention of a quality attribute during the thermal processing of conductive heating foods in brick-shaped containers.

A computerised method for the determination of the mass average retention during the thermal processing of conductive heating foods in cylindrical containers based on numerical integration of Eq. 1.9 considering 12 points inside the container was presented (Timbers and Hayakawa 1967). To develop the method all numerically significant terms on the analytical solutions of Fourier's equation for heating and cooling were considered. Six dimensionless groups were selected and tables prepared for the determination of the mass average sterilising value (1969). Similar procedures were derived by other authors (Lenz and Lund 1977b; Thijssen *et al.* 1978; Thijssen and Kochen 1980) the main improvements being the use of numerical solutions of the conduction equation. In Table 1.8 a summary of the published formula methods for the evaluation of the mass average lethality is presented.

Cohen and Wall (1971) presented a method for the calculation of the average lethality in cylindrical containers based on the calculation of the processing value, from time-temperature curves experimentally measured at several points of the container, using the General Method (Bigelow 1921) and subsequent integration over the total volume of the can. This method has been referred to as an average General Method (Lenz and Lund 1977b).

The use of numerical solutions of the heat conduction equation (1.5.2.) allow the calculation of the time-temperature evolution in any point of the container permitting then evaluation of the mass average sterilising value expressed by Eq. 1.9 for any kind of retort profile (*e.g.*, Teixeira *et al.* 1969a; Manson *et al.* 1970; Silva *et al.* 1993). A large number of studies on optimisation of the volume integrated (mass average) quality during the thermal processing of conductive heating foods make use of numerical solutions of the Fourier equation (*e.g.*, Teixeira *et al.* 1969b and 1975b; Ohlsson 1980a, 1980b and 1980c; Saguy and Karel 1979; Martens 1980; Nadkarni and Hatton 1985; Banga *et al.* 1991; Hendrickx *et al.* 1991a, 1991b, 1991c and 1992b).

1.7. Evaluation of thermal processes for variable boundary conditions (variable heating medium temperature)

Most of the methods discussed in the previous sections were developed for the evaluation of thermal processes consisting of a heating step at constant temperature followed by a cooling step at constant temperature. These methods, with the exception of the numerical solutions for conduction heating foods, do not provide means for the evaluation of thermal processes when a variable heating medium temperature is observed (*e.g.,* deviations in the scheduled processing temperature, variable retort temperature profiles).

Several methods have been derived in order to evaluate thermal processes when a variable boundary condition (variable heating medium temperature) is observed. The available methods can be divided into two groups: The methods based on solutions of the heat conduction equation (fact that limits their applicability to conductive heating foods) and methods where empirical solutions to describe the time-temperature evolution are used. Another possible distinction between the available methods can be made based on the way the variable boundary condition is handled. Some authors used Duhamel’s theorem to handle variable heating medium profiles (Gillespy 1953; Hayakawa 1971) while others used numerical solutions of the heat conduction equation (*e.g.,* Teixeira 1969a)

A tabular method using the Duhamel's theorem to handle variable heating medium temperature was suggested by Gillespy (1953). While originally developed for estimating the process attainment in the water legs of hydrostatic cookers it is a method of general applicability and can be used to deal with any variable heating medium temperature profile during the processing of conduction heating foods.

Hayakawa (1971) proposed the use of Duhamel's theorem, for the prediction of the time-temperature history of a food subjected to a variable heating medium temperature. To calculate the product temperature at time t, the time interval [0, t] is divided in a set of n intervals of length Δt= t/n, and the heating medium temperature, $T_s(t)$, is approximated at each of the intervals, by the temperature at the middle of the interval. Based on this approximations the integral in Eq. 1.18 is solved numerically as,

$$T(r,t) = T_0 + \sum_{i=1}^{n}\Big[\big(T_s\big[(i-0.5)\Delta t\big] - T_0\big)\Delta U(r)_{n-i+1}\Big] \qquad (1.37)$$

with,

$$\Delta U(r)_k = U\big(r,(k-1)\Delta t\big) - U\big(r,k\Delta t\big) \qquad (1.38)$$

where $T_s[(i-0.5)\Delta t]$ represents the surface temperature at (i-0.5)Δt, the mid point of interval [(i-1) Δt, i Δt], and $\Delta U(r)_k$, represents a dimensionless temperature difference, calculated from a dimensionless temperature history curve of a system subjected to a constant surface temperature. In this method, the empirical formulas developed by Hayakawa (Table 1.4) were used for the calculation of the dimensionless temperature differences.

The modification of the basic conduction model of Teixeira *et al.* (1969a), to allow for the prediction of temperatures of mixed mode heating foods has recently been proposed (Teixeira *et al.* 1992; Bichier and Teixeira 1993). The procedure is based on the fact that two log-linear heat penetration curves (x and y) having the same f value but different j-values lie parallel when plotted in a semi-logarithmic graph, with the time-shift between the curves equal to,

$$\Delta t = f \log\left(\frac{j_x}{j_y}\right) \qquad (1.39)$$

The authors considered the simple adjustment of the elapsed process time on the existing numerical heat conduction models for on-line process control by means of the use of a constant time delay (calculated from Eq. 1.39) in the calculations. The f_h value is implemented by considering an apparent thermal diffusivity. This approach produces good estimates of temperature in the case of constant heating medium temperature.

For the particular case of perfectly mixed foods, Eq. 1.16 allows the calculation of the temperature evolution when the heating medium temperature can be described by a set of linear segments. When the heating temperature is given by a set of discrete points numerical integration of Eq. 1.13 has been proposed (Bimbenet and Michiels 1974).

1.8. Implementation of the methods

Several approaches have been used for the calculation of thermal processes using the methods described in the previous sections. The most common approach relied on the use of pre-prepared tables and charts that allow a step-by-step calculation of the processing value (forward calculation) for a given set of processing conditions or the reverse calculation, the calculation of processing conditions that will give rise to a certain processing value. The use of tables and graphs was inevitable at the time the methods were developed. However the amount of information presented in tabular or graphical form is necessarily restricted due to space limitations. In some cases parameters with less pronounced effect on the final processing values were chosen to be omitted in order to reduce the number of working tables and graphs. With the computing power available today it is possible to avoid the limits posed by the use of tables and graphs. Computer implementation of a particular method should be performed by returning to the temperature prediction equations that form the basis of the method. The computer implementation of a method through the tabulated values in their original form or by means of regression equations is not considered appropriate, as it will transfer the limitations of the original tables to the computerised version of the method (Stoforos *et al.* 1994).

Several software packages for design and evaluation of thermal processes are commercially available. CAL Soft™ (TechniCAL Inc., Metaire, LA, USA) is a series of integrated, software modules for heat penetration studies (Swientek 1986). It includes thermal process calculations through General, Ball's and Stumbo's method.

PRO CALC Thermal Process Analysis System (PRO CALC Associates, Surrey, BC, Canada) allow the design and evaluation of thermal processes, using both the general method and formula method, using regression equations based in the tables developed by Ball and Olson. The Thermal Process Profiler (TPRO) software (Norback, J. and Johnson, C.E., Dept. Food Science, University of Wisconsin, Madison, WI, USA) allows the evaluation of thermal processes, combining the use of Ball's formula methods for the prediction of the temperature history in the cold spot of the food, with a numerical integration scheme for lethality calculations. NumeriCAL™ (TechniCAL Inc., Metaire, LA, USA) performs thermal process calculations, including evaluation of process deviations, by numerical simulation of the internal temperature data through input of the f_h and j_h parameters and the heating medium temperature history (Sperber 1989). Only limited information is available on the way the calculations are performed (Manson 1991, Manson 1992). CTemp (Campden & Chorleywood Food Research Association, Chipping Campden, Gloucestershire, UK) is a software package based on numerical solutions of the heat equation for various geometries that allows evaluation of thermal processes, including process deviations, for conductive heating products (Dobie *et al.* 1994).

1.9. Conclusions

The first order model of microbial destruction has been successfully used in the field of heat sterilisation and although more sophisticated models could be used, the first order model constitutes a good engineering tool for the design and evaluation of heat processes. Both the Arrhenius and the classical TDT model can be used to describe the dependence of the reaction rate with temperature. There is insufficient evidence in the literature to allow for a categorical decision in favour of one of the models.

Physical-mathematical methods are a valuable tool for the design and evaluation of thermal processes, greatly reducing the experimental effort needed. However the available physical-mathematical methods must be used critically. A knowledge of the assumptions made during the development and of the limitations of a particular method must precede its application for the design and evaluation of thermal processes.

The evaluation of thermal processes for conduction heating foods can be easily and accurately performed using analytical or numerical models available for the solution of the heat conduction equation. Variable processing temperatures and surface heat transfer coefficients can be easily accommodated by the available models allowing the evaluation of thermal processes for variable boundary conditions (e.g., deviations on the heating medium temperature) and to take into account the influences of different heating media (e.g., steam vs. steam-air mixtures) and packaging materials (e.g., plastic vs. metal containers). Numerical solutions of the conduction equation allow to calculate the product temperature at any point of the container making possible the evaluation of the process in terms of a volume integrated processing value. The available empirical models for the evaluation of thermal processes (e.g. Ball method) can predict accurately the processing values for conduction foods, as they are mostly based in solutions of the conduction equation.

For products where convection plays an important role in the heat transfer, liquid foods or mixtures of liquid and particulates, the number of alternative methods for the evaluation of thermal processes is limited. Methods based on the fundamental equations that describe the heat transfer when convection occur are scarce and when available the conditions for their applicability are restricted. For this kind of products the evaluation of thermal processes is usually conducted using methods that make use of an empirical description of the heat transfer. These methods are restricted for the evaluation of thermal processes consisting of one or two step changes in the medium temperature and do not allow for the accurate evaluation of thermal processes when a variable medium temperature is present (e.g., deviations on the scheduled process temperature and variable heating medium profiles). Moreover for methods using an empirical description of the heat penetration, the extrapolation of the empirical parameters between processing conditions must be done carefully. Changes in processing conditions might require a reevaluation of the empirical parameters.

Chapter 2. New semi-empirical approaches for the evaluation of thermal processes

2.1. Introduction

With the need for the evaluation of thermal processes where other than the classical type of profiles are used (*e.g.,* use of variable retort temperature profiles for the optimisation of thermal processes; Banga *et al.* 1991, Noronha *et al.* 1993), the evaluation of deviations of the scheduled process consisting in drops of the retort temperature, and to provide means for a better evaluation of the coming-up time (CUT) contribution on the total lethality of the process, there is a need for methods that can handle variable boundary conditions, that is, variable heating medium temperature profiles, for other than conduction heating foods.

Methods for the design and evaluation of thermal processes discussed in the previous chapter were, in their majority, developed considering processes consisting of a single step change (heating) or a combination of two step changes in the external medium temperature (heating followed by cooling).

In this chapter empirical methods are presented and tested against theoretical solutions for conductive and perfectly mixing heating. The experimental verification of the applicability of the method and its application for different case studies is presented in following chapters.

2.1.1. Coming-up time contribution

The empirical methods for the temperature evolution during in-pack sterilisation of foods, discussed in section 1.5.3., were developed considering a step change in the medium temperature. In batch-type sterilisation, the initial period necessary to heat the retort to the scheduled processing temperature cannot be taken into account by the available empirical methods. In order to estimate the lethality gain observed due to the existence of this come-up period several approaches have been followed.

The first attempt to deal with the retort coming-up time contribution to the total lethality of the process has been presented by Ball (1923). Based on heat penetration runs with boiling water, using No. 2 cans of corn and of 4% starch solutions, he concluded that 42% of the CUT could be considered as part of the process. That is the length of time necessary to process a can after the retort has reached processing temperature could be shortened by 42% of the time taken to bring the retort to processing temperature. The 42% correction factor was determined considering a linear increase of temperature during the CUT.

The duration of the come-up time and the shape of the retort temperature profiles during the come-up period have an influence on the j-value determined from the classical log-linear plots (Fig. 1.2), the f_h-value is not affected. There is a need for j_h-values that are transferable from one processing condition to another, therefore j_h-values must be stripped from come-up influence. The 42% correction factor has been commonly used for the determination of corrected zero times for the determination of corrected j-values (j_{hb}) from heat penetration data. However, the traditional approach of a 42% correction factor as a conservative procedure has been questioned (Berry 1983). Experimental cases were presented showing that the use of such correction factor can lead to underestimation of process times necessary to obtain product sterility (Berry 1983).

Several researchers derived relationships that allow the calculation of correction factors for the come-up time based on the process variables. It was pointed out that the correction factors could depend upon various parameters like food properties, microbial characteristics, as well as operational conditions (Hayakawa and Ball 1971). Regression equations for the prediction of correction factors for come-up heating, based either on critical point or mass average survivor concentration in cylindrical cans of foods heating by conduction, were presented (Uno and Hayakawa 1980 and 1981). The thermophysical properties and operational conditions which have an influence on the value of the correction factor of packaged liquids subjected to mechanical agitation were also evaluated, and regression equations relating the correction factors with the relevant process variables developed (Succar and Hayakawa 1982).

A simple experimental technique was presented for predicting the come-up time correction factor for a retort. The correction factors thus obtained were used for the correction of the j-values (Berry 1983). In this method it is sufficient to consider two sterilisation cycles where all the conditions (initial temperature, rotation,...), including the shape of the retort temperature profile during the coming-up period, remain the same with the exception of the come-up time duration. From the experimentally determined lethality and the come-up time duration of the two processes it is possible to evaluate the contribution of the come-up time in the lethality of the process.

The discussed approaches for the evaluation of the coming-up time contribution allow to calculate the contribution of the retort coming up time in the total lethality of the process. However, when used they do not allow the calculation of the temperature evolution inside the product. Ideal method though, would be the one that allows the prediction of the product temperatures when a come-up period is present.

2.1.2. Process deviations

During thermal processing, food temperatures can deviate significantly from their expected values because of deviations on the scheduled retort temperature. Such deviations can seriously endanger public safety due to under sterilisation of the food, or can be responsible for energy losses or reduction of product quality due to over-processing (Datta *et al.* 1986). If during a process a deviation in the scheduled retort temperature is observed (from a safety stand point, only temperature drops are of concern) then several alternative solutions are possible: reprocessing of the product, destruction of the product, holding of the product and future evaluation of the safety of the process or, if the deviation is detected before the end of the process, corrective action can be taken based on the scheduled process at the new retort temperature. Some of these alternatives, while valid from a safety standpoint, may have important economic costs or lead to considerable reduction in the product quality. To estimate the degree of sterilisation achieved in the cold spot of a container, methods are needed for the prediction of the temperature history at this location under conditions of variable heating medium temperature. The ideal case would be an on-line control of the retort temperature able to allow automatic corrective actions for possible deviations on the retort temperature.

2.1.3. Automatic control of sterilisation processes

Several computer-based retort control strategies, based on finite-difference solution of the conduction equation, for on-line correction of process deviations have been proposed (Teixeira and Manson 1982; Richardson and Holdsworth 1988; Datta *et al.*

1986; Gill *et al.* 1989; Simpson *et al.* 1990). These approaches have been shown to be valid for the on-line control of sterilisation processes for conduction heating foods. Their use is restricted to conduction heating foods as numerical solutions of the heat conduction were used in their development. There is a need for methods able to predict the temperature evolution under variable boundary conditions for foods that exhibit other modes of heat transfer in order to extend the available methodologies for the on-line control of sterilisation processes for this kind of products.

2.2. Calculation of transient temperatures during variable heating medium temperature

2.2.1. Existing approaches

As discussed in section 1.7. some authors presented methods that can be used for the evaluation of thermal processes when a variable retort temperature is observed (Gillespy 1953; Hayakawa 1971; Bichier and Teixeira 1993), however these methods present limitations that do not allow their general application for the evaluation of heat sterilisation processes. The methods using Duhamel's theorem do not allow changes on the heating characteristics of the product, such as when the product changes in its properties during processing (broken-heating products) or changes in the heating rate due to changes in the heat transfer coefficient between the product and the heating medium, when going from the heating to the cooling phase. On the other hand methods based on numerical solution of the heat conduction equation, that allow an easy incorporation of variable boundary conditions, can only be used for the evaluation of thermal processes for products heating by conduction.

In the method proposed by Hayakawa (1971) empirical formulas were used for the description of the temperature evolution, Duhamel's theorem was used to handle the variable heating medium temperature profile. In the method presented by Bichier and Teixeira (1993) discussed in section 1.7. means for incorporating the empirical parameters f_h and j_h in the conduction model were devised by considering an apparent thermal diffusivity and a time-shift, respectively. Here we propose another method for the incorporation of these empirical parameters in the conduction model that, as it will became apparent in the following sections of this chapter, will provide means for a better handling of variable heating medium temperatures.

2.2.2. The apparent position concept

When the temperature evolution measured at different points of a conductive heating body, initially at uniform temperature and suddenly immersed in a heating medium at a constant temperature, is plotted in log-linear co-ordinates (Fig. 1.2) it is observed that after an initial curvilinear portion the obtained curves can be described using straight-lines and that all the obtained straight-lines have the same slope (same f_h-values), but different intercepts (different j-values).

In section 1.5.3. expressions for the calculation of the empirical heat penetration parameters, f_h and j_h, for several geometries considering finite and infinite surface heat transfer coefficients (Tables 1.5 and 1.6) were introduced. Using these expressions, it is possible to determine a position in a conductive heating body that will have a certain j_h-value and an 'apparent' thermal diffusivity that will result in a given f_h-value.

Taken into account the available alternatives in Tables 1.5 and 1.6, the solution for a conductive heating sphere with infinite heat transfer coefficient was chosen. This case allows to cover a broad range of j-values (0 to 2), the broader range for geometries where the heat transfer is one dimensional. This range could be only slightly increased by using the solution for a conductive heating finite cylinder or brick what would increase the range to 2.04 or to 2.06 respectively. However, any of these options would imply the use of a more complex solution of the conduction problem. The use of solutions of the conduction equation considering finite heat transfer coefficient would also allow the incorporation of the empirical parameters in the conduction model by considering apparent Biot numbers for a fixed position. However, this option would lead to the use of solutions of the conduction equation more complex than those used when the heat transfer coefficient can be considered infinite (Tables 1.1 and 1.2).

The incorporation of the empirical f_h parameter in the conduction heating model was accomplished considering the relationship, between the thermal diffusivity and the f_h value given by Eq. 2.1. The incorporation of the j-value was accomplished taking into account the theoretical variation of j-value inside a conductive heating sphere presented by Ball an Olson (1957) (Eq. 2.2).

$$f_h = 0.233 \frac{R^2}{\alpha} \tag{2.1}$$

$$j(r) = 0.63662 \frac{R}{r} \sin\left(\frac{\pi r}{R}\right) \tag{2.2}$$

For any food with empirical heating parameters f_h and j_h it is then possible to find, an apparent position in a sphere, of thermal diffusivity given by Eq. 2.1, that shows the same heating parameters (j_h and f_h) as the food under consideration.

2.2.2.1. Analytical solution - Duhamel's theorem (ASDT)

In this method, as in the method proposed by Hayakawa (1971) described in section 1.7., Duhamel's theorem is used for the calculation of the temperature history of a food subjected to a variable heating medium temperature. While in the method proposed by Hayakawa empirical equations were used for the prediction of the dimensionless temperature differences to be used in Eq. 1.37, in this method the analytical solution of Fourier's second law for a sphere (Table 1.1) was applied. The empirical parameters were incorporated in the conduction model using the apparent position concept described in the previous section.

2.2.2.2. Apparent position - Numerical solution (APNS)[1]

When there are changes in the heating characteristics of the product during the process, caused for example by changes in f_h value in products that exhibit broken-heating curves, or changes in the surface transfer coefficients when moving from heating to cooling conditions, Duhamel's theorem is no longer applicable. Consequently the approach described above (2.2.2.1.) cannot be applied. Numerical solutions for the transient heat transfer in conductive heating foods are proved to be a fast and reliable way of dealing with the problem of heat conduction under variable retort temperature profiles, allowing changes to any of the variables, either separately or in combination (Tucker 1991). We will therefore try to combine the flexibility of numerical solutions with the empirical description of heat penetration curves.

[1] See Appendix I for a detailed description of the method.

This approach is a hybrid of the last method (ASDT) and the method proposed by Teixeira *et al.* (1992). It combines the flexibility of finite-difference with the empirical description of the heat penetration curves. The approach is differing from the one proposed by Teixeira *et al.* (1992) in the way it incorporates the empirical parameters in the conduction model. Here, the incorporation of the empirical parameters, f_h and j_h, is performed by taking into account the existing analogies between the empirical description of the time-temperature curves and the first term approximation of the analytical solution of the Fourier's equation for a sphere discussed previously. A position inside a conductive sphere, where the j_h-value equals the required one, is calculated and the time-temperature curve is simulated at this point using a finite-difference model for a sphere with the actual boundary condition (time variable heating medium temperature). The f_h value is incorporated by an 'apparent' thermal diffusivity.

2.3. Material and methods

2.3.1. Programs

In this section the developed computer programs are briefly discussed. All programs were written in the Pascal language and were run in a personal computer (PC) using the Turbo Pascal integrated environment (Turbo Pascal, Version 6.0, Borland International, Inc.).

2.3.1.1. Conduction heating - Finite-difference solution

For conduction heating, data were generated using finite-difference models (see section 1.5.2.) for various regular geometries (infinite slabs, infinite cylinders, sphere, finite cylinder, bricks), (Chau and Gaffney 1990, Silva *et al.* 1992a), from which the theoretical j-values can be derived from analogy between the Ball equation and the first term approximation of the analytical solutions of Fourier equation for each of the geometries (Table 1.5). The finite-difference program has been described in detail elsewhere (Silva *et al*. 1992a)

2.3.1.2. Perfectly mixed case -BIM (Bimbenet)

For the generation of the temperature history for perfectly mixed products subjected to a variable heating medium temperature, Bimbenet and Michiels's (1974) equations discussed in section 1.5.1.2. were implemented.

2.3.1.3. Hayakawa's method (1971) - HYK

A computer program was written for the implementation of the method proposed by Hayakawa (1971) for the determination of the temperature evolution in the product when subjected to a variable heating medium temperature (see section 1.7.) Duhamel's integral (Eq. 1.18) was approximated using Eqs. 1.37 and 1.38. For the determination of the temperature differences in Eq. 1.38 Hayakawa's empirical formulas (Table 1.4) were used.

2.3.1.4. Analytical solution with Duhamel's theorem - ASDT

A computer program was written for the implementation of the method described in section 2.2.2.2. Duhamel's integral (Eq. 1.18) was approximated using Eqs. 1.37 and 1.38. For the determination of the temperature differences in Eq. 1.38 the analytical solution for a conductive sphere initially at homogeneous temperature and subjected to a step change in the surface temperature was used (see Table 1.1). The apparent position inside the sphere showing a given j-value was determined by solving numerically Eq. 2.2 using Newton-Raphson's method (Dorn and McCracken 1972). The thermal apparent diffusivity was calculated from the f_h-value using Eq. 2.1.

2.3.1.5. Numerical solution with apparent position concept - APNS (apparent position numerical solution)

A finite-difference conduction model for a sphere, described elsewhere (Chau and Gaffney 1990, Silva *et al.* 1992a), was modified in such a way that the empirical parameters f_h and j_h could be incorporated. To perform this incorporation an apparent thermal diffusivity was calculated from the f_h value using Eq. 2.1 considering a sphere of unit length. The apparent position inside the sphere showing the target j_h-value was calculated from Eq. 2.2 as previously described. A repeated linear interpolation scheme (Dorn and McCracken 1972) was used to determine the temperature at this

TABLE 2.1 Retort temperature profiles considered for the simulations.

#	Process
1	60 min at 121°C.
2	20 min 60-121°C (ramp) + 40 min at 121°C
3	30 min at 121°C + 10 min at 110°C + 20 min at 121°C
4	50 min at 121°C + 30 min at 35°C.
5	30 min at 121°C + 30 min at 110°C
6	20 min at 121°C + 10 min at 110°C + 10 min (ramp) 110°C to 121°C + 20 min at 121°C.
7	20 min at 121°C + 10 min (ramp) 121°C to 110°C + 10 min at 110°C + 20 min at 121°C.
8	20 min at 121°C + 10 min at 110°C + 30 min at 115°C

exact location inside the sphere from the temperatures calculated for each time step from three nodes of the finite difference's grid.

2.3.1.6. Numerical solution with time-shift - ATNS (apparent time numerical solution)

A program was written to calculate the time-temperature history for a food showing a j-value in the interval [0,2] using the method proposed by Teixeira *et al.* (1992). In this program a finite-difference conduction model for a sphere was used to perform the calculations and the calculated time-temperature history was shifted considering the time delay on Eq. 1.39. The shifting in the time was only performed once at the start of the process.

2.4. Results and discussion

The performance of four methods for the determination of the product temperature evolution when subjected to a variable heating medium temperature (Hayakawa's method-HYK; Apparent time numerical position-ATNS; Analytical solution Duhamel's theorem -ASDT and Apparent position numerical solution-APNS) were tested against theoretically generated case studies for both conduction (several geometries) and perfectly mixed heating.

Different types of processing conditions were considered: (i) constant retort temperature (Table 2.1, #1) (ii) a linear come up behaviour followed by a constant retort temperature (Table 2.1, #2), (iii) constant heating temperature followed by constant cooling temperature (Table 2.1, #4) and (iv) different process deviations during the holding phase (Table 2.1, #3 and #5 to #8). The predicted product temperature response, using the different methods was calculated and compared with the reference methods: finite-difference conduction model or Bimbenet and Michiel's equations. In all the simulations a homogeneous initial product temperature of 40°C was assumed. For the calculation of the processing value (F_0) the reference temperature was 121°C and a z value of 10°C. All the reported F_0 values were calculated by numerical integration of Eq. 1.7, using Simpson's rule (Carnahan *et al.* 1969).

In Figs. 2.1 to 2.4 the time-temperature curves obtained with the different methods, for the centre of infinite cylinders and slabs with different f_h values, are compared with the temperatures calculated using a finite-difference model for conduction. It can be observed that for a single step change in the retort temperature (Fig. 2.1) all the methods are able to predict accurately the transient temperature history. It can also be observed in the first line of Tables 2.2 to 2.5, where the case of constant retort temperature (Table 2.1, #1) is shown, that the error in the calculation of the processing values from the time-temperature data curves generated using the different methods is negligible. When a cooling step is considered (Fig. 2.2) all the methods, with the exception of the method that uses the apparent time concept (time delay), are able to follow closely the temperature curves generated using the finite-difference method. Again it can be observed that the error in the predicted F_0 values is negligible for all the methods with the exception of the method that uses the time delay in the calculations (Tables 2.2 to 2.5, #5), where, as it could be expected from the temperature overestimation during the cooling section, this method overestimates the processing value. For the other examples (Fig. 2.3 and Fig. 2.4) there is close agreement between the temperatures predicted by the different methods when compared to the finite-difference solution, again with exception of the method using the time delay concept. For this method it was observed that when the external (retort) temperature suddenly changes (Fig. 2.2 and Fig. 2.4) or gradually changes (Fig. 2.3) the method is not a good predictor of the product time-temperature course. Lower or higher temperatures

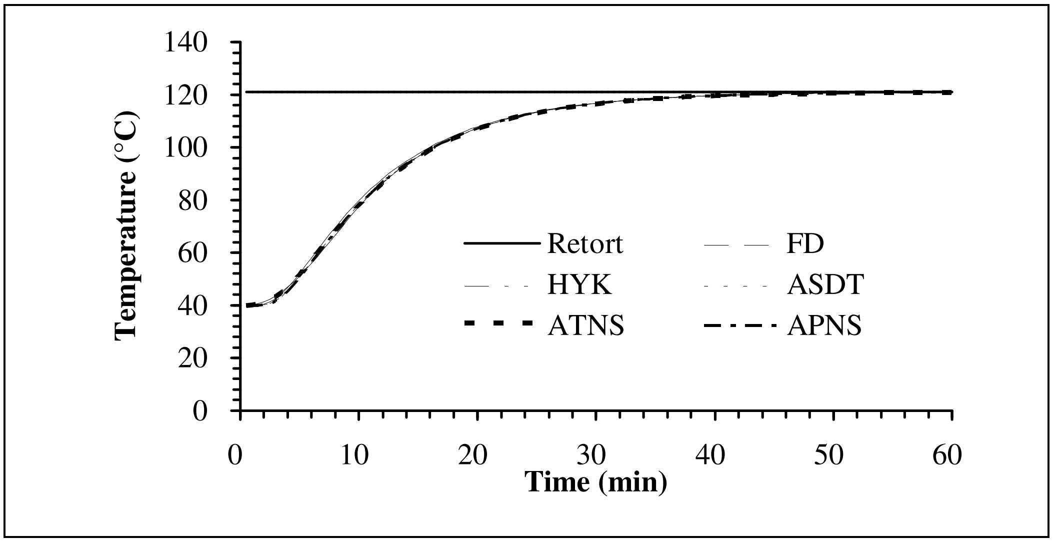

FIGURE 2.1 Time-temperature profiles predicted using the different methods compared with the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite cylinder. f_h= 20 min. Theoretical j-value = 1.60128. Some of the curves are partially superimposed. FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

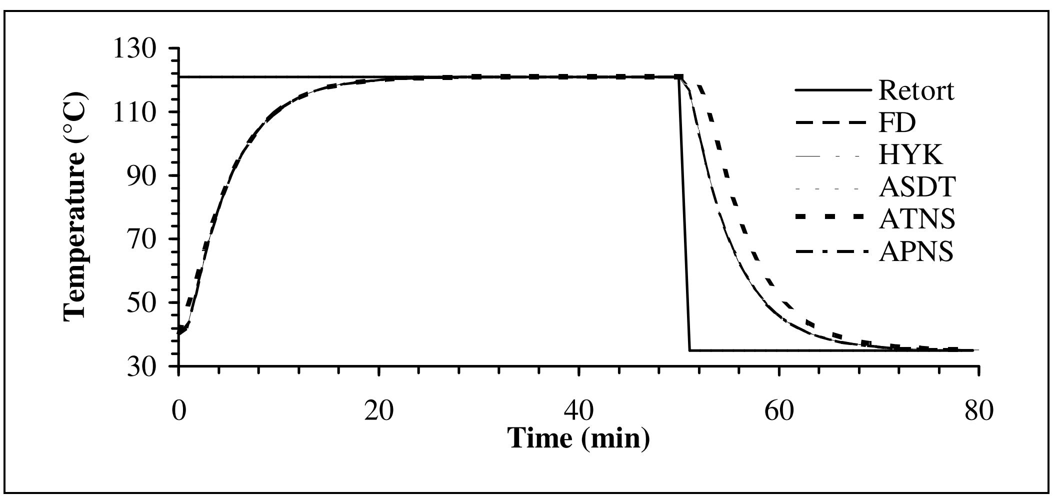

FIGURE 2.2 Time-temperature profiles predicted using the different methods compared with the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite slab. f_h= 20 min. Theoretical j-value = 1.27324. Some of the curves are partially superimposed. FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

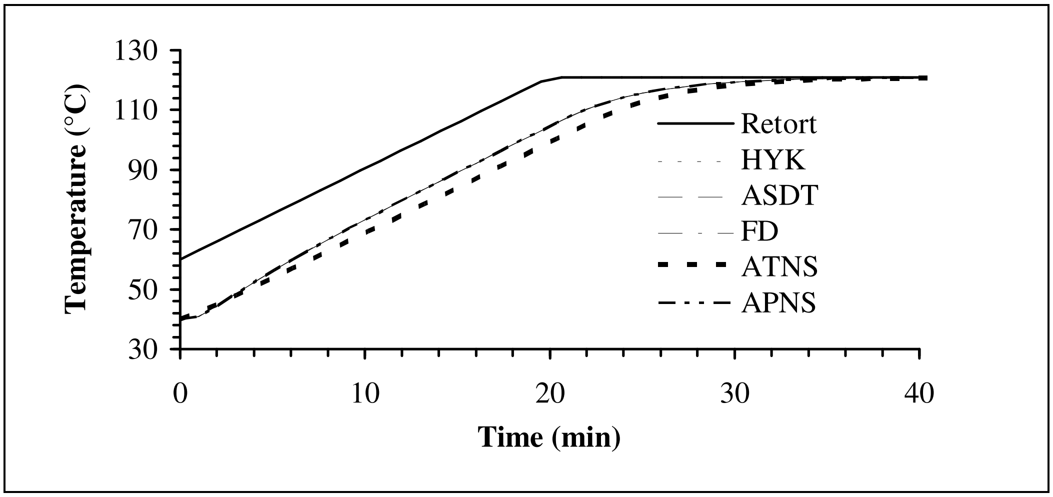

FIGURE 2.3 Time-temperature profiles predicted using the different methods compared with the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite slab. f_h= 10 min. Theoretical j-value = 1.27324. Some of the curves are partially superimposed. FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

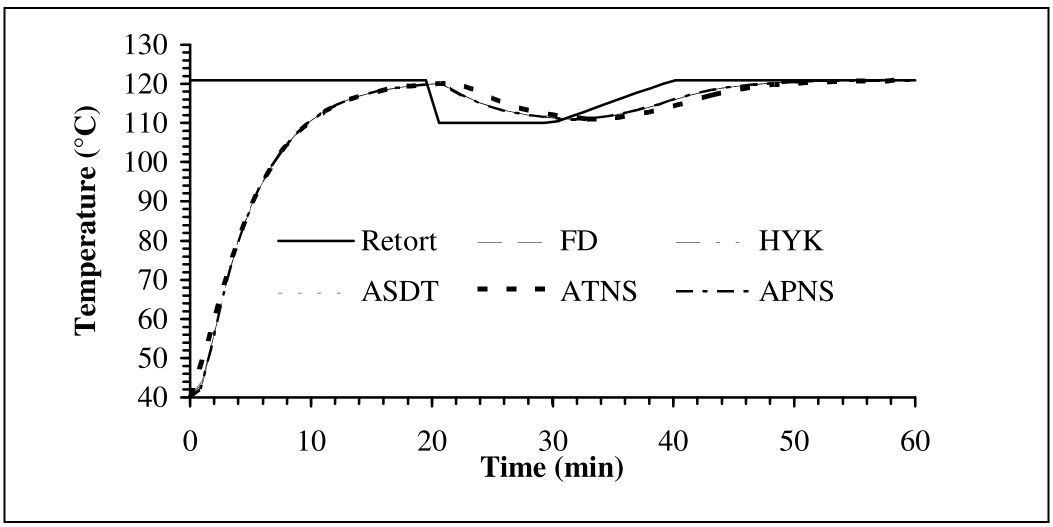

FIGURE 2.4 Time-temperature profiles predicted using the different methods compared with the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite cylinder f_h= 10 min. Theoretical j-value = 1.60218. Some of the curves are partially superimposed. FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

than those obtained using a finite-difference method are predicted, respectively for an increase or a decrease in the process temperature.

The reason for this phenomenon is the incorrect way for taking into account the j_h-value. Each time that the boundary condition changes there is a lag period before the cold spot temperature respond to these changes, which is reflected by the j_h-value. The time delay concept as used here only considers the correct j-value at time zero. At all the other time moments the response of the model is as a system with j_h-value = 2.0 (centre of a sphere). This means that the correct application of the time delay concept leads to a time correction factor each time the boundary condition deviates from a constant value. The time correction should be done according to the j_h-value of the system at the moment the boundary condition changes. Since temperature gradients exist during the process, j_h-values cannot be predicted. This problem can be overcome by the use of an apparent position concept.

In Tables 2.2 to 2.5 the processing values calculated from the time-temperature history determined for each of the described methods are presented. These values are compared with processing values calculated from the time-temperature history determined using the reference method. For each of the different processes and calculation method the error observed in relation to the finite-difference based processing value is presented, and for each case the maximum percent error is outlined using bold type to enable an easy comparison between the accuracy of the different methods.

From these results it is easily seen that the methods based on the application of Duhamel's theorem and/or on the application of the apparent position concept allow a good prediction of the processing values during the sterilisation of conduction heating foods. The deviation observed when comparing the processing values calculated using these methods with the values obtained by integration of lethalities under the time-temperature curve obtained with the finite-difference methods never exceeds 1.25% (Table 2.2, #2). When the method based on the application of the apparent time concept is applied process values up to 25% larger (Table 2.3, #5) than the predicted with finite-difference can be found.

TABLE 2.[illegible] Process values (in minutes) calculated from the time-temperature profiles predicted using the different models, as compared with the process value calculated using the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite cylinder, f_h= [illegible] min. Theoretical j_h-value = [illegible]. See Table 2.1 for definition of process. % error = (F_0^{method}- F_0^{FD}) /F^{FD} · 100.

Process #	FD (min)	HYK (min)	error (%)	ATNS (min)	error (%)	ASDT (min)	error (%)	APNS (min)	error (%)
1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
3	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
6	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
7	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
8	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

TABLE 2.5 Process values (in minutes) calculated from the time-temperature profiles predicted using the different models, as compared with the process value calculated using the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite slab. f_h= 10 min. Theoretical j_h-value = 1.27324. See Table 2.1 for definition of process. % error = (F_0^{method}- F_0^{FD}) /F^{FD} · 100

Process #	FD (min)	HYK (min)	error (%)	ATNS (min)	error (%)	ASDT (min)	error (%)	APNS (min)	error (%)
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
6	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

TABLE 2.3 Process values (in minutes) calculated from the time-temperature profiles predicted using the different models, as compared with the process value calculated using the finite-difference solution. Case study: Temperatures at the geometrical centre of an infinite slab. f_h= 20 min. Theoretical j_h-value = 1.27324. See Table 2.1 for definition of process. % error = (F_0^{method}- F_0^{FD}) /F^{FD} · 100

Process #	FD (min)	HYK (min)	error (%)	ATNS (min)	error (%)	ASDT (min)	error (%)	APNS (min)	error (%)
1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
3	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
5	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
6	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
7	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
8	7.08	7.12	0.56	7.77	9.75	7.12	0.56	7.07	-0.14

FD - Finite-difference; HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

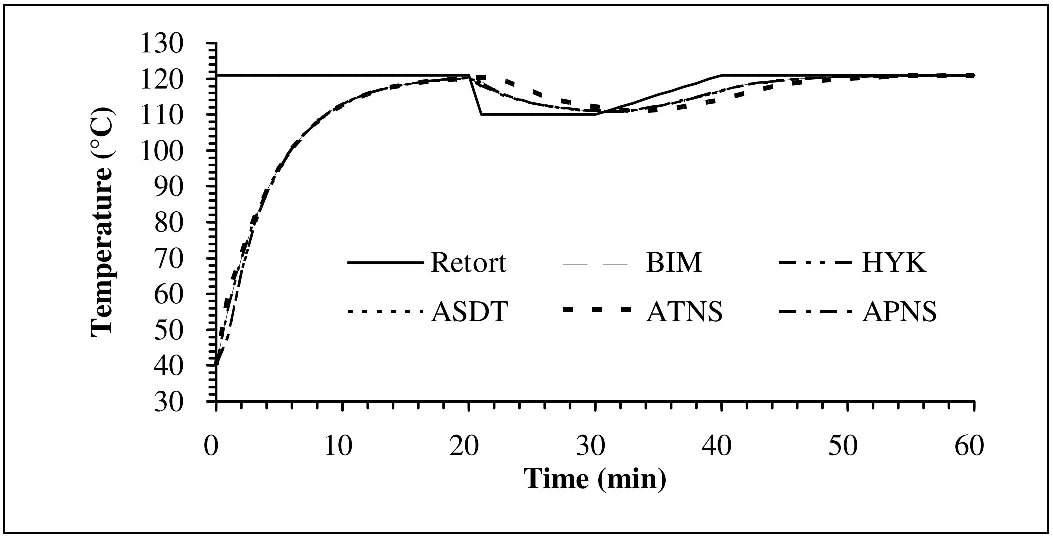

FIGURE 2.5 Time-temperature profiles predicted using the different methods compared with the results obtained using Bimbenet and Michiel's method. Case study: Perfectly mixed liquid. f_h= 10 min. Theoretical j-value = 1.0. Some of the curves are partially superimposed. BIM - Bimbenet and Michiel's method; HYK - Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution

In Fig. 2.5 the temperature evolution predicted with the four different methods are compared with the temperature evolution predicted with the solution for a perfectly mixed liquid calculated using Eq. 1.16. With the exception of the method using the apparent time-shift for the incorporation of the j_h-value, a good prediction of the temperatures could be achieved.

In Table 2.6 results obtained for the four alternatives are compared with results obtained using the formulas of Bimbenet and Michiels (1974) for the calculation of the transient temperature of perfectly mixed liquids with j_h-values equal to 1.0. In the case of perfectly mixed liquids Hayakawa's method (1971) produced the best results. In this method Hayakawa's empirical formulas for the calculation of the temperature history in the curvilinear portion of the heat penetration curves are applied. This can explain the superiority of this approach since these formulas were developed considering heat penetration data from products covering a wide range of j_h-values. The two methods that use the apparent position concept (ASDT and APNS) also allow a good prediction of the processing values during the sterilisation of perfectly mixed liquids. For the cases studied, here the maximum error observed for these methods is

TABLE 2.6 Process values (in minutes) calculated from the time-temperature profiles predicted using the different models, as compared with the process value calculated using the temperatures calculated accordingly to Bimbenet and Michiel's method. Case study: Perfectly mixed liquid: f_h= 10 min. Theoretical j_h-value = 1.0. See Table 2.1 for definition of process. % error = $(F_0^{method} - F_0^{FD}) / F^{FD} \cdot 100$

Process #	BIM (min)	HYK (min)	error (%)	ATNS (min)	error (%)	ASDT (min)	error (%)	APNS (min)	error (%)
1	44.79	44.79	0.00	44.72	-0.16	44.77	-0.04	44.72	-0.16
2	32.65	32.64	-0.03	36.44	11.61	32.60	-0.15	32.57	-0.25
3	31.38	31.38	0.00	31.08	-0.96	31.55	0.54	31.49	0.35
4	35.02	35.04	**0.06**	36.93	5.45	35.47	1.28	35.41	**1.11**
5	19.20	19.20	0.00	21.52	**12.08**	19.47	1.41	19.45	1.30
6	26.38	26.38	0.00	25.84	-2.05	26.50	0.45	26.42	0.15
7	25.95	25.95	0.00	25.62	-1.27	26.08	0.50	25.99	0.15
8	14.69	14.69	0.00	16.34	11.23	14.91	**1.50**	14.87	1.23

BIM - Bimbenet and Michiel's method; HYK - Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.

1.5% (Table 2.6, #8). As in the case of conduction heating foods the use of the apparent time concept leads to larger deviations, in our case studies, up to 12% (Table 2.6, #5)compared to the method of Bimbenet and Michiels (1974).

For the intermediate case of thermal processing of mixed mode heating foods (convection/conduction) the theoretical assessment of the methods' performance was not conducted due to the lack of reliable algorithms for the simulation of the theoretical heat transfer under these conditions. For products exhibiting mixed mode heat transfer experimental studies must be carried out to validate the presented methods.

In Table 2.7 the performances of the proposed methods are compared in terms of computing time. The methods using the finite-differences models (ATNS and APNS) show computing times significantly inferior to the ones presented by the methods that use numerical implementations of Duhamel´s theorem to handle variable boundary conditions. It is also noticeable from the results presented that the ASDT method presents computing times superior to the ones achieved by the HYK method. This higher computing times are due to the fact that in the first method there is the need to

TABLE 2.7 Computing time for the different methods. Times necessary to simulate a sterilisation process consisting of 15 min CUT followed by 60 minutes at processing temperature (120°C).

Method *	f_h (min)	j_h	Computing Time# (sec)
ASDT	25	1.5	21.42
ASDT	10	1.0	43.87
HYK	25	1.5	6.76
HYK	10	1.0	5.88
ATNS	25	1.5	0.27
ATNS	10	1.0	1.10
APNS	25	1.5	0.31
APNS	10	1.0	0.66

* HYK- Hayakawa's method; ASDT - Analytical Solution Duhamel's Theorem; ATNS - Apparent Time Numerical Solution; APNS- Apparent Position Numerical Solution.
# All calculations were performed in a PC DX2 running at 66MHz.

evaluate all the relevant terms of a series (Table 1.1) for the calculation the relevant temperatures in Eq. 1.38 while in the second method this is done by the direct application of Hayakawa´s formulas (Table 1.4).

2.5. Conclusions

Three of the methods tested for the prediction of temperature evolution under variable retort temperature (HYK, ASDT and APNS) allowed a good prediction of the temperature history in the cold spot of the product when compared to theoretical solutions for conduction heating foods and perfectly mixed liquid foods.

Comparing the different methods for flexibility and calculation time one can conclude that the numerical solution using the apparent position concept (APNS) is the most promising method. The APNS method allows an easy incorporation of changes in the heating characteristics. Changes in the f_h-value, cases of broken-heating curves or when the f-value changes from heating to cooling, can be incorporated by changing the apparent thermal diffusivity. Changes in the j-value (heating to cooling), while more involving, can be accommodated by the calculation of a new apparent position based on the new j-value, and by considering a new initial, uniform, temperature equal to the temperature at the time of the change in position. This flexibility can only be realised by the APNS approach. As stated before the methods that use the Duhamel's theorem cannot handle changes in the heating characteristics. Moreover the APNS method is the fastest one, in terms of computation time, allowing an easy incorporation in on-line retort control logic.

The method using the apparent position concept (APNS) associated to a numerical solution of the conduction equation allows the determination of the temperature evolution at a single point in the product (*e.g.,* cold spot) for variable boundary conditions, requiring as input only the heat penetration parameters (f_h and j_h) obtained from heat penetration tests together with the retort temperature profile. However, the method should be used with caution because it is empirical in nature and is not intended to simulate the heat transfer mechanisms during the sterilisation. The method relies on a correct determination data (to be discussed in the following chapter) of the heat penetration parameters (f_h and j_h) under the same conditions (viscosity, head space, agitation,...) expected during the actual sterilisation process.

The APNS method presents some limitations similar to the ones observed with other methods that make use of empirical parameters for the description of the heating behaviour of the product, namely the necessity of determinate the empirical parameters from heat penetration and the problems associated with the transferability of the empirical parameters to other processing conditions (container dimensions, headspace,...). However, the method allows to handle variable retort temperature profiles using empirical parameters determined for a single step change in the heating medium temperature.

Chapter 3. Strategies for the determination of empirical heating parameters

3.1. Introduction

In the previous chapter, empirical methods were presented for the determination of the product temperature when subjected to a variable heating medium temperature. In order to use those methods it is necessary to have an *a priori* knowledge of the heating characteristics of the product in the form of the empirical parameters f_h and j_h.

In the methods proposed in the previous chapter, it is assumed that the heat penetration parameters are determined under conditions of a step change of the heating medium (i.e., no come-up period). In the methods that make use of Duhamel's theorem this constraint is bound to the conditions of applicability of the theorem, where the solution for the transient temperature history evolution under conditions of a single step change in the surface temperature is used for the calculation of the temperature evolution under conditions of variable heating medium temperature. In the methods that make use of the apparent position concept the need for j_h-values determined under the appropriate conditions arises from the relationships used for the calculation of an apparent position from a given j-value (see Table 1.5) derived assuming a step change in the medium temperature.

The classical determination of the empirical parameters from experimental data consists in plotting the difference between the heating medium temperature (a constant value) and the temperature observed in the product (usually the slowest heating point) in an inverse semi-log graph (see Fig. 1.2). From this kind of graphs it is possible to determine graphically the two parameters (f_h and j_h for the heating curve, and f_c and j_c for the cooling curve) necessary for the empirical description of a straight line heating curve (for broken-line heating curves it is also necessary to determine two extra parameters for the complete characterisation of the heating curve: a second f_h value and the time at which the break, change in the f_h values, occurs). In the empirical description of heating and cooling curves the determination of the heating and cooling parameters (f_h, j_h and f_c, j_c) is based on the assumption of an instantaneous change in the medium temperature (to the heating or cooling temperature).

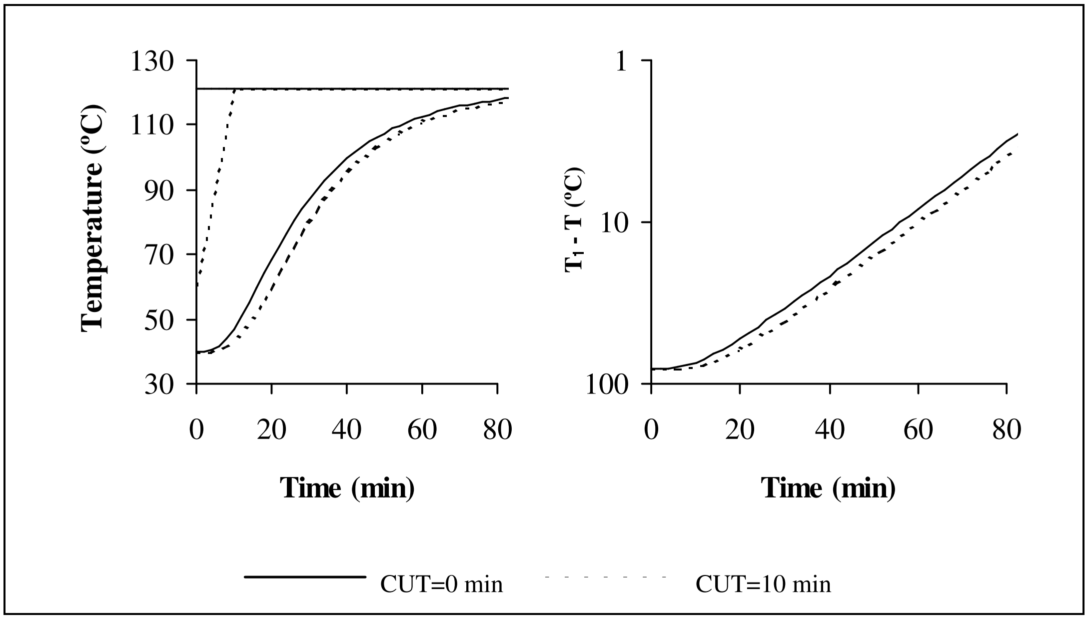

FIGURE 3.1 Influence of the retort come-up time in the heat penetration parameters. The f_h does not change with the come-up time duration (48 min in both cases), the j_h value increases from 1.76 (CUT = 0 min, full-line) to 2.05 (CUT = 10 min, dotted line). Conductive cylinder (73 mm x 110 mm), thermal diffusivity 1.6 x 10-7 m2/s.

Several factors influence the j_h-value. Besides the variation with the position inside the product, which constitutes the basic idea behind the APNS method discussed in chapter 2, the surface heat transfer coefficient, the existence of an initial temperature distribution in the product and the type and duration of the come-up-time will influence the j_h-value. When a CUT is present, a corrected zero time (42% rule) is commonly used for the determination of a corrected j_{hb}-value.

Theoretically, j_h-values cannot be lower than 1.0 (perfectly mixed) and no greater than 2.064 (conduction heating brick, Table 1.5), for the centre of products with uniform initial temperature subjected to a step change in heating medium temperature, if it is assumed that the heat transfer is limited to conduction or convection with infinite surface heat transfer coefficient (a finite surface heat transfer coefficient will lower j_h). During the analysis of heat penetration data, j_h-values outside the range 1.0-2.0 are often found. This is due to the experimental conditions, used in collecting the necessary temperature data. In particular, the presence of a come-up-time during the heat penetration experiments will greatly influence the j_h-value (Fig. 3.1).

The j_h-values determined using the classical procedure are not appropriate in the context of the methods proposed in chapter 2, as they depend on the CUT (the use of the 42% correction factor does not always delivers j-values independent of the CUT, see section 2.1.1.). In order to use these methods, there is a need of determining corrected j-values, independent of the come-up-time. These corrected j-values are defined as the j-values for an ideal condition, where at time zero the autoclave is turned on and is immediately at the operating temperature (Pflug 1987a).

The ideal condition of zero come-up time is not attainable in most of the available retorts. The obvious solution would be to determine the heat penetration parameters under laboratory conditions where a zero come-up time can be easily achieved, e.g., sudden immersion of the test can in a water or oil bath. However, as the empirical parameters, f_h and j_h, are related to the processing conditions they must be determined under processing conditions as close as possible to the ones expected during the actual process.

In the following sections, methods for the determination of the corrected f_h and j_h parameters to be used with the methods discussed in the previous chapter, are presented. The methods were tested using heat penetration data generated using numerical models for cases where the theoretical values were known. The methods were used for the determination of the corrected empirical parameters from experimental heat penetration data. Process deviations, consisting on drops on the heating medium temperature during the holding phase of the process, were evaluated using the corrected empirical values.

3.2. Mathematical procedures and computer programs

The procedures presented here for the calculation of corrected empirical heat penetration parameters from heat penetration data, do not make use of correction factors to handle the variable heating medium temperature during the come-up period. A model able to predict the temperature evolution at the centre of the product under variable boundary conditions, using f_h and j_h as parameters, is the core of the procedure (any of the models discussed in the previous chapter can be used for this purpose). The objective is to find values of j_h and f_h that minimise the sum of the squared differences between the experimental temperature and the product temperatures predicted by the model taking into account the experimental heating medium temperature profile.

The initial approach consisted in determining the appropriate j_h-value for a fixed value of f_h. This was based on the fact that, for conductive heating bodies, the existence and duration of a come-up time would only affect the j_h-value and not the f_h-value. As it was observed that small errors on the determination of the f_h value can affect the determination of the j_h-values, methods that allow the simultaneous determination of the two parameters were considered. A reason in favour of the simultaneous determination of f_h and j_h-values lies on the fact that f_h values determined from log-linear plots are calculated based on a constant heating medium temperature. In a real experiment the heating medium temperature the retort temperature will vary with time (apart from the obvious variation of retort temperature during the come-up period there are always small variations on the retort temperature once the processing temperature is reached), this will lead to small errors on the calculated f_h value. If both parameters are determined simultaneously taken into account the actual retort temperature with its small variations, better estimates for f_h and consequently for j_h can be achieved.

3.2.1. Classical determination of the empirical heat penetration parameters

The determination of the empirical parameters is classically done (Ball and Olson 1957) by manually plotting the data from a heat penetration experiment in log-linear coordinates and then determining the heat penetration parameters from the inverse of the slope of the obtained straight line (f_h) and the j-value from the intercept of the line with the vertical axis (Fig. 1.2).

Using this manual procedure heat penetration factors, determined independently by different individuals from the same set of time-temperature data, may differ because each individual may select a slightly different 'best fit' of the straight line segments to the data. The use of automated procedures eliminates the human error, assuring that each process is handled identically in the selection of the appropriate line segments and subsequent heat penetration factors (Berry and Bush 1987).

A computer program was written for the automatic plotting of heat penetration data and determination of the heat penetration factors. The program plots the heat penetration data in a log-linear-graph (decimal logarithm of the difference between the processing and product temperature in the y-axis *versus* time in the x-axis). The program automatically selects the linear portion of the heat penetration curve and from the slope and intercept of the determined line calculates the f_h and j_h values. The automatic determination of the linear segment was performed by the sequential elimination of the points on the initial curvilinear portion of the heat penetration curves until no significant increase (i.e., smaller than 0.001%) in the coefficient of correlation of a linear regressions performed on the remaining points (R^2) was detected.

The program calculates two different j-values: The first one based on the experimental zero time (steam-on), the j_h-value and the second one, j_{hb}-value, based on the corrected zero time according to Ball's 42% rule (Anonymous, 1967).

3.2.2. Determination of corrected j_h-value for a fixed f_h-value

The corrected j_h-value was defined as the value that (for a fixed f_h-value) allows the minimisation of the differences between the experimental temperatures and the temperatures predicted by a method able to predict the product temperature evolution under variable boundary conditions (variable heating medium temperature).

To determine the corrected j_h-value a univariate-search routine is used (Davies-Swann Campey method; Saguy 1983). The routine searches for a j_h-value that allows the minimisation of an objective function defined as,

$$\text{Objective function} = \sum \left(T_{\exp} - T_{pred} \right)^2 \tag{3.1}$$

where T_{exp} are the experimentally measured temperatures and T_{pred} the predicted temperatures.

Any of the three methods discussed in Chapter 2 (HYK, section 2.3.1.3.; ASDT, section 2.3.1.4. or APNS, section 2.3.1.5.) can be used for the calculation of the product temperature evolution (T_{pred}) using the experimental retort temperature profile as the boundary condition.

As the initial guess for the search routine the j_{hb} -value, as determined using the program described in the previous section, was used. The f_h determined by the same

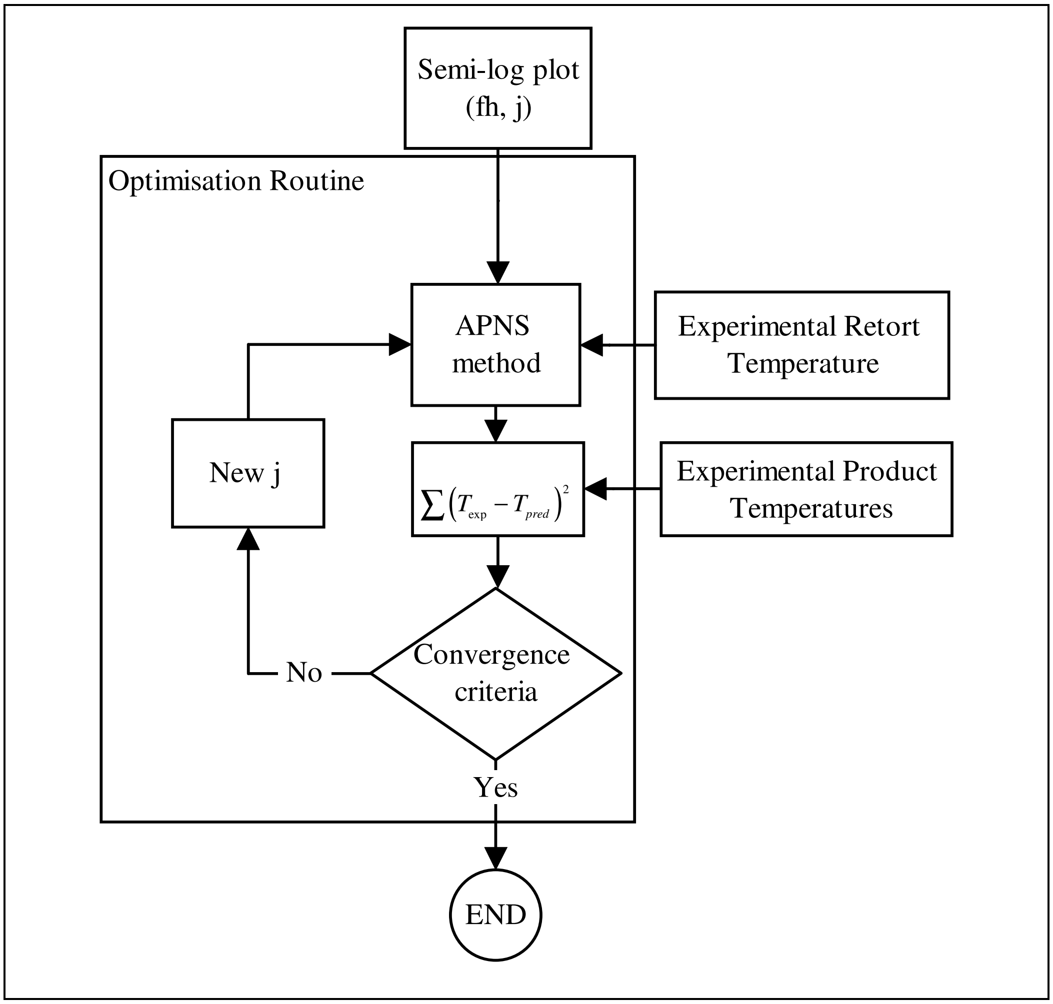

FIGURE 3.2 Flow-chart showing the principal steps in the determination of the corrected j_h-value from experimental time-temperature data.

program was used as the fixed value for f_h. In Fig. 3.2 the principal steps involved in the procedure are illustrated.

3.2.3. Simultaneous determination of corrected f_h and j_h-values

The simultaneous determination of corrected f_h and j_h values consists in finding the f_h and j_h value that allows the minimisation of Eq. 3.1. As before, the calculation of the predicted temperatures (T_{pred}) can be performed using any of the methods presented in Chapter 2. In this case, as two 'decision variables' are involved (f_h and j_h), the univariate search procedure used in the previous method is not appropriate. There is a need for methods that allow the simultaneous determination of the two variables of interest.

Two different approaches were followed for the simultaneous determination of the f_h and j_h value. The first one was based on the use of the Levenberg-Marquardt method for non-linear regression (Myers, 1980) and the second on a modified version of Box's COMPLEX method, a constrained simplex optimisation method (Saguy 1983).

In the first approach the procedure NLIN from the commercial software package SAS (SAS Institute Inc. 1982) was used. In this approach the HYK and the ASDT methods (discussed in Chapter 2) were used for the calculation of the product temperature evolution (T_{pred}). Both methods had to be programmed using the SAS programming language (SAS Institute Inc. 1982) in order to be used together with procedure NLIN.

Due the difficulties found in programming the APNS method in the SAS language a second approach was followed for the simultaneous determination of the f_h and j_h parameters when using the APNS for the calculation of the product temperature evolution. A modified version of Box's COMPLEX method (Saguy 1983), an optimisation routine, was used to this purpose.

As an initial step in the optimisation routine a bidimensional 'search area' was defined. Typically the search area was defined by considering j_h values in the 0 to 2.0 range and f_h values in the f_h*±5.0 min or f_h*±10.0 min. f_h* being the value determined from the semi-log plot.

Four points (defined by an f_h and an j_h co-ordinate) were randomly selected in the selected domain and the objective function (Eq. 3.1) determined at each point. The point where the objective function presented the higher value was substituted by a new point determined by considering a reflection through the geometrical centre of the remaining points. This procedure was repeated while reduction in the value of the objective function could be achieved. When no reduction in the objective function could be achieved by the simple reflection through the geometrical centre or if the reflected point would fall outside the defined domain the new point was corrected using an appropriate correction factor. The procedure was repeated until a convergence criteria, based both in the relative and absolute difference between the maximum and minimum values of the objective function for the four points, was achieved

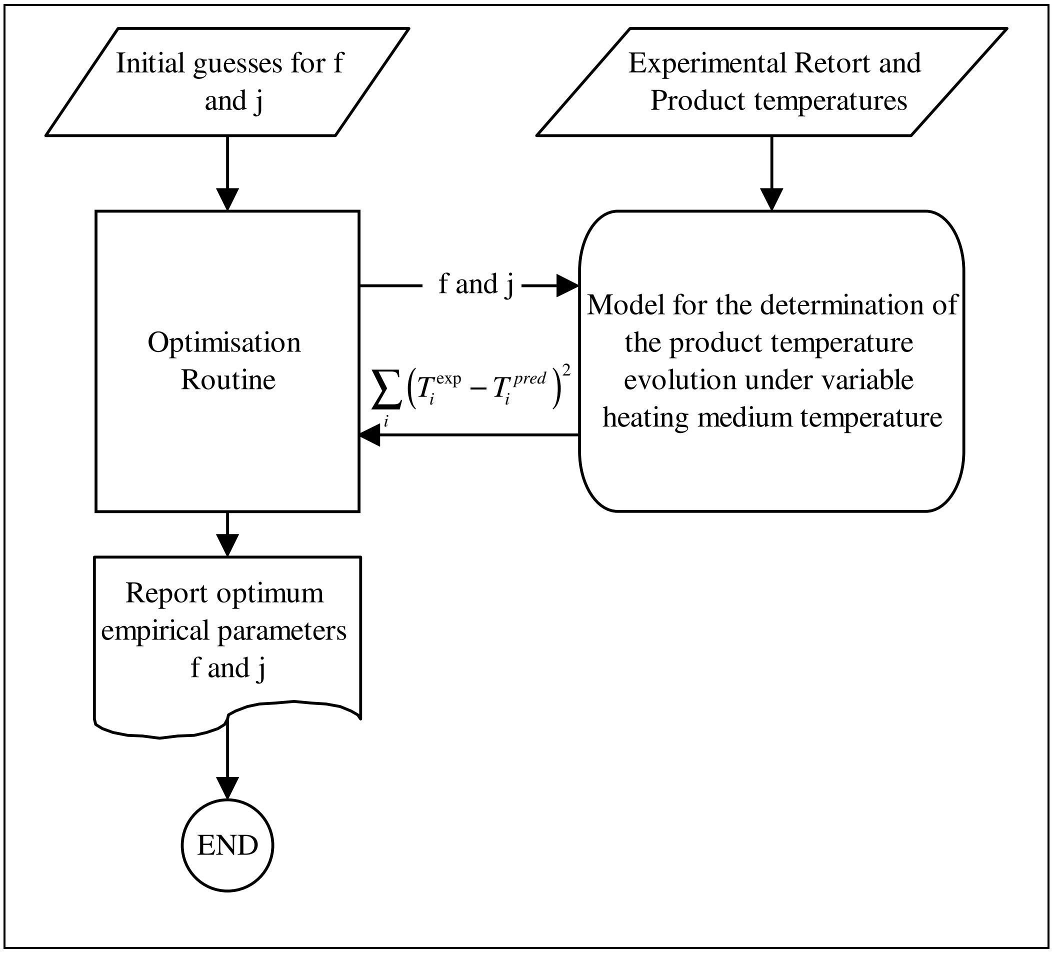

FIGURE 3.3 Flow-chart showing the principal components of the programs used for the determination of the empirical parameters from experimental time-temperature data.

A Pascal version of the APNS method was used for the calculation of the product temperature evolution. In Fig. 3.3 a flow chart of the program developed is shown. The f_h and j_{hb} values determined as described in section 3.2.1. were used as initial guesses for the procedure.

3.3. Theoretical case studies

The proposed methods for the determination of j_h-values from heat penetration data were tested using data obtained through simulation using finite-difference solutions of the conduction equation for one-dimensional geometries, where the theoretical f_h and j_h-values could be derived from the thermal characteristics and geometry (see Table 1.5).

3.3.1. Material and methods

Theoretical heat penetration curves for infinite slabs and infinite cylinders were generated using a one-dimensional finite-difference model described elsewhere (Silva *et al.* 1992). On all simulations an initial homogeneous product temperature of 40ºC and heating medium temperature of 121ºC (after the come-up time) were considered. Unless otherwise stated, the heating medium temperature increased linearly with time during the come-up period, and an initial heating medium temperature of 40ºC was used. An infinite surface heat transfer coefficient was used on all simulations.

The f_h and j_{hb}-values determined using the classical procedure (3.2.1.) were used as initial guesses for the determination of the corrected empirical parameters using the proposed procedures.

3.3.2. Results and discussion

3.3.2.1. Determination of corrected j_h-value for a fixed f_h-value

In Tables 3.1 and 3.2 the j_h-values determined, for different come-up times, according to the classical procedure and to the three proposed methods, for an infinite cylinder and an infinite slab, are presented. When the j_h-values (determined from the actual experimental zero time) are considered, their dependence on the come-up duration is clear from the presented results, an increase on the j_h-values is observed when the CUT increases. The use of a corrected zero time (Ball's 42% rule) produces j_{hb}-values that are independent of the CUT duration but deviate from the theoretical values (1.60 for the infinite cylinder and 1.27 for the infinite slab). These problems do not arise when the three proposed methods for the determination of corrected j_h-values are used. It can easily be seen from Tables 3.1 and 3.2 that these methods allow the determination of the j_h-values with a high degree of accuracy independently of the duration of the come-up-time

In order to study the influence of the 'shape' of the retort temperature during the come-up period, heat penetration curves for an infinite cylinder were simulated for

TABLE 3.1 Determination of the j_h-value for different retort coming-up time using three different methods. Case study: Temperatures in the centre of a conductive heating infinite cylinder. f_h= 28.6 min. Theoretical j_h-value =1.60218

	Classical analysis			HYK	ASDT	APNS
CUT (min)	f_h (min)	j_h*	j_{hb}**	j_h	j_h	j_h
0	28.64	1.58	1.58	1.62	1.64	1.63
10	28.60	2.33	1.46	1.61	1.64	1.62
15	28.62	2.90	1.44	1.62	1.64	1.62
20	28.64	3.05	1.44	1.62	1.63	1.62

* Calculated graphically at the beginning of the process.
** Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.2 Determination of the j_h-value for different retort coming-up time using three different methods. Case study: Temperatures in the centre of a conductive infinite slab. f_h= 66.83 min. Theoretical j_h-value =1.27324

	Classical Analysis			HYK	ASDT	APNS
CUT (min)	f_h * (min)	j_h*	j_{hb}**	j_h	j_h	j_h
0	66.90	1.27	1.27	1.27	1.27	1.27
10	66.93	1.48	1.10	1.27	1.27	1.27
15	66.93	1.61	1.19	1.27	1.27	1.27
20	67.00	1.75	1.18	1.27	1.27	1.27

* Calculated graphically at the beginning of the process.
** Calculated graphically considering Ball's 42 % correction factor for the CUT.

different retort come-up profiles. Different come-up profiles, for the same CUT duration, were generated considering the following power function,

$$\begin{cases} T_R(t) = T_{R,0} + (T_1 - T_{R,0})\left(\dfrac{t}{CUT}\right)^n & \text{for } 0 \le t < CUT \\ T_R(t) = T_1 & \text{for } t \ge CUT \end{cases} \tag{3.2}$$

where T_R represents the retort temperature and $T_{R,0}$ the initial retort temperature.

In Fig. 3.4 the CUT profiles obtained by varying the parameter n in Eq. 3.2 are depicted. The results of the analysis of the heat penetration curves resulting from the different profiles using the classical procedure and one of the proposed methods for the determination of the j-value are given on Table 3.3. It is observed that both the j_h and j_{hb} (with 42% correction) depend on the shape of retort temperature during the CUT (it should be remembered that the 42% correction factor was derived for linear come-up profiles, see section 2.1.1.). When the proposed method for the determination of j_h-values is applied it is observed that the obtained values are independent on the shape the retort temperature during the come up period, and that the calculated j_h-values are very close to the theoretical predicted value for an infinite cylinder (1.60).

3.3.2.2. Simultaneous determination of corrected f_h and j_h values

The methods for the simultaneous determination of corrected f_h and j_h values discussed in section 3.2.3. were applied to determinate the empirical parameters for the cases discussed in the previous section.

In Tables 3.4 and 3.5, the results of the simultaneous determination of the empirical heating parameters f_h and j_h using the proposed approaches are compared with the empirical parameters calculated using the computerised version of the classical approach discussed in section 3.2.1. For both cases the proposed methods allowed the calculation of f_h and j_h-value independent of the CUT duration and close to the theoretical values expected for zero CUT.

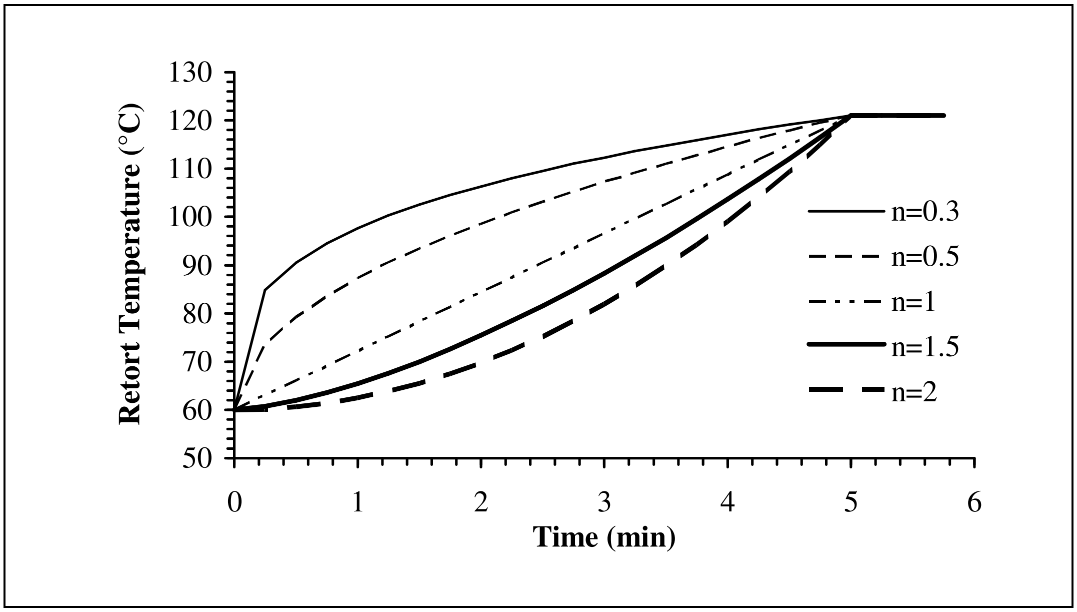

FIGURE 3.4 Retort coming-up-time shapes generated considering different values of the parameter n in Eq. 3.2. CUT = 5 min, T_1= 121°C and $T_{R,0}$ = 60 min.

TABLE 3.3 Determination of the j_h-value using the APNS method. Case study: Temperatures in the centre of a conductive infinite cylinder. f_h= 20 min. Theoretical j_h-value = 1.60218. Retort temperature defined by Eq. 3.2. CUT = 5 min, T_1 = 121°C and $T_{R,0}$ = 60 min.

	Classical Analysis			APNS
$n^{\#}$	f_h (min)	j_h*	j_{hb}**	j_h
0.3	20.25	1.77	1.27	1.63
0.5	20.25	1.85	1.33	1.64
1.0	20.24	2.00	1.44	1.64
1.5	20.24	2.09	1.50	1.64
2.0	20.24	2.14	1.54	1.64

exponent in Eq. 3.2.
* Calculated graphically at the beginning of the process.
** Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.4 Simultaneous determination of f_h and j_h-values for different retort coming-up times. Case study: Temperatures in the centre of a conductive infinite cylinder. f_h= 28.60, Theoretical j-value = 1.602

	Classical Analysis			HYK		ASDT		APNS	
CUT (min)	f_h (min)	j_h*	j_{hb}#	f_h (min)	j_h	f_h (min)	j_h	f_h (min)	j_h
0	28.64	1.58	1.58	28.45	1.62	27.97	1.64	28.18	1.66
10	28.60	2.33	1.46	28.22	1.64	28.02	1.63	28.18	1.67
15	28.62	2.90	1.44	28.09	1.65	28.04	1.63	28.20	1.67
20	28.64	3.05	1.44	28.08	1.66	28.07	1.63	28.24	1.66

* Calculated graphically at the beginning of the process.
# Calculated graphically considering Ball's 42 % correction factor for the CUT.

The APNS method was used for the simultaneous determination of f_h and j_h-values from heat penetration curves resulting from the different retort profiles depicted in Fig. 3.4. In Table 3.6 the obtained results are presented. With the present method f_h and j_h-values close to the theoretically predicted values could be found. Moreover the empirical heat parameters thus determined were found to be independent of the CUT profile opposite to what is observed when the classical approach for the determination of the empirical parameters is used.

The methods for the simultaneous determination of the empirical parameters, f_h and j_h, were able to determine accurately the corrected parameters from theoretical generated heat penetration curves. Independently of the duration and the type of come-up type (linear, power function) the proposed methods were able to accurately determine the theoretically predictable empirical parameters.

TABLE 3.5 Simultaneous determination of f_h and j_h-values for different retort coming-up times. Case study: Temperatures in the centre of a conductive infinite slab. f_h= 67.0, Theoretical j-value = 1.27

	Classical Analysis			HYK		ASDT		APNS	
CUT (min)	f_h (min)	j_h*	j_{hb}#	f_h (min)	j_h	f_h (min)	j_h	f_h (min)	j_h
0	66.90	1.27	1.27	67.04	1.27	66.69	1.28	66.89	1.27
10	66.93	1.48	1.21	66.82	1.27	66.68	1.27	66.75	1.28
15	66.93	1.61	1.19	66.74	1.28	66.76	1.27	66.91	1.27
20	67.00	1.75	1.18	66.03	1.28	66.71	1.27	66.87	1.28

* Calculated graphically at the beginning of the process.
# Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.6 Simultaneous determination of f_h and j_h-values using the APNS method. Case study: Temperatures in the centre of a conductive infinite cylinder. f_h= 20 min. Theoretical j_h-value = 1.60218. Retort temperature defined by Eq. 3.2. CUT = 5 min, T_1 = 121°C and $T_{R,0}$ = 60°C.

	Classical Analysis			APNS	
n	f_h (min)	j_h*	j_{hb}#	f_h (min)	j_h
0.3	20.25	1.77	1.27	19.75	1.66
0.5	20.25	1.85	1.33	19.76	1.66
1.0	20.24	2.00	1.44	19.74	1.66
1.5	20.24	2.09	1.50	19.75	1.66
2.0	20.24	2.14	1.54	19.74	1.66

* Calculated graphically at the beginning of the process.
# Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.7 Influence of addition of noise to the time-temperature data in the simultaneous determination of f_h and j. Case study: Finite Cylinder, f_h=30 min. CUT = 5 min, T_1 = 121°C and $T_{R,0}$ = 60°C.

	No Noise [1]		Noise (±0.5°C)[2]		Noise (±1.0°C)[3]	
Replicate[*]	f_h (min)	j_h	f_h (min)	j_h	f_h (min)	j_h
1	28.8	1.8	29.5	1.9	27.9	1.9
2	27.5	1.9	29.4	1.9	27.4	1.9
3	29.5	1.9	27.8	1.9	27.9	1.9
4	29.9	1.9	29.7	1.9	30.9	1.9

[*] For each data set the determination of the parameters was repeated four times.
[1] Time temperature data with no added noise.
[2] Time temperature data with uniformly distributed noise, ±0.5°C, added to both retort and product temperatures.
[3] The same as above with noise ±1.0 °C

In order to test the robustness of the proposed method of the empirical parameters the empirical parameters were determined from data sets where uniformly distributed noise was added. In Table 3.7 we present the results obtained for the simultaneous determination of the empirical heat penetration parameters from a data set with no added noise and from two data sets obtained from the first and where different levels of noise were added. For each data set thus obtained the empirical parameters were determined using the APNS based method. The analysis of the data using ANOVA (analysis of variance) shows that there is no significant difference between the parameters determined from the different data sets, this shows the robustness of the method to the presence of noise.

3.4. Experimental validation

In order to test the validity of the proposed methods for the determination of heat penetration parameters from experimental data, experiments were carried out with food simulants in order to avoid the intrisic variability associated with real foods. Products that heat mainly by conduction (Bentonite suspensions) and products that present different degrees of convective heating were considered. The products chosen for the experimental validation cover a range of f_h values similar to the one found with real foods.

Heat penetration tests were conducted in a process simulator. Both processes in pure steam and in water cascading mode were considered. However, in order to test the influence of the come-up period on the determined process parameters only experiments in the water cascading processing mode were considered due to impossibility, with the available process simulator, of controlling the come-up time duration when in pure steam mode.

3.4.1. Material and methods

In this section we will describe the preparation of the food simulants, the containers, the pilot plant, the probes and data-logging equipment used in the experimental runs. In addition, some preliminary results on the determination of the coldest-spot are presented.

3.4.1.1. Food simulants

The experiments were performed in metal cans (450 ml - 110 mm height, 73 mm diameter, 0.23 mm thickness, CMB, Machelen, Belgium) closed using a manual operated closing machine (Lanico-Maschinenbau, Otto Niemsch GmbH, Braunschweig) and in glass jars (600 ml - 172 mm height, 40.5 mm radius, about 2.6 mm wall thickness; Carnaud-Giralt, Laporta S.A., Spain). A gross headspace of 10 mm was used in all experiments.

3.4.1.1.1. Bentonite suspensions in cans

Various bentonite suspensions (x%, x g/ 100 ml), were prepared by mixing dried bentonite powder (Sigma Chemicals Co., USA) with the required amount of distilled water under constant mixing. To allow for a complete hydration of bentonite the suspensions were stored overnight at 4º C (at least for 16 hours) (Niekamp *et al.* 1984).

3.4.1.1.2. Water in glass jars

Glass jars were filled with distilled water, at ambient temperature, to a final gross headspace of 10 mm.

3.4.1.1.3. Silicone oil in glass jars

Glass jars were filled, at ambient temperature, with silicon oil (350 cp at 25°C, density = 970 Kg/m^3; Lamers-Pleugen, 's- Hertogenbosh, The Netherlands or 1070 cp at 25°C, Fluka Chemie, Bornem, Belgium) to a final gross headspace of 10 mm.

3.4.1.1.4. Carboxymethylcellulose(CMC) solutions in glass jars

Low-viscosity carboxymethylcellulose solutions (4%) were prepared by carefully dissolving sodium salt-carboxymethylcellulose (Sigma Chemie, Bornem, Belgium) in distilled water under continuous agitation. The solutions were stored overnight and afterwards immersed in an ultrasonic-bath (Brandsonic-220, Germany) for 20 min in order to force the release of entrapped air bubbles. Glass jars were filled, at ambient temperature, with the CMC solutions.

3.4.1.2. Process simulator

Experiments were conducted in a modified Barriquand Steriflow process simulator (Barriquand, Roanne, France), a 0.9 m diameter and 0.8 m deep, stainless steel vessel where water cascade, pure steam and water immersion sterilisation processes can be performed. The system allows the processing in still and rotating mode (end-over-end and axial rotation). In the cooling step water cascading is used. When appropriate the equipment allows to control of pressure in the vessel in order to preserve container integrity.

3.4.1.3. Experimental acquisition of temperatures

Thermocouples used were copper-constantan (Type T). Conventional thermocouples for liquids and air (SSR-60020-G700-SF, 20x6 mm, Ellab, Copenhagen, Denmark) were used to measure the external (heating or cooling) temperatures. Needle-type thermocouples (SSA-12080-G700-SF, 80x1.2 mm, Ellab, Copenhagen, Denmark) were used for the measurement of temperatures inside the containers. Four point thermocouples able to measure simultaneously the temperature at four locations in the container separated by 1 cm (ST4-11120-G700-SL, Ellab, Copenhagen, Denmark) were used for the determination of the location of the slowest heating point in the container. A CMC-92 multi-channel data acquisition system (TR9216, Ellab, Copenhagen, Denmark), connected to a personal computer for storing and manipulating the data, was used. Temperatures were measured at 15 or 30 second intervals. Thermocouples were calibrated against a standard mercury-in-glass thermometer in ice water as well as at the maximum processing temperature (Pflug 1987a). Only thermocouples with an accuracy of ± 0.2 °C were used. The data logger was calibrated against a thermocouple voltage calibrator (PVG 77, Ellab, Copenhagen, Denmark).

A computer program was developed to convert the time-temperature data to a standard file format. The data on this file-format was used as input to all the programs for further data analysis.

3.4.1.4. Cold spot determination

Preliminary heat penetration tests were conducted for the determination of the slowest heating point. The temperature evolution at different locations along the central axis of the container was measured. The lethality achieved at each location was calculated by numerical integration of lethality for the entire (heating and cooling phases) process. For the calculation of the lethalities a reference temperature of 121°C and a z-value of 10°C were used. In Table 3.8 the results for the cold spot determination for low-viscosity carboxymethylcellulose solutions (4%) in glass jars are presented. Four replicates were performed.

Using a similar procedure the cold spot was determined for the other products. For Bentonite suspensions in cans the cold spot was near the geometrical centre of the can, as expected for a conduction product, for water and silicone processed in glass jars the cold spot was found to be located at 10 mm from the bottom of the glass jar as for the case of CMC solutions processed in glass jars.

3.4.2. Results and discussion.

In Tables 3.9 to 3.11 we present the empirical parameters obtained for three different products (bentonite suspensions (10%) processed in metal cans, water and silicone oil solutions processed in glass jars) determined using the methods discussed in section 3.2.3. The empirical parameters determined using the classical approach (log-linear plot of the time temperature-data) were used as initial guess for each of the methods.

TABLE 3.8 Determination of the cold spot for low-viscosity solutions of carboxymethilcellulose (4%)

Process 1 *		Process 2 #	
Distance from the bottom (mm)	F_0 (General Method) (min)	Distance from the bottom (mm)	F_0 (General Method) (min)
10	**7.35**	**10**	**7.26**
20	9.66	20	9.39
30	8.23	30	8.09
40	9.20	40	9.09

* CUT = 8.0 min; Holding Time = 26 min; Th =120º C
# CUT =9.5 min; Holding Time = 25 min; Th =120º C

The proposed methods were able to calculate empirical parameters that are not influenced by the duration of the retort come-up-time. For the tested products and the range of come-up-times tested, the proposed methods could resolve the come-up time influence and produce j_h values that are independent of the heating medium temperature evolution. The small differences observed in the value of the heat penetration parameters between different come-up times were attributed to experimental variability as no relationship between these values and the come-up duration could be observed.

As no significant differences could be found between the corrected empirical parameters calculated using the three different methods the APNS method was selected for further experimental validation due to his superior performance in terms of computational speed. In tables 3.12 and 3.13 the empirical parameters determined using this method are presented for two food simulants, CMC solutions (4%) and silicon oil processed (1070 cp) processed in glass jars.

As in the previous examples it was possible, using the APNS based method, to determine heat penetration factors that are independent of the CUT duration. The small differences observed between the empirical parameters determined for the different CUTs were attributed to experimental variation, as no relationship between the determined values and the CUT duration could be found.

TABLE 3.9 Simultaneous determination of f_h and j_h-values for different retort coming-up times. Case study: Bentonite suspensions (10%) in metal cans processed in water cascading mode at 121°C.

	Classical Analysis #		HYK #		ASDT #		APNS #	
CUT (min)	f_h (min)	j_{hb} *	f_h (min)	j_h	f_h (min)	j_h	f_h (min)	j_h
8	32.3(1.69)	3.1(0.61)	39.0(0.22)	2.0(0.01)	40.1(0.19)	1.9(0.02)	40.0(0.45)	1.9(0.01)
15	33.1(0.42)	2.4(0.03)	38.7(0.12)	2.1(0.04)	40.0(0.32)	1.9(0.02)	39.9(0.29)	2.0(0.01)
20	34.8(0.45)	2.4(0.11)	38.2(0.26)	2.1(0.04)	39.9(0.32)	2.0(0.03)	39.8(0.25)	2.0(0.03)
25	32.9(0.79)	2.9(0.15)	37.9(0.39)	2.2(0.03)	39.6(0.78)	2.0(0.01)	39.5(0.25)	2.0(0.02)

Average of 4 observations (standard deviation).
* Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.10 Simultaneous determination of f_h and j_h-values for different coming-up times. Case study: Distilled water in glass jars processed in water cascading mode at 121°C.

	Classical Analysis #		HYK #		ASDT #		APNS #	
CUT (min)	f_h (min)	j_{hb} *	f_h (min)	j_h	f_h (min)	j_h	f_h (min)	j_h
9	10.3(0.31)	1.4(0.06)	11.0(0.56)	1.4(0.07)	10.9(0.49)	1.4(0.06)	10.9(0.45)	1.4(0.05)
11	10.3(0.53)	1.7(0.05)	10.7(0.67)	1.5(0.13)	10.6(0.68)	1.6(0.11)	10.6(0.59)	1.6(0.11)
13	10.3(0.70)	1.7(0.05)	10.5(0.90)	1.6(0.05)	10.5(0.88)	1.6(0.05)	10.5(0.62)	1.6(0.04)
15	10.5(0.78)	1.7(0.05)	10.3(0.67)	1.7(0.01)	10.3(0.69)	1.7(0.00)	10.3(0.52)	1.7(0.01)
17	10.40(0.35)	1.86(0.01)	9.87(0.23)	1.85(0.09)	10.00(0.26)	1.79(0.07)	9.94(1.02)	1.81(0.21)
19	10.28(0.38)	1.94(0.05)	10.01(0.20)	1.7(0.05)	10.03(0.30)	1.69(0.02)	10.35(0.70)	1.63(0.09)

Average of 4 observations (standard deviation).
* Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.11 Simultaneous determination of f_h and j_h-values for different coming-up times. Case study: Silicone oil (350 cp)in glass jars processed in water cascading mode at 121°C

	Classical Analysis [#]		HYK [#]		ASDT [#]		APNS [#]	
CUT (min)	f_h (min)	j_{hb} [*]	f_h (min)	j_h	f_h (min)	j_h	f_h (min)	j_h
9	18.5 [a]	1.4[a]	19.1 [a]	1.5 [a]	18.9 [a]	1.5 [a]	19.0 [a]	1.5 [a]
11	18.5 [a]	1.4 [a]	18.7 [a]	1.6 [a]	18.4 [a]	1.6 [a]	18.4 [a]	1.6 [a]
13	18.7(0.22)	1.4(0.10)	19.6(0.17)	1.4(0.12)	19.4(1.32)	1.5(0.14)	19.4(1.09)	1.5(0.12)
15	18.9(0.84)	1.4(0.25)	19.9(1.41)	1.4(0.22)	19.7(1.54	1.4(0.25)	19.8(1.15)	1.4(0.21)
17	19.0(0.26)	1.4(0.08)	18.4(0.47)	1.6(0.03)	18.0(0.66)	1.6(0.06)	18.0(0.58)	1.6(0.06)
19	18.8(0.22)	1.4(0.08)	17.9(0.30)	1.7(0.15)	17.7(0.33)	1.7(0.14)	17.6(0.15)	1.8(0.11)

[#] Average of 4 observations (standard deviation) except for [a].
* Calculated graphically considering Ball's 42 % correction factor for the CUT.

TABLE 3.12 Simultaneous determination of f_h and j_h-values for different coming-up times using the APNS method. Case study: CMC (4%) solution in glass jars processed in water cascading mode at 121°C.

	Classical analysis		APNS	
CUT (min)	f_h (min)	j_{hb} [*]	f_h (min)	j_h
8.0	13.3	1.5	13.3	1.7
9.5	13.4	1.4	13.3	1.7
11.0	12.5	1.8	12.6	1.8
15.0	12.6	2.0	12.4	1.9

* Calculated graphically considering Ball's 42 % correction factor for the CUT.
The reported values are average values for 2 observation.

TABLE 3.13 Simultaneous determination of f_h and j_h-values for different coming-up times using the APNS method. Case study: Silicon oil (1070 cp) in glass jars processed in water cascading mode at 121°C.

	Classical analysis		APNS	
CUT (min)	f_h (min)	j_{hb} *	f_h (min)	j_h
7.5	23.1	1.5	23.8	1.6
8.0	23.3	1.4	23.8	1.6
11.0	23.3	1.5	23.1	1.7
13.0	23.4	1.5	23.7	1.6
15.0	24.1	1.5	23.7	1.7

* Calculated graphically considering Ball's 42 % correction factor for the CUT.

3.5. Evaluation of process deviations

The evaluation of the product temperature evolution when a drop in retort temperature occurs during the holding phase of the sterilisation process was the main objective of this chapter.

In the previous sections of this chapter methods for the determination of empirical heat penetration parameters that are independent of the retort come-up time were set forward. These heat penetration parameters corrected for the CUT can be used with the methods developed in chapter 2 for the evaluation of the product temperature evolution under variable heating medium temperature conditions.

In this section results of the use of the APNS method for the evaluation of process deviations are presented. Temperature drops in the heating phase of the process were programmed in a retort simulator and both the retort and product temperature registered. Several products and different types of temperature drops were considered. The experimental retort temperatures and the corrected heat penetration parameters were used to determine the predicted temperature evolution using the APNS method.

3.5.1. Material and methods.

Food simulants were prepared as described in sections 3.4.1.1. The retort simulator used was described in section 3.4.1.2. Temperatures were measured as described in section 3.4.1.3.

For the determination of the temperature evolution under variable heating medium temperature the APNS method described in section 2.2.2.2. was used.

3.5.2. Results and discussion

In Figs. 3.5 to 3.9 some typical examples of the programmed process deviations are presented.

When in water cascading mode, due to the large thermal capacity of the system, in order to be able to produce noticeable drops on the heating medium temperature it was necessary to program very long deviations. The obtained deviations consisted of a very slow decrease in the heating medium temperature from the moment the heating was turned off (e.g. Fig. 3.6). In order to achieve a faster decrease in the medium temperature (e.g. Fig. 3.8) it was necessary to program the retort to use cooling water. Drops up to 10°C in the retort temperature were programmed.

When processing in pure steam the deviations were achieved by opening the venting valve, thus decreasing the internal pressure (temperature), until the required drops in retort temperature were achieved (Fig. 3.7).

Inspection of Figs. 3.5 to 3.9 shows a good agreement between the experimental and the temperatures predicted using the APNS. Using the proposed methodology for the determination of corrected empirical parameters it was possible to find empirical values that allowed a good prediction of the temperature evolution when using the APNS method. The APNS method could, for all the cases presented, predict accurately the product temperature evolution under process deviations.

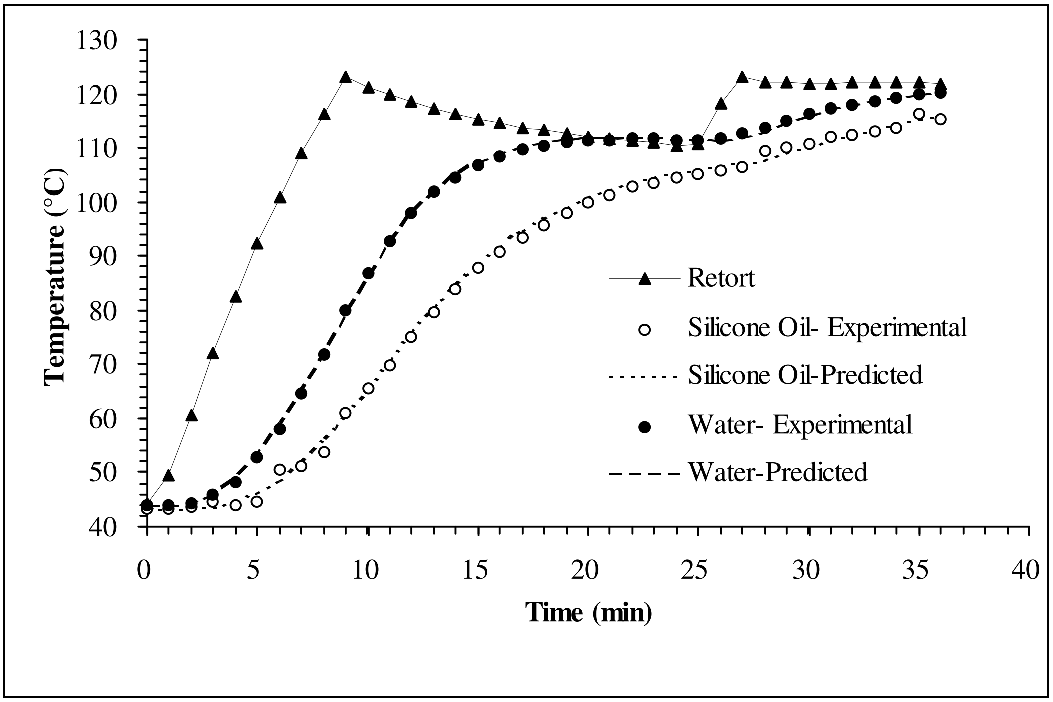

FIGURE 3.5 Evaluation of process deviations using the APNS method. Case study water and silicone oil in glass jars processed in water cascading.

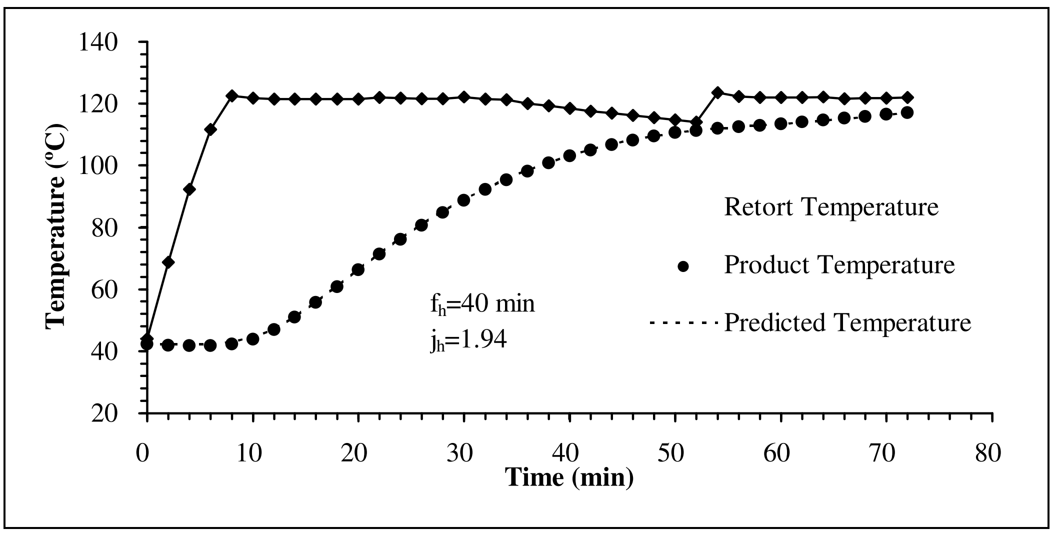

FIGURE 3.6 Evaluation of Process deviations using the APNS method. Case study: Bentonite (5%) processed in metal cans under water cascading.

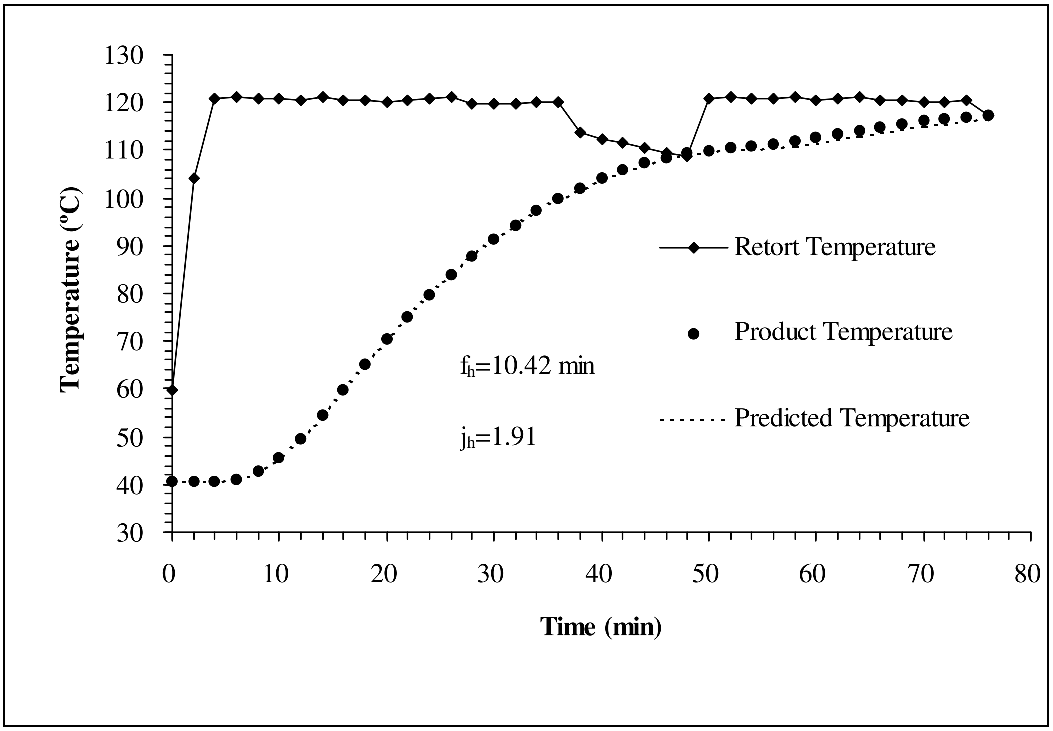

FIGURE 3.7 Evaluation of Process deviations using the APNS method. Case study: Bentonite (5%) processed in metal cans processed in pure steam.

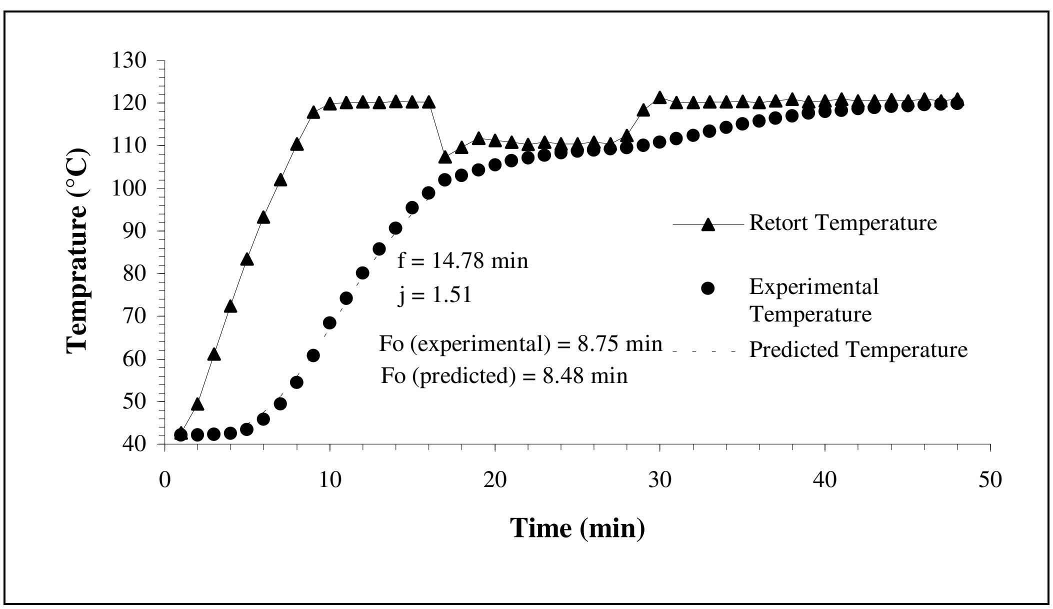

FIGURE 3.8 Evaluation of process deviations using the APNS method. Case study: CMC solutions in glass jars processed in water cascading.

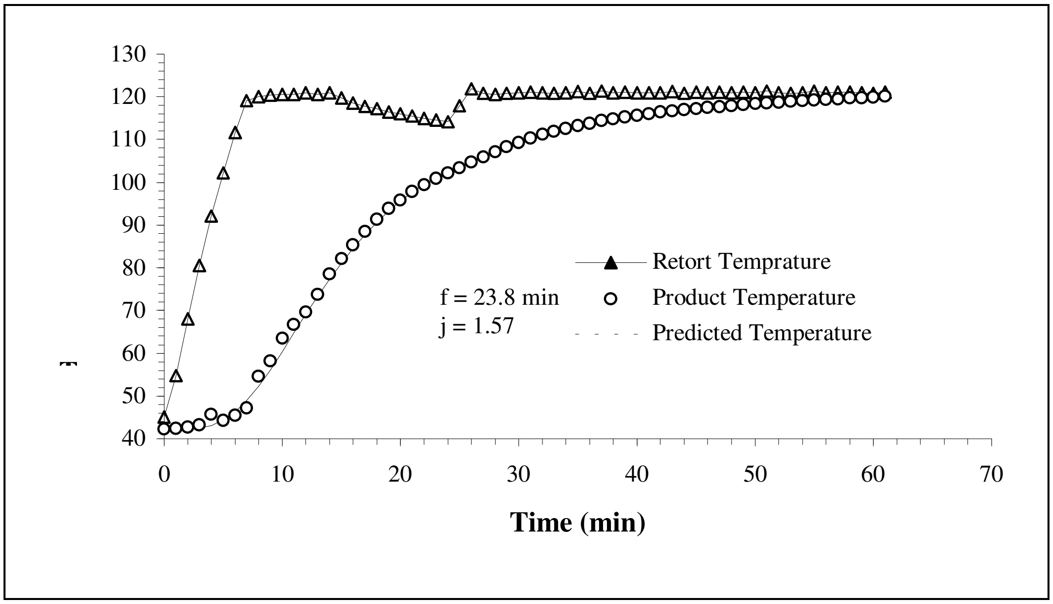

FIGURE 3.9 Evaluation of process deviations using the APNS method. Case study: Silicone oil in glass jars processed in water cascading.

As referred previously small variations on the determined heat penetration parameters were observed. The empirical parameters did not always converge to a single value. This can be due to experimental errors in the measurements of the temperature, or to failures in the method used for the determination of the parameters. The relevance of the observed variability in the heat penetration parameters in the evaluation of thermal process was tested experimentally. Several runs in the pilot plant installation with drops on the heating medium temperature during the heating phase were performed. For each of the processes the achieved processing value was calculated from the experimental measured temperatures. The processing values were also calculated using the temperatures predicted by the APNS method using the empirical parameters determined from experimental data. In Table 3.14 the F_0 determined from the experimental data and from the temperatures calculated from the empirical parameters determined from the heat penetration curves for the lower and higher retort coming-up-time are presented. The observed differences on the calculated empirical parameters do not have a major influence on the final lethalities of the processes. The maximum difference observed in the calculated processing values (0.25 min) is in the range of experimental variability for the processing value observed in practice (Pflug and Odlaug 1978).

TABLE 3.14 Influence of the observed scattering on the determined parameters on the process value calculated for several process deviations.

Case Study	F_0 (exp) (min)	F_0 (low) * (min)	F_0 (high) * (min)	$\lvert F_0$ (high) - F (low)$\rvert$ (min)
Bentonite 10%	5.8	5.7	5.9	0.2
Bentonite 5%	5.3	4.9	4.9	0.0
Silicon oil (1)	1.5	1.3	1.4	0.1
Silicon oil (2)	1.7	1.7	1.6	0.1
Water (2)	5.4	5.9	5.6	0.2
Water (2)	7.4	7.8	8.0	0.2

* low and high refer respectively to the higher and lower retort come-up-times used in the experimental heat penetration tests conducted for the determination of the empirical parameters.

3.6. Conclusions

A general methodology for the determination of the empirical parameters (f_h and j_h) from heat penetration data was proposed and tested against theoretical generated data and experimental case studies. The determination of the empirical parameters using the proposed methods are based on the minimisation of the sum of squares of the differences between experimental temperatures and the temperatures predicted by a model able to handle variable heating medium temperatures.

The proposed methods are able to calculate appropriate empirical parameters to be used with the methods for temperature prediction presented in the previous chapter. The heat penetration parameters determined used the classical graphical procedure cannot be used with those methods due to the contribution of the CUT on the determined parameters. The methods proposed in this chapter are able to determine empirical heat penetration parameters independent of the type and duration of the CUT.

When the present methodologies were used with the methods for temperature evolution under variable heating medium temperature empirical parameters could be found that allow a good match between the experimental and predicted temperatures.

The methodology presented allows to solve several problems on process evaluation that could not be handled by the existing methodologies to design and evaluate thermal processes. The evaluation of deviations on the heating medium temperature and of the contribution of the retort come-up-time on the lethality of the process are examples of problems that can be easily handled with the presented methodologies.

The methodologies presented can be used for the on-line evaluation and control of thermal processes. The reduced number of parameters that need to be experimentally determined and the reduced calculation effort makes the present methodology appropriate for the on-line control of thermal processes.

The main disadvantages associated with the present methodologies lie in the use of an empirical description of the heat transfer. The modification of any parameters on the process that influence the values of the empirical parameters implies a new evaluation of the empirical parameters from heat penetration experiments in order for a proper use of the methods. The method is also limited for the evaluation of thermal processes for products that show a log-linear heating behaviour ('broken-heating' products included). For products showing different kinds of heat penetration curves alternative strategies should be considered (*e.g.,* heat penetration curves for canned liquids under rotation cannot accurately be described using the empirical f_h-j_h description).

Chapter 4. Evaluation of thermal processes: Broken- heating curves

4.1. Introduction

In the two previous chapters new methods for the evaluation of thermal processes and procedures for the determination of empirical parameters from heat penetration data were presented. The procedures were used for the evaluation of deviations in the heating medium temperature. Due to its speed and flexibility the APNS (apparent position numerical solution method) was selected. Several restrictions, however, limit the general applicability of the APNS method for the evaluation of thermal processes. The APNS method as presented in chapter 2 is limited to products that exhibit a single heating rate (single f_h) and only a single type of process deviations (drops in the heating medium temperature) can be handled with this method.

Several products exhibit a change in the heating rate during the heating process, due to changes in the product properties (e.g. gelatinization). This change in the heating rate leads to heat penetration curves that show two distinct linear segments. This type of heating is commonly described as broken-heating behaviour, and associated heat penetration curves as broken-heating curves. In this chapter we will try to extend the applicability of the APNS method to products that present broken-heating behaviour.

A sudden change in processing conditions that influence heat transfer (e.g. drops in rotational speed) can also lead to broken-heating behaviour. A special case of process deviations, drops in the rotation during rotary-sterilisation will be dealt with in this chapter.

4.1.1. Broken heating curves

To characterise broken-heating curves using an empirical description it is necessary to determine the four empirical parameters. Two parameters to characterise the first linear portion: the initial lag (j_h) and the slope of the first linear segment (f_{h1}); and two extra parameters necessary to define the second linear segment of the broken-heating curve: the time when the break occurs (X_b) and the slope of the second segment (f_{h2}).

The determination of the parameters that describe broken-heating curves can be done by plotting the heat penetration data in log-linear coordinates, followed by the determination (*e.g.,* by visual inspection) of the different linear segments. The f_h-values of the two straight lines (f_{h1} and f_{h2}) and the j_h-value can be easily determined from the graph. The value of the fourth factor, X_b, is, in this graphical procedure, defined as the time correspondent to the intersection of the two linear segments (Lopez 1987).

The determination of the empirical parameters for broken-heating curves by different individuals is prone to lead to significant differences on the determined parameters. The difficulties on defining the appropriate linear segments and on defining the localisation of the break point makes the manual determination of the empirical parameters particularly difficult. Statistical methods comprised of least squares, rational functions, min-max and cubic splines, have been used in conjunction with comparisons of ratios of slopes and coefficient of determination to define the location of the 'break' in the broken line heating curves associated with the heating of canned beans and potato products (Wiese and Wiese 1992). These numerical methods allow a good approximation of the observed temperatures and the determination of the break-time. However when no distinct break is observed, i.e., when the heating curve shows a gradual curvilinear change from the first to the second slope, all these methods develop complications in locating the point of the break (Wiese and Wiese 1992).

In this chapter a method for the determination of the empirical heat penetration parameters for broken heating curves is presented. The method represents a natural extension of the procedures presented in Chapter 3.

4.1.2. Drops in rotation

Agitation allows to increase the rates of heat transfer during the thermal processing of packed liquid foods or liquid foods with particulates. Using agitating retorts liquid products benefit from induced convection currents that will lead to an increase in the heating rates.

Rotation, by increasing the rates of heat transfer and by not allowing the development of severe temperature gradients inside the container during the process, allows the use of higher processing temperatures without the concomitant quality destruction at the surface observed when the heat transfer is mainly processed by conduction. As a result the use of rotation allows the design of high-temperature-short-time (HTST) processes that allow higher quality retention. The reduction of processing time with associated increase of product throughput and in some cases the reduction of energy consumption constitute further advantages for the use of rotation during the thermal processing of liquid and liquid with particulates foods.

Rotational speed, as it influences directly the rates of heat penetration, is a critical variable in the process and needs to be continuously monitored to guarantee that the scheduled process is delivered. Drops in rotational speed during the process are considered as a process deviation and there is a need for methods able to assess the impact of this special kind of deviations on the processing value.

A drop in the rotational speed during the process leads to a decrease of the rate of heat transfer. When the differences between the retort temperature and the product temperatures, observed when a drop in rotation occurs during the process, are plotted in a semi-log graph the decrease on the rate of heat transfer is apparent (Fig. 4.1). The obtained curve is similar to the ones obtained for broken-heating products exhibiting the initial curvilinear portion followed by two distinct linear segments. The curve can be characterised using the same four empirical-parameters used to characterise broken-heating curves: j_h, f_{h1}, f_{h2} and X_b.

Taken into account the existing analogies between the heat penetration curve characteristics of broken-heating products and the heat penetration curves obtained when a drop of rotation occurs, the use of the APNS method to evaluate this kind of process deviations was investigated.

4.2. Material and methods

4.2.1. Mathematical procedures and computer programs

4.2.1.1. Extension of the APNS method to allow for changes in the heat penetration parameters.

As implemented in section 2.3.1.5. the APNS method is restricted to a single f_h and j_h value providing no means of handling changes in the heat penetration rates (changes in the f_h value).

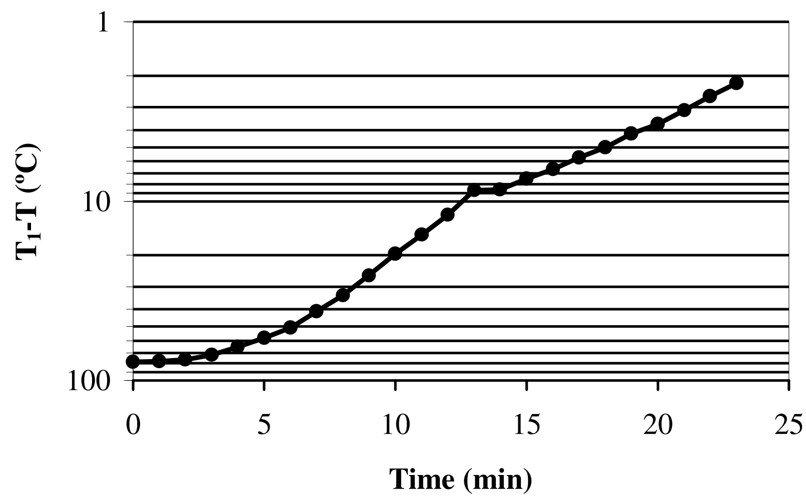

FIGURE 4.1 Typical heat penetration curve obtained when a drop in rotation is observed. Case Study: White beans processed in glass jars. Initial rotation 15 r.p.m., rotation discontinued at minute 13.

The program described in section 2.3.1.5. was modified to allow changes in the empirical heat penetration parameters. Changes in the f_h-value (f_{h1} to f_{h2}) were accomplished by changing the apparent thermal diffusivity (using Eq. 2.1 with the new f_h-value) used in the numerical calculations.

This modification allows to use the APNS method for the prediction of the temperature evolution for broken-heating products (by performing the change in the f_h-value at the time the break-occurs, X_b) and for drops in the rotational speed (by correcting the f_h at the time the deviation occurs).

4.2.1.2. Determination of the empirical parameters for broken-heating curves.

The method proposed for the determination of the parameters that describe the broken-heating curve represents a natural extension of the method used for the determination of the parameters for simple heat penetration curves described in section 3.2.3.

The problem of characterising a given broken-heating curve can be formulated as the determination of the four parameters, j_h, f_{h1}, f_{h2}, and X_b (X_b, representing the time when the break occurs) that when used with the extension of the APNS described in the previous section allow the minimisation of the sum of squares of the differences between the predicted and experimental temperatures.

The modified version of the COMPLEX method described in section 3.2.3. was used for the determination of the appropriate set of parameters (j_h, f_{h1}, f_{h2}, X_b) that minimise the sum of squares of the differences between the experimental temperatures and the temperatures predicted using the APNS method. As initial guesses for the procedure the empirical parameters determined using the graphical procedure described in section 3.2.1. were used.

4.2.2. Preparation of food model systems

4.2.2.1. Bentonite suspensions

Bentonite suspensions were prepared as described in section 3.4.1.1.1.

4.2.2.2. Starch suspensions in glass jars

Starch suspensions were prepared by mixing the appropriate quantities of starch with distilled and dimineralised water until an homogeneous suspension was formed. Glass jars were filled with the suspension to a final head space of 10 mm.

4.2.2.3. Starch suspensions in metal cans

Starch suspensions were prepared by mixing the appropriate quantities of starch with distilled and dimineralised water until an homogeneous suspension was formed. Metal cans were filled with the starch suspensions to a final gross headspace of 10 mm.

4.2.2.4. White beans in glass jars

Dried white beans, *Phaseolus vulgaris* were soaked in distilled and demineralised water at 15°C for at least 16 hours. Glass jars were filled with 450 g of beans, before weighing the beans the excess of water was removed by letting the beans stand in a sieve for approximately 1 min. Distilled water was added to a final headspace of 10 mm. The glass jars were closed manually.

4.2.2.5. Carboxymethylcellulose solutions in glass jars

See section 3.4.1.1.4.

4.2.2.6. Water in glass jars

See section 3.4.1.1.2.

4.3. Results and discussion

4.3.1. Determination of the empirical parameters for broken-heating curves

In order to test the feasibility of the proposed methodology for the determination of empirical parameters for broken-heating curves experiments with products that show broken-heating behaviour were performed. Bentonite suspensions and starch solutions were selected as model products.

4.3.1.1. Bentonite suspensions in metal cans.

In order to select the appropriate concentration for bentonite suspensions, that show a broken-heating behaviour, heat penetration tests for different bentonite concentrations in metal cans were performed both in pure steam and in water cascading mode. To test the stability of the bentonite suspensions they were subjected to consecutive runs by programming a processing temperature of 121°C during 50 min (excluding the CUT duration) followed by cooling with water at room temperature. After four runs it was observed that the product started to leak from the thermocouple insertion point and the containers were not subjected to further processing.

In Tables 4.1 and 4.2 the empirical parameters determined when the product was processed in pure steam and in water cascading respectively are presented. For both cases it was observed that, in the range of concentrations tested, only the 3% bentonite suspensions presented a noticeable brake-point after the four runs. For higher concentrations it was observed that when the bentonite cans were reprocessed the broken-heating behaviour gave rise to straight line behaviour. Lower concentrations were not tested due to literature evidence showing that for lower bentonite concentrations broken-heating behaviour is not observed (Ball and Olson 1957).

The fact that small variations in the bentonite suspensions concentration lead to a rapid variation on the heating characteristics of the suspensions, a variation from 3.00% to 3.25% is sufficient to go from a broken-heating to a straight-line behaviour, implies an extreme care in the preparation of the suspensions in order to obtain reproducible results. On the other hand, even when a consistent broken-heating

TABLE 4.1 Empirical parameters for bentonite suspensions in metal cans processed in pure steam. Process 1 to 4 refer to the successive runs at 121°C for 50 min the containers were subjected to.

Concentration (%)	Process #	j_h (42%) *	f_{h1} * (min)	f_{h2} * (min)	X_b * (min)
3.00	1	1.1	4.5	6.8	7.5
	2	1.1	7.0	38.7	10.8
	3	1.1	9.3	54.0	12.3
	4	1.2	11.4	41.4	11.3
3.25	1	2.0	6.1	34.1	8.3
	2	1.0	17.4	41.8	41.1
	3	1.9	43.1	-	
	4	1.9	40.8	-	
3.50%	1	1.1	6.1	34.1	8.3
	2	2.2	17.4	41.8	12.8
	3	1.7	43.0	-	-
	4	1.87	40.75	-	-
3.75%	1	1.2	7.8	37.6	7.3
	2	1.9	40.8	-	-
	3	1.8	41.3	-	-
	4	1.9	40.8	-	-
4.00%	1	1.4	17.2	39.9	8.8
	2	1.9	40.6	-	-
	3	1.8	40.9	-	-
	4	1.9	40.3	-	-

* Average of four observations

behaviour is observed it is necessary to process extensively the product in order to obtain consistent heat penetration-parameters. Due to the above reasons bentonite suspensions were abandoned as a model system for studying broken-heating behaviour. Nevertheless when observed the broken heating behaviour could be described using the proposed methodology.

TABLE 4.2 Empirical parameter for bentonite suspensions in metal cans processed in water cascading. Process 1 to 4 refer to the successive runs at 121°C for 50 min the containers were subjected to.

Concentration (%)	Process #	j_h (42%) *	f_{h1} * (min)	f_{h2} * (min)	X_b * (min)
3.00	1	1.0	5.6	7.7	9.5
	2	1.3	8.2	38.8	11.8
	3	1.1	11.7	36.7	15.8
	4	1.2	13.4	36.8	16.0
3.25	1	1.0	7.2	37.5	12.5
	2	1.3	13.7	41.4	14.5
	3	2.1	19.8	40.3	20.8
	4	1.6	40.9	-	-
3.50%	1	1.0	7.8	44.9	11.5
	2	2.0	40.8	-	-
	3	2.0	41.0	-	-
	4	2.0	40.7	-	-
3.75%	1	1.0	9.4	39.5	9.8
	2	2.0	40.3	-	-
	3	1.9	40.5	-	-
	4	2.0	40.0	-	-
4.00%	1	1.2	10.9	39.2	9.0
	2	1.9	40.2	-	-
	3	1.9	40.3	-	-
	4	1.9	39.9	-	-

* Average of four observations

4.3.1.2. Starch solutions

Starch solutions in both glass jars and cans were processed at 121°C in water cascading mode. A CUT of approximately 8 min was observed in all the runs. Due to the gelatinisation of the starch it was necessary to process the product under rotation in order to prevent the deposition of the starch at the bottom of the container.

TABLE 4.3 Empirical parameters determined graphically for starch solutions processed in metal cans in water cascading mode. T_1= 121 °C. CUT = 8 min

rotation (r.p.m.)	concentration (g/100 ml)	j_{hb} *		f_{h1} * (min)		f_{h2} * (min)		X_b * (min)	
		avg.	std.	avg.	std.	avg.	std	avg.	std.
4	3	0.6	0.02	10.9	0.26	33.7	1.65	9.6	0.25
8	3	0.6	0.01	12.1	0.15	25.1	0.75	8.9	0.71
4	4	0.6	0.01	13.8	0.34	39.2	0.25	5.4	0.35
4	4	0.6	0.02	25.5	0.67	39.4	2.70	8.1	0.29
4	4	0.6	0.03	24.9	3.13	37.3	1.84	8.3	0.52
8	4	0.6	0.02	13.7	0.85	31.8	0.76	5.5	0.14
8	4	0.6	0.02	20.8	0.84	29.5	1.51	8.7	0.50

* Average and standard deviation calculated from four replicates.

TABLE 4.4 Empirical parameters determined graphically for starch solutions processed in glass jars in water cascading mode. Rotational speed 4 r.p.m. T_1= 121 °C. CUT = 8 min.

Concentration (g/100 ml)	j_h (42%)		f_{h1} (min)		f_{h2} (min)		X_b (min)	
	avg.	std. *	avg. *	std. *	avg. *	std *	avg. *	std. *
2	0.8	0.04	11.8	0.24	#	#	#	#
3	0.8	0.01	16.4	0.80	33.6	7.83	10.1	0.66
3	0.7	0.01	17.0	0.68	27.0	2.18	7.5	0.35
4	0.7	-	17.3	-	31.1	-	8.4	-
4	0.8	0.01	19.3	1.28	40.1	8.52	80.3	0.76
4	0.7	0.01	31.9	1.82	41.4	3.98	11.9	0.28
4	0.8	0.01	20.9	1.18	65.7	8.51	7.4	0.58
4	0.64	0.03	17.16	0.64	37.59	3.62	6.38	0.25
5	0.77	0.01	20.76	0.35	50.99	6.48	7.75	0.5
5	0.75	0.01	20.50	1.15	52.76	8.58	7.25	0.00
5	0.65	-	31.9	-	60.10	-	11.25	-
5	0.74	0.00	21.78	0.76	66.49	0.83	7.00	0.35

* Average and standard deviation calculated from four replicates.
# No broken-heating behaviour was observed for 2% solutions.

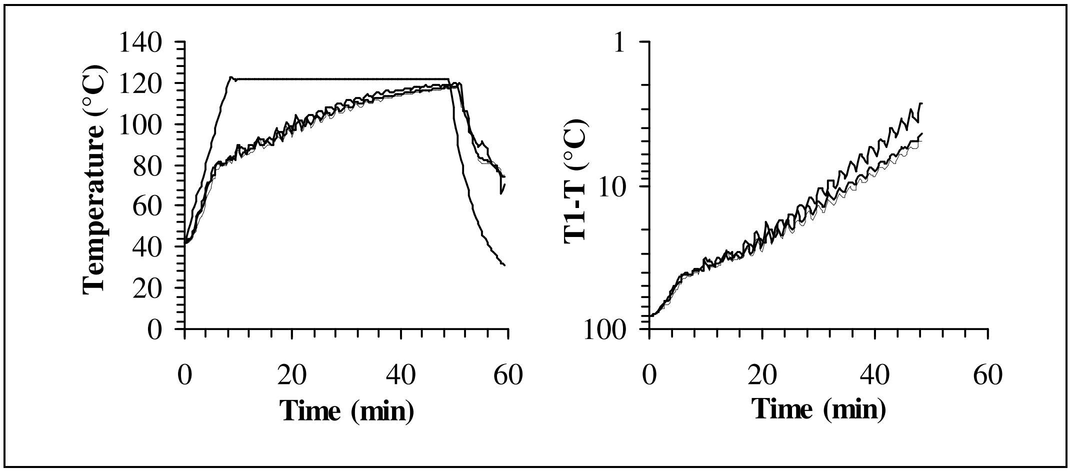

FIGURE 4.2 Time-temperature curves obtained for starch solutions (4%) processed in metal cans under end-over-end rotation. Process conditions: CUT =8 min, 4 r.p.m, T_1=121 °C. Results for three cans processed simultaneously are presented.

In Tables 4.3 and 4.4 the empirical heat penetration parameters determined graphically for starch solutions processed in metal cans and in glass jars, respectively, are given. A broken heating behaviour was observed for both processes in glass jar and in metal cans for starch concentrations equal or above 3%.

In Fig. 4.2 a typical heat penetration curve for starch solutions is given. The broken-heating behaviour is easily observed in this figure. A major problem that arises in the analysis of such heat penetration curves is the definition of the linear segments necessary for the determination of the heat penetration parameters. This explains in part the high variability of the parameters presented in Tables 4.3 and 4.4. It is also observed that after the occurrence of the break a fluctuation on the product temperature is observed. The observed fluctuations contribute also to the referred variability on the parameters.

The empirical parameters for the starch solutions were determined using the procedure proposed for the determination of the empirical parameters for broken-heating products. In Tables 4.5 and 4.6 the empirical parameters (j_h, f_{h1} and f_{h2}) and the time when the break occurs (X_b) are presented for the starch solution processed in metal cans and in glass jars, respectively. The proposed method allowed the automatic determination of the empirical parameters necessary to characterise the experimental broken heating curves.

TABLE 4.5 Empirical parameters for starch solutions processed in metal cans determined using the optimisation procedure.

conc. (%)	rotation (r.p.m.)	CUT (min)	j_h *	f_{h1} * (min)	f_{h2} * (min)	X_b * (min)
3	4	8	0.2 (±0.04)	27.8 (±0.15)	43.4 (±3.22)	10.4 (±6.14)
3	8	8	0.4 (±0.03)	6.4 (±1.09)	28.9 (±0.57)	5.9 (±0.06)
4	4	8	0.9 (±0.01)	3.5 (±0.47)	45.8 (±0.54)	5.0 (±0.21)
4	4	12	1.7 (±0.14)	3.5 (±0.49)	37.4 (±0.49)	8.3 (±0.37)
4	8	8	2.0 (±0.00)	2.3 (±0.32)	30.2 (±0.81)	5.4 (±0.22)
4	8	12	1.9 (±0.09)	2.5 (±0.53)	26.6 (±1.13)	7.9 (±0.41)

* Average of four observation. Standard deviation between brackets.

TABLE 4.6 Empirical parameters for starch solutions processed in glass jars determined using the optimisation procedure.

conc. (%)	rotation (r.p.m.)	CUT (min)	j_h *	f_{h1} * (min)	f_{h2} * (min)	X_b * (min)
3	4	8	0.7 (±0.05)	14.6 (±2.11)	35.9 (±7.34)	8.5 (±0.36)
3	4	8	0.4 (±0.08)	27.2 (±8.52)	34.8 (±7.03)	10.2 (3.18)
4	4	8	2.0 (±0.14)	4.9 (±0.33)	39.4 (±6.62)	6.6 (±0.23)
4	4	15	1.5 (±0.57)	8.8 (±3.85)	42.5 (±10.93)	11.5 (±0.81)
5	4	15	1.4	6.9	57.7	11.0
5	4	8	1.7 (±0.03)	5.1 (±0.11)	52.4 (±5.99)	6.3 (±0.15)

* Average of four observation. Standard deviation between brackets.

In Fig. 4.3 the temperatures predicted by the APNS method using the determined parameters are compared with the experimental temperatures for 4% starch solution processed in metal can under agitation. The calculated and predicted temperatures are compared both in a linear and in a semi-log graph. A good agreement between the predicted and the experimental temperatures can be observed in the linear graph. The apparent discrepancies between the predicted and experimental temperature in the end of the heating phase observed in the log-linear graph are due to the use of a logarithmic scale that amplifies the small differences in temperature observed.

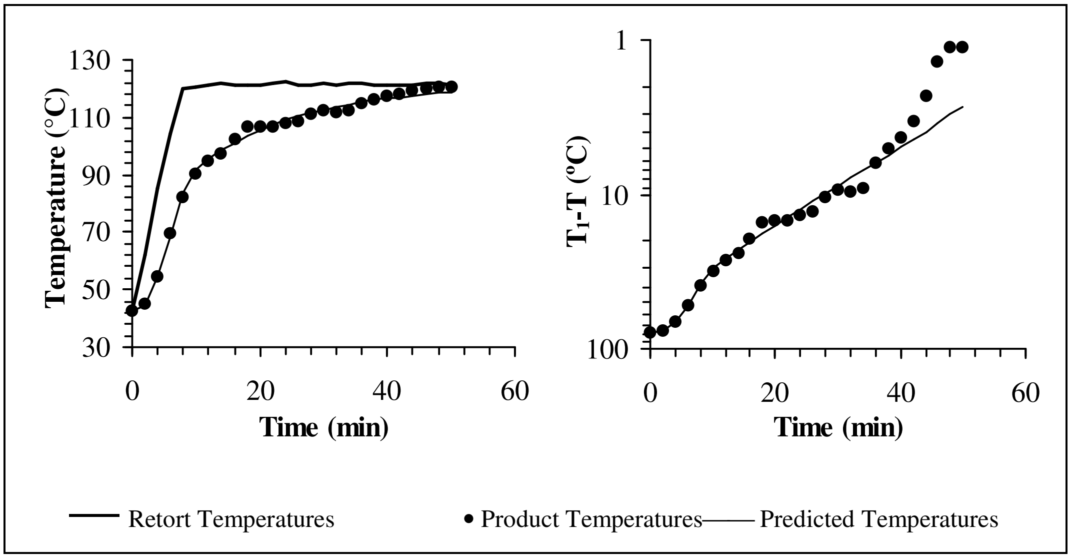

FIGURE 4.3 Experimental product temperatures vs. temperatures predicted by the APNS method when the calculated empirical parameters are used in the simulation. Case Study: Starch solution (4%) in metal can . CUT = 8 min, 4 r.p.m., T_1 = 121°C

The methodology presented for the determination of heat penetration parameters for broken heating curves allows the determination of parameters that accurately describe the experimental time temperature curves. However care must be taken when transferring the obtained parameters to other processing conditions. Experimental work must be carried out in a case by case basis as the mechanisms responsible for the occurrence of the break will vary for different products.

4.3.2. Evaluation of process deviations consisting of drops in rotations

As mentioned before, the degree of mechanical agitation a container is subjected to will have an influence in the heat penetration rate. For liquid foods an increase in the mechanical agitation promotes, to a certain extent, an increase in the heat penetration rate (decrease in the f_h-value, see Table 4.7). When a drop in the rotation occurs it is expected the heat penetration rate will decrease (increase in the f_h-value).

The possibilities of using the APNS method for the evaluation of process deviations consisting of drops in the rotational speed were tested for two case studies: Distilled water processed in glass jars and white beans in distilled water processed in glass jars.

TABLE 4.7 Water in glass jars. Heat penetration parameters for the different rotations

Rotation (r.p.m)	j_h *	f_h * (min)
0	1.4 (±0.03)	10.2 (±0.53)
10	1.0 (±0.07)	8.3 (±1.08)
15	0.9 (±0.00)	7.9 (±0.68)
25	0.9 (±0.03)	7.4 (±0.88)

* Average of four replicates. Standard deviation between brackets.

4.3.2.1. Water in glass jars

Empirical parameters for water in glass jars were determined at different rotational rates. The method discussed in section 3.2.3. was used for the parameters estimation. On Table 4.7, the empirical heat penetration parameters for several rotational speeds are shown.

Several process deviations consisting in drops in the rotational speed were carried out in the available simulator. The process started at a constant rotational speed and at a definite time the rotation was discontinued. The rotational speed was discontinued after the end of the CUT so that the induced break occurs in the linear portion of the heating curve. The APNS method was used to predict the temperature evolution of the simulated processes. The parameters on Table 4.7 were used to simulate the process. Before the drop in rotation the parameters correspondent to the initial rotation were used for the simulation of the temperatures in the container. After the drop in rotation the f_h-value for 0 rotation was used. The process value was calculated from integration of the lethality calculated from the predicted temperature evolution. In Fig. 4.4 the temperature predicted by the APNS method is compared with the temperature measured in two different containers. A good agreement is found between the experimental parameters and the temperature predicted by the APNS method.

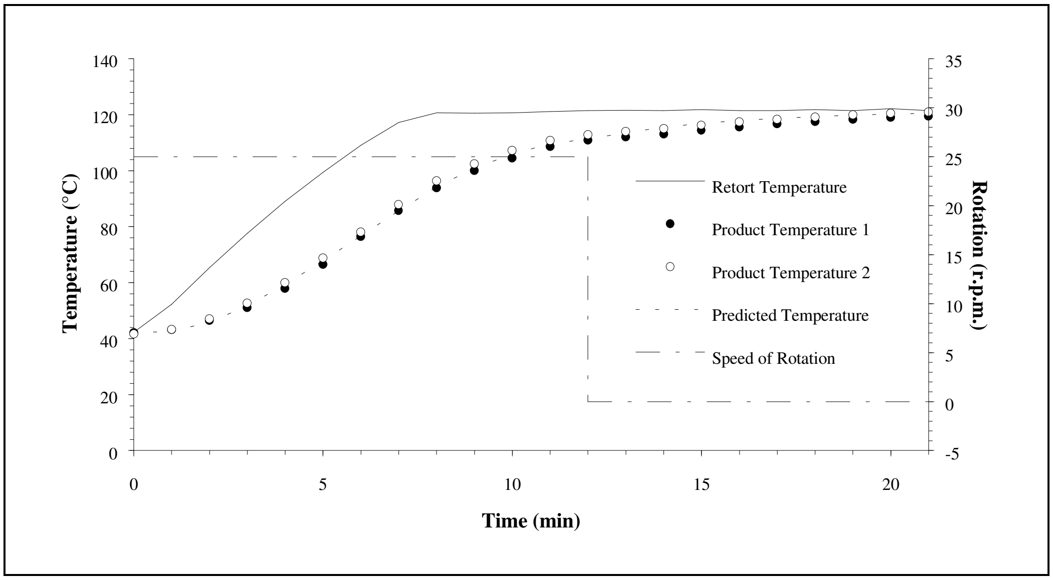

FIGURE 4.4 Use of the APNS method for the evaluation of a deviation on the process consisting in a drop in rotational speed. Case study: Water processed in glass jar. Product Temperature 1 and 2 refer to the time-temperature evolution observed in two different glass jars. Parameters used in the simulation: $j_h = 0.9$, 4 $f_{h1} = 7.4$ min, $f_{h2} = 10.2$ min. Drop in rotation occurs 12 minutes after the beginning of the process.

On Table 4.8, the processing values predicted for several process deviations are compared with the processing values calculated from the experimental temperature evolution measured at two different containers during the process. A good agreement could be found between the processing values predicted using the APNS method and the ones calculated from the experimental time-temperature curves. The contribution of the cooling phase was not taken into account in the calculation of the processing values.

4.3.2.2. White beans in distilled water

The j_h-value and the first f_h-value were determined from a heat penetration experiment at constant rotational speed using the method described in section 3.2.3. For the determination of the f_h-value to be used after the drop in rotation (f_{h2}), three different strategies were tested.

TABLE 4.8 Processing values predicted by the APNS method for process deviations consisting in drops in rotations. Case study: Water in glass jars.

Deviation	F_0 (experimental 1) * (min)	F_0 (experimental 2) * (min)	F_0 (predicted) (min)
From 10 r.p.m. to 0 r.p.m.	5.0	7.1	7.0
From 15 r.p.m. to 0 r.p.m.	3.7	5.3	5.5
From 25 r.p.m. to 0 r.p.m.	3.2	4.7	4.7

* processing values for two different containers.

In the first case, as in the evaluation of drops in rotation with water in glass jars, the second f_h-value was determined from a heat penetration curve from a process with no rotation. In the second alternative, the product was first processed at given rotation and then reprocessed at 0 r.p.m. In the third case, the parameters were determined from a heat penetration curve obtained from reprocessing the product at 0 r.p.m after the deviation occurred. For each individual heat penetration curve the heat penetration parameters were determined using the APNS based method for the simultaneous determination of the heat penetration parameters described in section 3.2.3. In Figs. 4.5 to 4.7 the three different alternatives used for the determination of the process parameters are compared for the evaluation of a process deviation consisting of an initial period at 25 r.p.m. followed by a period at 0 r.p.m.

When the f_h-value used to simulate the temperature after the drop in rotation is determined from a heat penetration curve obtained under no rotation it is observed that after the drop in rotation the APNS method over predicts the temperatures (Fig. 4.5). The same temperature over-prediction is observed when the f_h-value used after the drop in rotation is determined from a heat penetration run where the product is first processed at 25 r.p.m and then reprocessed at 0 r.p.m. (Fig. 4.6). When the second f_h-value is determined from a heat penetration run using the product previously subjected to the deviation a good agreement between experimental and predicted temperatures could be found (Fig. 4.7).

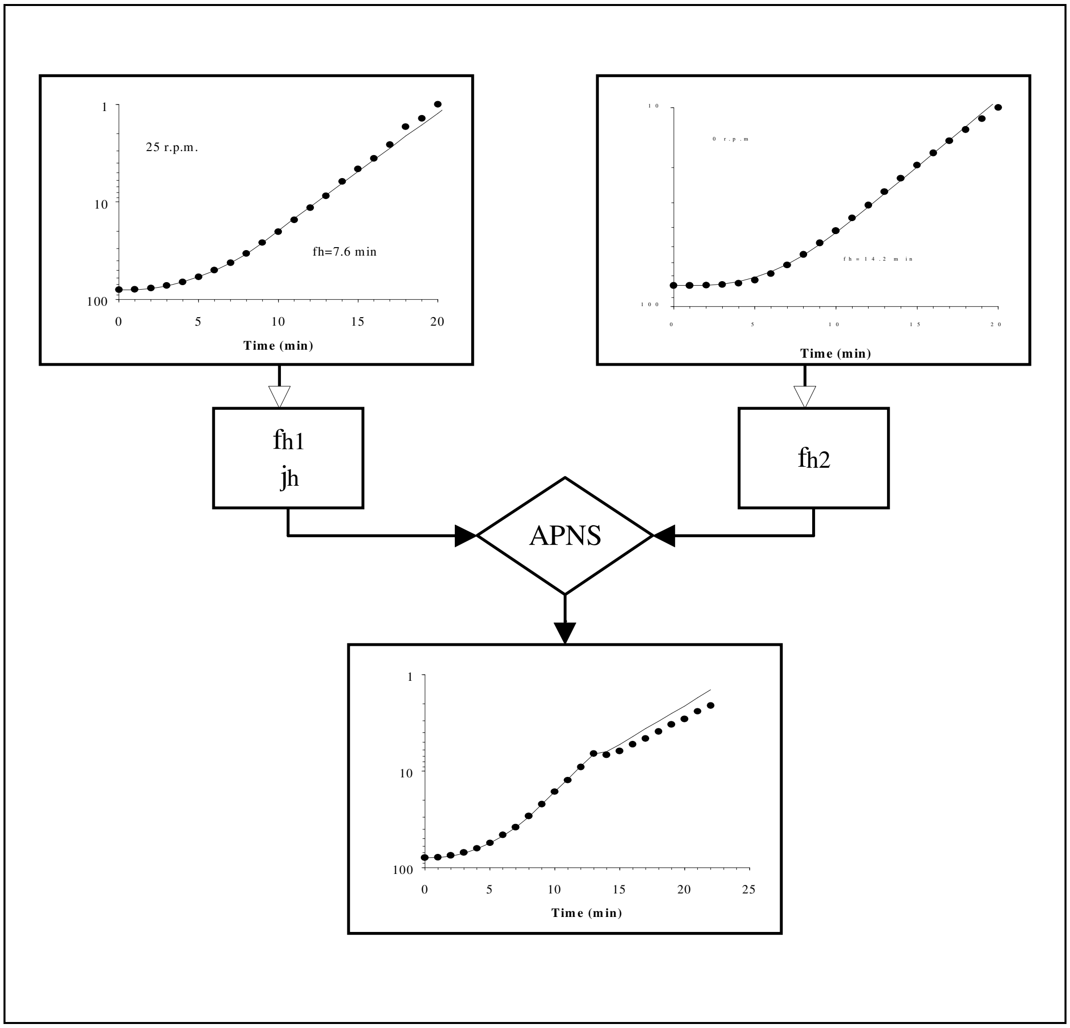

FIGURE 4.5 Determination of the appropriate empirical parameters for the evaluation of process deviations consisting of drops in the rotational speed for white beans processed in glass jars. Second f_h-value determined from an independent experiment.

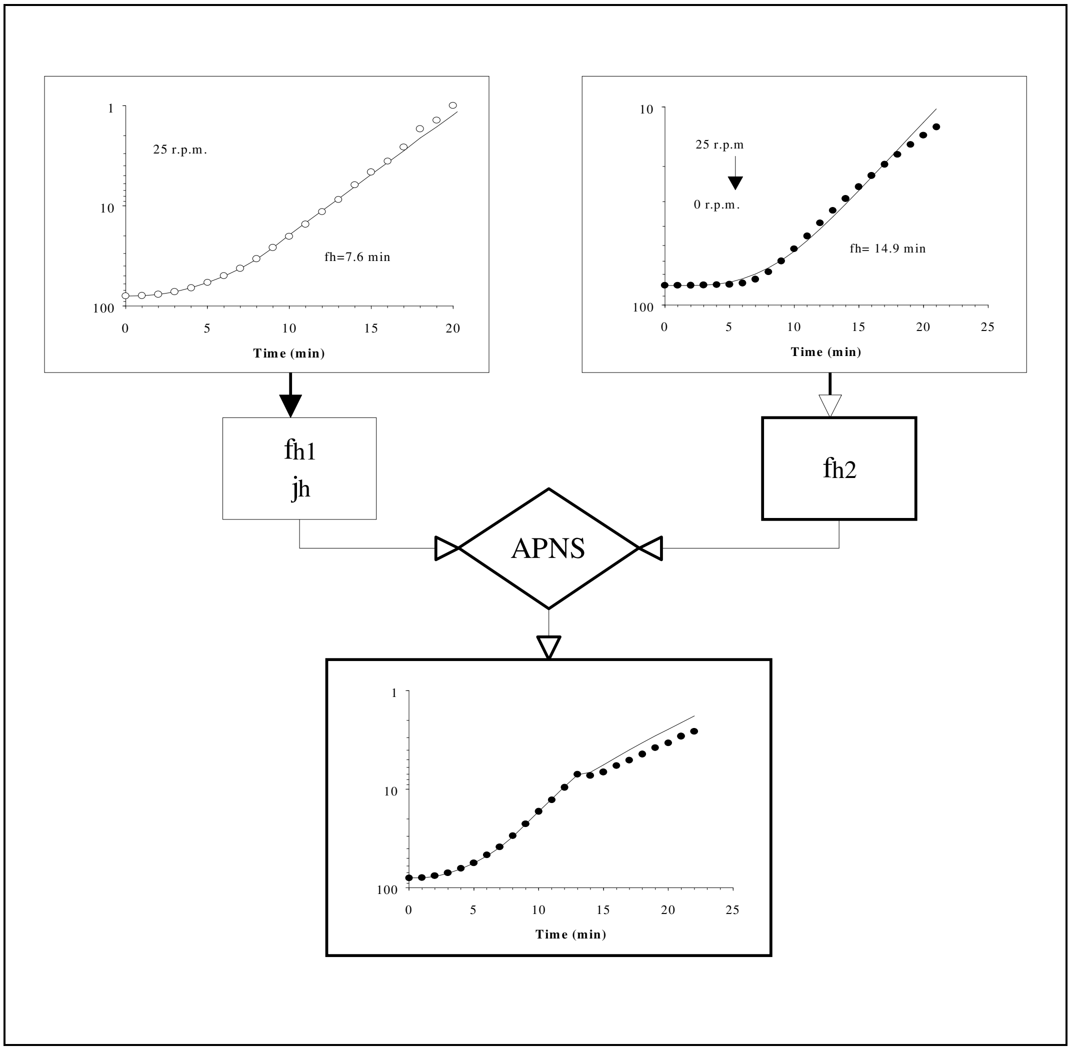

FIGURE 4.6 Determination of the appropriate empirical parameters for the evaluation of process deviations consisting of drops in the rotational speed for white beans processed in glass jars. Second f_h-value calculated by reprocessing the product.

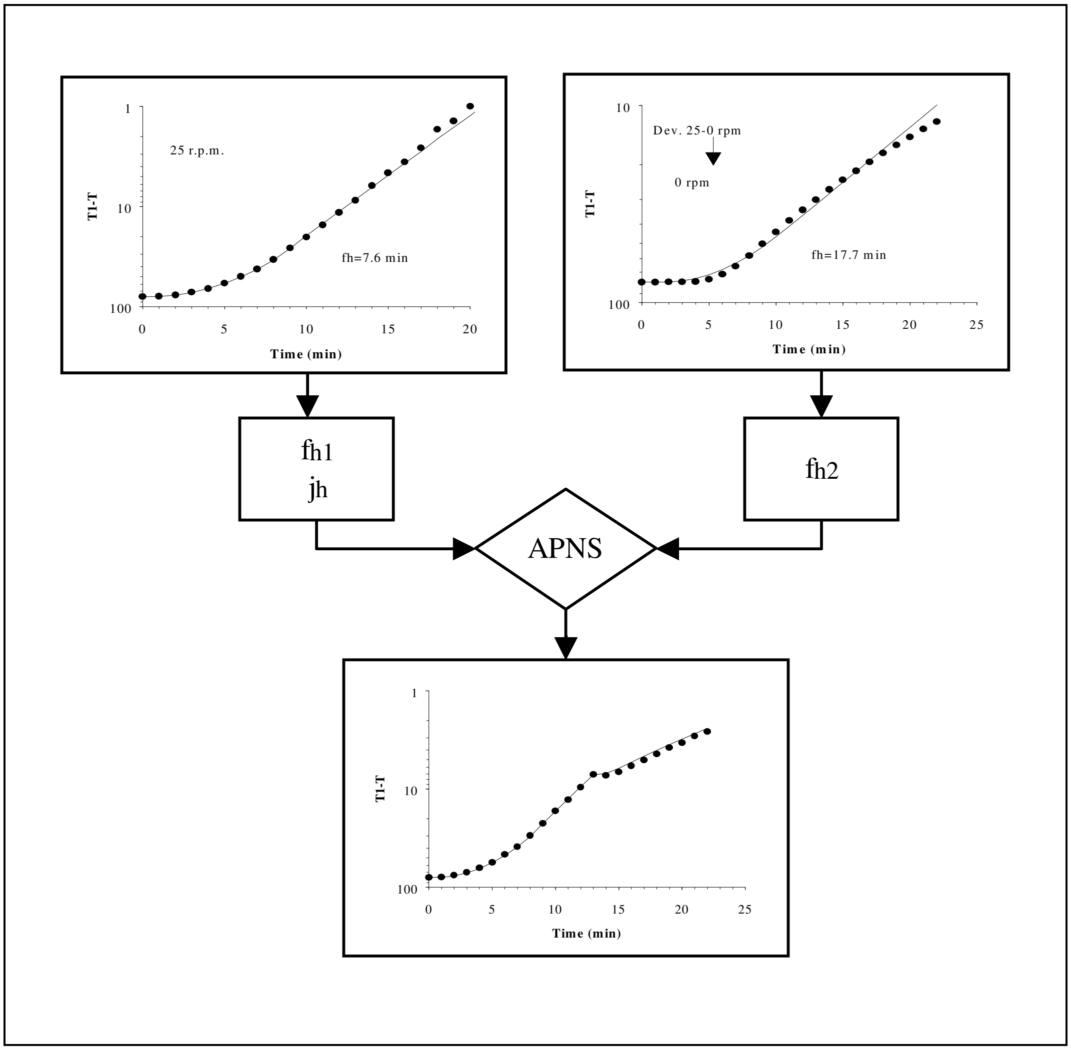

FIGURE 4.7 Determination of the appropriate empirical parameters for the evaluation of process deviations consisting of drops in the rotational speed for white beans processed in glass jars. Second f_h-value calculated by reprocessing the product after the deviation

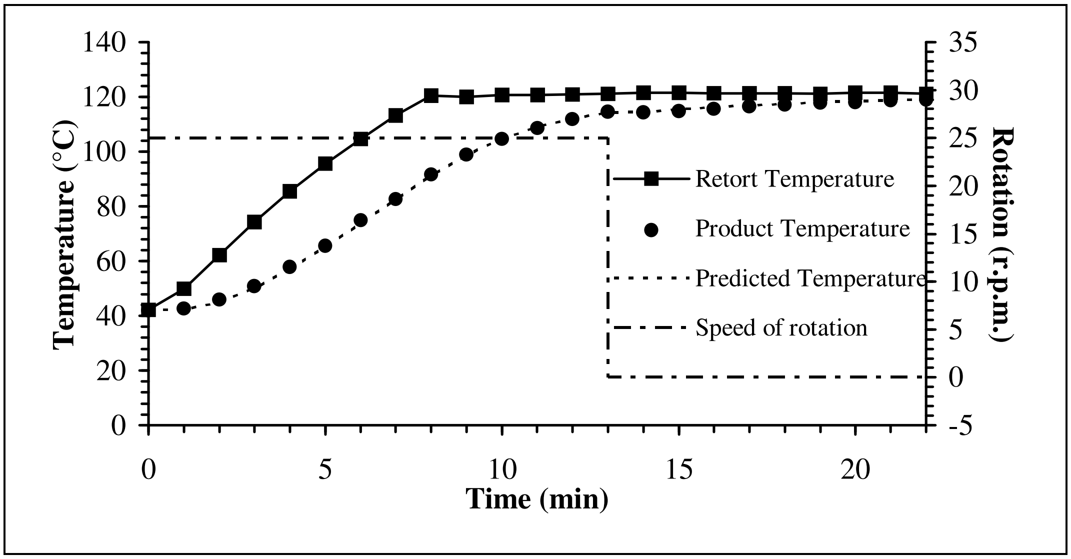

FIGURE 4.8 Use of the APNS method for the evaluation of a deviation on the process consisting in a drop in rotational speed. Case study: White beans processed in glass jar. Parameters used in the simulation: j_h = 1.0,
f_{h1} = 7.6 min, f_{h2} = 17.7 min. Drop in rotation occurs 13 minutes after the beginning of the process.

In Fig. 4.8, the temperatures predicted by the APNS method, using the empirical parameters expressed in Table 4.10 (#3), are compared with the temperatures determined experimentally for beans in glass jar processed with an initial rotational speed of 25 r.p.m. discontinued 13 min after the beginning of the process. A good agreement between the experimental and predicted temperatures can be observed. The APNS method can be used for the evaluation of deviations of thermal processes when a drop in rotational speed is observed during the process if proper parameters are used for the simulation of the temperatures.

On Tables 4.9 and 4.10, the process parameters used by the three different approaches, and the correspondent F_0-values (calculated using the temperatures predicted by the APNS method for each set of empirical parameters) are summarised. When the different processing values are compared with the processing values calculated from the experimental temperatures it is found that the third alternative produces the most reliable predictions of the process value.

TABLE 4.9 Process parameters used for the evaluation of a process deviation consisting of a drop of rotation from 15 r.p.m. to 0 r.p.m.. Case study: White beans in water. Experimental F_0-value = 3.33 min.

	j_h	f_{h1} (min)	f_{h2} (min)	X_b (min)	F_0 (predicted) * (min)
1	1.0	8.8	13.1	13.0	4.6
2	1.0	8.8	14.7	13.0	4.3
3	1.0	8.8	17.6	13.0	3.8

#1. f_{h2}-value determined from an independent experiment.
#2. f_{h2}-value determined by reprocessing the product at 0 r.p.m. after process at 15 r.p.m.
#3. f_{h2}-value determined by reprocessing the product after the actual deviation occur.
* Calculated using the temperatures predicted by the APNS method.

TABLE 4.10 Process parameters used for the evaluation of a process deviations consisting of a drop of rotation from 25 r.p.m. to 0 r.p.m.. Case study: White beans in water. Experimental F_0-value = 4.08 min

#	j_h	f_{h1} (min)	f_{h2} (min)	X_b (min)	F_0 (predicted) (min)
1	1.1	7.6	14.2	13.0	4.9
2	1.1	7.6	14.9	13.0	4.8
3	1.1	7.6	17.7	13.0	4.3

#1. f_{h2}-value determined from an independent experiment.
#2. f_{h2}-value determined by reprocessing the product at 0 r.p.m. after process at 25 r.p.m..
#3. f_{h2}-value determined by reprocessing the product after the actual deviation occur.
* Calculated using the temperatures predicted by the APNS method.

Considering the three different alternatives tested, it was found that for drops in rotation during the processing of white beans in glass jars the f_h-value that allows a better simulation of the temperatures that occur after the break in the rotational speed is the one determined from a heat penetration test with no rotation following the deviation itself.

Further research, covering a more extensive range of process conditions and products, is needed in order to validate the use of the APNS method for the evaluation of process deviations consisting on drops on the rotation. From the limited experience acquired with the two tested products it seems that the determination of the appropriate parameters to be used for the evaluation of the process should be carried on a case-by-case basis. No general rules could be set in order for the proper determination of the parameters to be used with the APNS method for the evaluation of this special kind of deviations.

4.4. Conclusions.

The methodology presented presents a valuable alternative for the determination of the parameters necessary for the description of broken-heating curves. Even for cases that did not present a sharp break, the method allowed for the determination of a set parameters that associated with the APNS method produce good estimates of the temperature evolution. The possibilities of extrapolating the determined parameters to different processing conditions (*e.g.*, other retort and initial product temperatures) must be assessed.

The APNS method seems a promising method for the evaluation of thermal process when deviations consisting on drops of the rotation occur. The main problem associated with this methodology is the evaluation of the correct empirical parameters to be used with the method after the occurrence of the deviation in the rotational speed. Further research is needed covering a more extensive range of process conditions and products in order to validate the proposed method for the evaluation of process deviations consisting on drops on the rotation.

The APNS method combines the flexibility of numerical solutions for the solution of the heat transport equation in handling variable boundary conditions with the empirical description of heat penetration curves. This flexibility allows the use of the APNS method for the evaluation of process deviations consisting on deviations on the heating medium temperature or in the rotational speed on rotational processes. The use of the method relies on the appropriate determination of a reduced set of parameters from experimental data. The APNS method is limited to products whose heat penetration curves present a straight-line behaviour or that could be accurately described by a set of linear segments.

Chapter 5. Optimisation of surface quality retention during the thermal processing of conduction heating foods using variable temperature retort profiles

5.1. Introduction

The first goal in designing a heat sterilisation process is to achieve a reduction in the number of undesirable micro-organisms, leading to a safe product with increased shelf-life. Because of the applied heat treatment, a concomitant decrease in the quality attributes (essential nutrients, colour, ...) is observed (Lund 1982).

Due to differences in temperature dependence between spore inactivation and degradation of quality factors (Table 5.1), the use of high-temperature-short-time (HTST) processes leads to sterilised products with a high quality retention. This is true in aseptic processing of liquids or other pumpable foods or in the case of rotary retorts, cases where the rate of heat penetration in the food is considerably high. However, for packed solid foods the observed slow rate of heat transfer does not allow the use of HTST processes. Very high temperatures will cause severe thermal degradation of the food near the surface before the food at the centre of the container has risen significantly in temperature. On the other hand a relatively low retort temperature will cause great quality losses because of the long time it will take to obtain commercial sterility (Ohlsson 1980d). Consequently there is an optimum time-temperature relationship, that will minimise the quality losses, still providing a microbiological safe food.

The idea of minimising quality losses during thermal processing of foods is not new. Since the presentation of the first study using computer simulation in 1969 (Teixeira *et al.* 1969a) the idea has been widely documented in literature (Teixeira *et al.* 1969b, 1975a and 1975b, Manson *et al.* 1970, Lund 1977 and 1982, Thijssen *et al.* 1978, Saguy and Karel 1979 and 1980, Ohlsson 1980a,b,c, Martens 1980, Thijssen and Kochem 1980, Norback 1980, Holdsworth 1985, Nadkarni and Hatton 1985, Bhowmik and Hayakawa 1989, Hendrickx *et al.* 1990, 1991a, 1991b, 1991c and 1992b, Banga *et al.* 1991, Silva *et al.* 1992a and 1992b). Optimal sterilisation processes leading to a maximisation of overall quality retention have been calculated

TABLE 5.1 Kinetic parameters for the wet-heat inactivation of several quality and safety factors (Lund 1977).

Quality/ Safety factor	z (°C)	E_a (Kcal/mol)	D_{121} (min)
Vitamins	25-31	20-30	100-1000
Colour, Texture, Flavour	25-45	10-30	5-500
Enzymes	7-56	12-100	1-10
Vegetative Cells	5-7	100-120	0.002-0.02
Spores	7-12	53-83	0.1-5.0

using systematic search procedures (Teixeira *et al.* 1969b and 1975b, Bhowmik and Hayakawa 1989), graphical optimisation (Ohlsson 1980a, 1980b and 1980c) and mathematical optimisation techniques (Saguy and Karel 1979, Martens 1980, Nadkarni and Hatton 1985, Banga *et al.* 1991, Hendrickx *et al.* 1991a and 1992b).

The use of variable retort profiles (VRT) to improve overall (mass average) quality retention has been investigated thoroughly. Recently, a critical review of commonly used objective functions has been presented (Silva *et al.* 1992b). The use of selected types of retort time-temperature functions (step, ramp and sinusoidal functions) did not lead to significant improvements over the use of constant retort profiles (Teixeira *et al.* 1975b, Bhowmik and Hayakawa 1989). The application of the maximum principle theory to the calculation of the optimum time-temperature profile (Saguy and Karel 1980), showed the possibility of finding an optimum (unique) profile. However, the small improvement in quality retention achieved does not encourage the use of this type of profiles. The application of the Pontryagin's minimum principle to a distributed parameter model for the optimisation of overall nutrient retention (Nadkarni and Hatton 1985), leads to the conclusion that the use of a bang-bang control strategy, where the rates of heating and cooling of the heating medium should be as fast as the equipment limitations allow for, with one single heating-cooling cycle was the best strategy to adopt. The available literature information on optimisation of mass average quality clearly demonstrates that optimal CRT profiles are as good as optimal VRT profiles when the optimisation of the overall quality is of concern. Only when minimisation of process time is of interest, VRT profiles show some advantages (Teixeira *et al.* 1975b, Bhowmik and Hayakawa 1989, Banga *et al.* 1991).

Optimal constant retort temperatures (CRT) have been calculated for the case of optimisation of surface quality of canned foods (Ohlsson 1980a, 1980b and 1980c, Hendrickx *et al.* 1990 and 1992b, Banga *et al.* 1991). Semi-empirical formulas relating the optimal sterilisation temperatures and all the relevant process variables (food properties, processing conditions and sterilisation criteria) for 'one-dimensional' containers were proposed (Hendrickx *et al.* 1990, 1991a and 1992b) and confirmed for three-dimensional case studies (Hendrickx *et al.* 1991b and 1991c). The use of modern optimisation techniques to solve the problem of finding the optimal retort profile for the optimisation of surface retention (Banga *et al.* 1991) leads to the conclusion that the use of VRT profiles represents a valuable policy. An appreciable increase in the surface quality retention (20%), over the optimal CRT profile could be achieved. A considerable reduction in the process time could also be achieved using VRT profiles. These conclusions were based on a limited number of case studies.

In the first sections of this chapter the possibilities of variable retort temperature (VRT) as a mode of increasing the surface retention of quality factors and in decreasing the process time during the sterilisation of pure conduction-heating foods were further explored. A range of z values for quality factors, target lethalities and food heating characteristics, relevant to conduction heating foods, was considered.

Based on the calculated optimum variable retort temperature profiles an empirical equation able to reduce the number of parameters necessary to characterise the optimum variable retort temperature profiles was developed. This equation allowed to reduce the calculation effort necessary for the calculation of optimum VRT profiles.

5.2. Material and methods

5.2.1. Conduction heat transfer model

The calculation of the transient temperature-history inside the food, was performed using explicit finite-difference models for one-dimensional, homogeneous and isotropic conduction heating foods, described in section 1.5.2.

5.2.2. Optimisation of constant retort temperature profiles (CRT)

5.2.2.1. Definition of CRT profiles

In the present work, CRT profiles are defined as profiles existing of a come up period (the time needed for the heating medium to obtain the actual sterilisation temperature), a holding time (t_h) at constant heating temperature (T_h), followed by a cooling period (t_{cw}) at constant cooling temperature (T_{cw}), sufficiently low to bring the centre of the product below a pre-defined temperature (T_p^t). In this study the come-up-time of the retort was considered to be zero, this means that at time zero the retort was at temperature T_h. The total process time (t_p) was defined as the summation of the holding time (t_h) and the cooling time (t_{cw}).

5.2.2.2. Formulation of optimisation problems

The mathematical formulation, of the objective function, for the maximisation of the surface retention (RETS) was as follows,

Maximise with respect to T_h (design variable),

$$RETS = 10^{-\frac{C}{D_{Tref,q}}} \text{ x } 100 \tag{5.1}$$

with,

$$C = \int_0^{t_p} 10^{\frac{T_s(t)-T_{ref,q}}{z_q}} dt \tag{5.2}$$

subjected to,

(i) A microbial constraint at $t = t_p$,

$$F_{ce} = \int_0^{t_p} 10^{\frac{T_{ce}(t)-T_{ref,m}}{z_m}} dt \geq F_{ce}^t \tag{5.3}$$

where F_{ce}^t is the target lethality at the centre (cold spot) of the product.

(ii) A constraint in the final temperature at the centre of the product,

$$T_{ce}(t_p) \leq T_p^t \tag{5.4}$$

where $T_{ce}(t_p)$ represents the temperature at the centre of the food at the end of the process time. T_p^t is a temperature (target value) sufficiently low so that the rate of destruction of micro-organisms became negligible. This constraint assures that the product is sufficiently cooled at the end of the process.

5.2.2.3. Optimisation approach and algorithm

To calculate the optimal CRT profiles (holding temperature, T_h, resulting in a maximum quality retention) an optimisation routine using the Davies-Swann-Campey method (Silva *et al.* 1992a, Saguy 1983) was applied to find the value of T_h for a minimum C-value (Eq. 5.2). The procedure was initialised with a starting value for T_h as determined using previously developed (Hendrickx *et al.* 1991a and 1992b) semi-empirical formula to calculate optimal sterilisation temperatures (Eq. 5.5).

$$T_h^{opt} = 107.8 - 9.74\log(f_h) + 9.8\log(F_{ce}^t) + 9.3\ln(z_q) - \frac{3.06}{Bi} + 0.41\frac{z_q}{Bi} \tag{5.5}$$

For each T_h^{opt}, the associated t_p, necessary to satisfy the microbial constraint (Eq. 5.3), was calculated using a Pascal program. The program calculated t_h iteratively, starting from zero, and incremented this value by Δt_h (Eq. 5.6) (Hendrickx *et al.* 1991a), until the target lethality including the cooling part was reached. A cooling medium temperature of 20°C was used in all the simulations. The cooling was simulated until the final temperature constraint (Eq. 5.4) was satisfied.

$$\Delta t_h = \frac{F_{ce}^t - F_{ce}}{10^{\frac{T_h - T_{ref,m}}{z_m}}} \tag{5.6}$$

5.2.3. Optimisation of variable retort temperature profiles (VRT)

5.2.3.1. Definition of VRT profiles

VRT profiles are defined as profiles in which no *a priori* assumptions are made in the dependence of the retort temperature with time. Variable retort temperature profiles were approximated by a set of linear pieces. To reduce the number of variables to be optimised a constant time step was used in the description of the retort profile. The retort profile was described by a vector of temperatures, equally spaced in time. Intermediate temperatures were calculated by linear interpolation. This approach reduces the estimation of an optimal continuous function to a multi-dimensional variable optimisation problem.

5.2.3.2. Formulation of optimisation problems

In the optimisation of VRT profiles two objectives were considered: (a) optimisation of the quality retention for a fixed process time, and (b) optimisation of the process time with a constraint in the quality retention.

The optimisation of the quality retention (for a fixed process time) using VRT was mathematically defined as: the maximisation, with respect to the vector of retort temperature, T_r, of the surface quality (Eq. 5.1), subjected to the following constraints:

(i) Microbiological sterility (Eq. 5.3)

(ii) Final temperature at the centre (Eq. 5.4)

Both constraints were incorporated in the objective function by means of a penalty function, P,

$$P = W_1 (T_{ce}(t_p) - T_{ce}^t)^2 + W_2 (F_{ce} - F_{ce}^t)^2 \qquad (5.7)$$

where, W_1 and W_2 represent positive weighing factors.

The maximisation of the surface retention was dealt as a minimisation problem considering the objective function:

$$\text{Objective Function} = -\text{RETS} + \text{P} \qquad (5.8)$$

When the optimisation (minimisation) of the process time with a constraint on the surface quality was the objective, the problem was to find the retort profile that minimised t_p subject to the constraints:

(i) Microbiological sterility (Eq. 5.3)

(ii) Final temperature at the centre (Eq. 5.4)

(iii) Quality surface retention (RETS) larger or equal than a prefixed target value (RETSmin),

$$RETS \geq RETS_{min} \tag{5.9}$$

where $RETS_{min}$ represents the minimum acceptable value of surface retention for the quality factor.

5.2.3.3. Optimisation approach and algorithms

A FORTRAN program using a quasi-Newton multi-variable optimisation subroutine (E04JBF, NAG 1983) was used to calculate the optimum VRT profiles for a fixed process time. For the calculation of the objective function (Eq. 5.8), a subroutine able to perform the calculation of the transient temperatures inside the food, the quality surface retention and the processing value at the centre of the product, was written.

The choice of the weighing factors W_1 and W_2 (on Eq. 5.7) revealed to be crucial in the optimisation process. It was found that a fixed value of 1.0 for W_1 was suited for the resolution of most of the optimisation problems. Regarding W_2 it was found that solving the optimisation problem in several steps, taking as the initial guess for one step the solution of the previous step, starting with a small value of W_2 and increasing it in each step, was a satisfactory way to reach the optimum. The number of variables to be optimised, was made dependent on the process time. The number of variables was varied between 10 and 30, respectively for short and long process times (i.e., about 5 to 300 min). The optimum CRT profiles were taken as the initial guess to calculate the optimum VRT profiles.

To reduce the mathematical complexity, the problem of finding the minimum process time with a constraint on quality retention (Eq. 5.9) was solved by splitting it into a series of optimisation problems for fixed process time. For a set of processing times the optimisation of surface quality was carried out using the procedure described above, i.e. for each considered processing time the optimum VRT profile was calculated. Graphical presentation of the optimal surface retention associated with these optimum profiles against the process time, allow the determination of the minimum process time meeting the constraint on surface retention (Eq. 5.9). Each determined process time has an associated optimal VRT profile.

5.3. Results and discussion

The optimisation procedures discussed above were tested against the results previously presented by Banga *et al.* (1991). Since in the present work only one-dimensional finite-difference models were considered and the examples presented by Banga *et al.* referred to finite cylinders, the simulations were performed on infinite cylinders showing the same f_h-values (product heating rate) as Banga *et al.*'s case studies. In spite of the differences between the two optimisation schemes, the optimal VRT profiles obtained by Banga *et al.* were confirmed using the present approach. Differences of less than 0.5% in the optimal surface retention were observed. The optimum profiles obtained were similar to the profiles presented by Banga *et al.* (1991).

The optimisation procedures proposed were applied to a vast number of case studies, and the optimum VRT profile was found for each case. Only cases where the Biot number can be approximated as infinite and geometry that show one-dimensional heat transfer by conduction (infinite cylinder, infinite slab, and sphere) were considered for the sake of simplicity. Values of z_q covering the range of values found in literature were considered (Lund 1982, Ohlsson 1980d). Values of thermal diffusivity in the range of values normally encountered in foods were used in the simulations (George 1990). In all the cases studied for the calculation of the surface retention a D value of 178.6 min (Banga *et al.* 1991) for the quality factor was assumed. The calculation of the microbiological lethality was based on a z-value of 10°C.

5.3.1. Optimisation of the surface retention using VRT policy

Tables 5.2 to 5.4 summarise the results obtained for the optimisation of the retort temperature profile, considering the objective function surface retention. To compare the optimal VRT and the corresponding optimal CRT, the VRT profiles calculated for process times equal to the corresponding optimal CRT profiles were used.

The comparison of the optimum CRT's with the optimum VRT's for the same process time (Tables 5.2 to 5.4) show that it is possible to get improvement in the quality retention at the surface up to 13 percentage points (absolute) or up to 20% in relative terms (Table 5.2), using the VRT policy. From the case studies there is no straightforward relation between the achieved improvements and the z_q value or target microbial lethality. Fig. 5.1 shows typical results for the best CRT and the best VRT with the same process time.

One of the possible drawbacks for the practical implementation of these VRT profiles is the fine temperature control necessary to achieve the maximum retention and at the same time reaching the correct F_0 value at the centre. Small differences in temperature inside the retort can lead to large variability in the F_0 value. Table 5.5 shows typical simulation results of increasing and decreasing the calculated optimum temperature profiles by one degree over the entire process time. The effects on F_0, C and surface retention are presented.

5.3.2. Optimisation of the total process time

For some of the case studies the optimisation of process time was performed. As stated above, the strategy chosen to deal with this problem, consisted in calculating the optimal retention for different pre-set process times and then to plot the retention as a function of process time.

In Fig. 5.2 two examples of such cases are presented. It must be stressed that each point in these graphs represents not only the maximum possible retention for a certain process time, but is also associated with a unique optimum variable retort profile. In Fig. 5.2 the process time and the retention of the corresponding optimum CRT profiles are also presented so that the superior performance of VRT versus CRT can be noticed. One interesting feature showed in Fig. 5.2 is that for high values of process time an increase in the process time is not followed by an increase in surface retention, the surface retention becomes almost constant. This can be explained considering that

TABLE 5.2 Comparison of surface retention for optimal VRT and optimal CRT profiles Infinite Cylinders, α = 1.6E-07 (m²/s), T_0 = 40°C.

radius (m)	F^t_{ce} (min)	z_q (°C)	T_{opt} * (°C)	t_p * (min)	CRT (%)	VRT (%)	Gain (abs)	Gain (%)
0.050	6.0	25	109.11	304.75	34.6	41.0	6.4	18.5
0.025	6.0	25	115.00	78.70	62.5	69.4	6.9	11.1
0.025	6.0	30	116.84	69.70	60.1	66.8	6.7	11.1
0.025	6.0	35	118.37	64.52	58.9	65.3	6.4	10.8
0.025	6.0	15	109.66	137.00	76.1	81.1	5.0	6.6
0.025	12.0	30	119.63	71.55	52.4	58.9	6.5	12.4
0.025	9.0	30	118.72	69.70	55.7	62.7	7.0	12.5
0.025	9.0	15	111.61	134.30	62.8	75.8	13.0	20.7
0.025	12.0	15	112.80	135.60	64.7	71.5	6.9	10.6
0.015	6.0	25	119.44	28.77	77.3	81.9	4.5	5.9
0.035	6.0	25	112.31	143.90	51.0	57.5	6.5	12.7
0.035	12.0	30	116.97	136.16	36.7	45.8	9.1	17.8

* Temperature and process time of the optimum constant retort temperature (CRT) process.

TABLE 5.3 Comparison of surface retention for optimal VRT and optimal CRT profiles. Spheres, α= 1.54E-07 (m²/s), T_0 = 40°C.

radius (m)	F^t_{ce} (min)	z_q (°C)	T_{opt} * (°C)	t_p * (min)	CRT (%)	VRT (%)	gain (abs)	gain (%)
0.016	6.0	15	115.57	36.22	83.9	87.0	3.1	3.7
0.016	6.0	20	118.46	25.99	81.5	85.3	3.8	4.7
0.016	6.0	30	122.54	19.17	81.0	85.1	4.0	5.0
0.016	6.0	35	123.90	17.86	81.4	84.9	3.5	4.3
0.016	9.0	15	117.18	37.15	79.4	83.1	3.7	4.6
0.016	9.0	20	120.36	25.79	77.7	83.0	5.3	6.8
0.016	9.0	30	124.13	19.48	78.5	82.9	4.4	5.7
0.016	9.0	35	125.59	18.04	79.3	83.5	4.2	5.3
0.016	12.0	15	118.71	35.86	75.6	80.9	5.3	7.0
0.016	12.0	20	121.60	25.87	74.7	80.6	5.9	7.9
0.016	12.0	30	125.40	19.54	76.6	81.5	4.9	6.4
0.016	12.0	35	126.85	18.11	77.6	82.2	4.6	5.9
0.032	9.0	30	118.16	76.11	54.8	62.9	8.1	14.8
0.008	9.0	30	130.00	5.01	90.7	92.8	2.1	2.3

* Temperature and process time of the optimum constant retort temperature (CRT) process.

TABLE 5.4 Comparison of surface retention for optimal VRT and optimal CRT profiles. Infinite Slabs, α = 1.6E-07 (m²/s), T_0 = 40°C.

Half thickness	F_{ce}^{t}	z_q	T_{opt} *	t_p *	CRT	VRT	gain	gain
(m)	(min)	(°C)	(°C)	(min)	(%)	(%)	(abs)	(%)
0.02	6.0	15	108.24	189.81	73.4	78.5	5.1	6.9
0.02	6.0	20	111.37	131.28	62.0	69.5	7.4	11.9
0.02	6.0	30	115.28	96.81	52.3	58.4	6.1	11.6
0.02	6.0	35	117.01	87.99	50.4	53.0	2.6	5.2
0.02	9.0	15	109.99	190.98	66.6	73.1	6.4	9.7
0.02	9.0	20	113.06	132.99	55.6	62.9	7.3	13.1
0.02	9.0	30	117.05	97.48	47.4	55.9	8.5	17.9
0.02	9.0	35	118.73	88.89	46.2	53.8	7.7	16.6
0.02	12.0	15	111.18	193.20	61.1	68.2	7.1	11.6
0.02	12.0	20	114.38	132.56	50.7	59.5	8.9	17.5
0.02	12.0	30	118.27	98.17	43.9	52.7	8.8	20.0
0.02	12.0	35	119.89	89.77	43.0	51.3	8.3	19.3
0.01	9.0	30	122.98	25.11	74.0	79.1	5.1	6.9
0.04	9.0	30	111.32	373.16	15.8	23.0	7.2	45.3

* Temperature and process time of the optimum constant retort temperature (CRT) process.

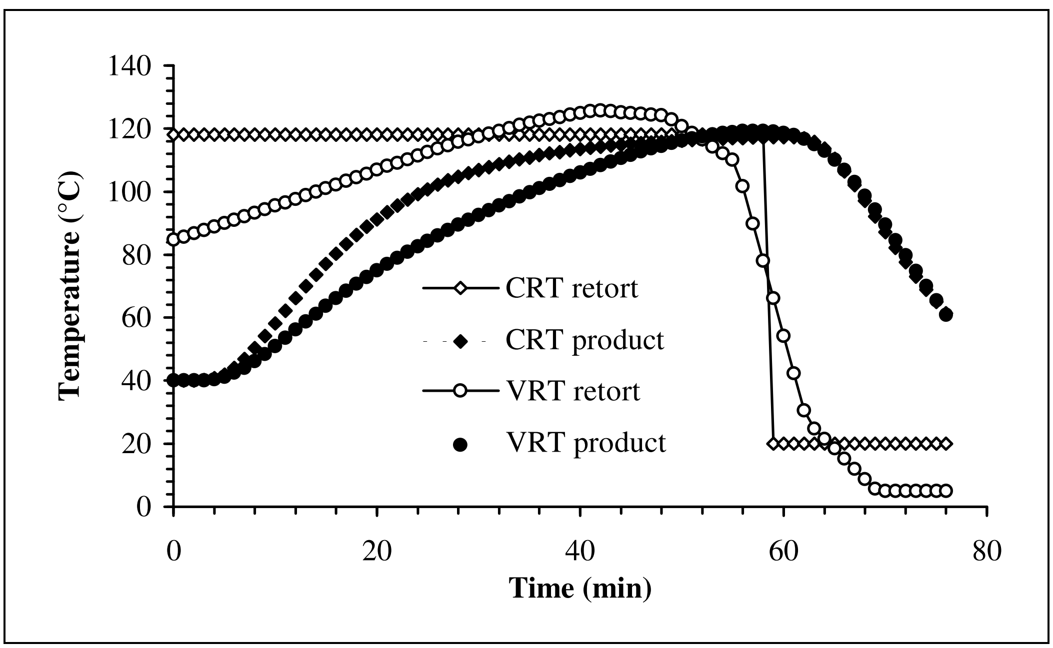

FIGURE 5.1 Optimum VRT and CRT profiles, and corresponding temperature profiles at the centre of the product, for the same total process time.

TABLE 5.5 Effect of deviations (±1°C) in the optimal variable retort temperature profiles on the F, C and surface retention values

	C-value			F value			Surface Retention		
	(-1°C) (min)	Optimum (min)	(+1°C) (min)	(-1°C) (min)	Optimum (min)	(+1°C) (min)	(-1°C) (%)	Optimum (%)	(+1°C) (%)
A	18.3	21.5	25.0	7.2	9.0	11.34	78.9	75.8	72.4
B	33.3	36.0	38.9	6.8	9.0	10.74	65.0	62.9	60.6
C	36.1	40.2	45.1	9.7	12.0	15.1	62.8	59.5	55.9

A - Infinite cylinder, radius = 0.025 m, F^t=9.0 min, z_q = 15 °C.
B - Sphere, radius = 0.032 m, F^t = 9.0 min, z_q = 30 °C.
C - Infinite slab, radius = 0.02 m, F^t = 12.0 min, z_q = 20 °C.

after a certain value of process time the variable process time is no longer a constraint (Banga *et al.* 1991), the global optimum is reached.

By comparing the time of the best CRT and optimal VRT process that achieves the same surface retention (the time corresponding to the interception of the horizontal line and the curve), one can calculate the gain in process time that can be achieved using a VRT policy. In the two examples presented improvements around 27% in the process time were observed (e.g., 88.9 min for the CRT profile and 65 min for the VRT profile).

In Table 5.6 the results obtained for all the cases studied are summarised. The use of VRT was found to be interesting in terms of the optimisation of process time. Optimum VRT profiles achieving the same surface retention as the best CRT profile with a reduction between 23% and 45% of the CRT process time (Table 5.6) could be achieved. The best results in terms of process time reduction were achieved for low z_q values (high temperature sensitive quality factors). Target F_0 was less important.

The retort profiles and the associated product centre temperatures for the optimal CRT and the optimal VRT that can achieve the same surface retention of the best CRT in a minimum process time for a typical case study are illustrated in Fig. 5.3.

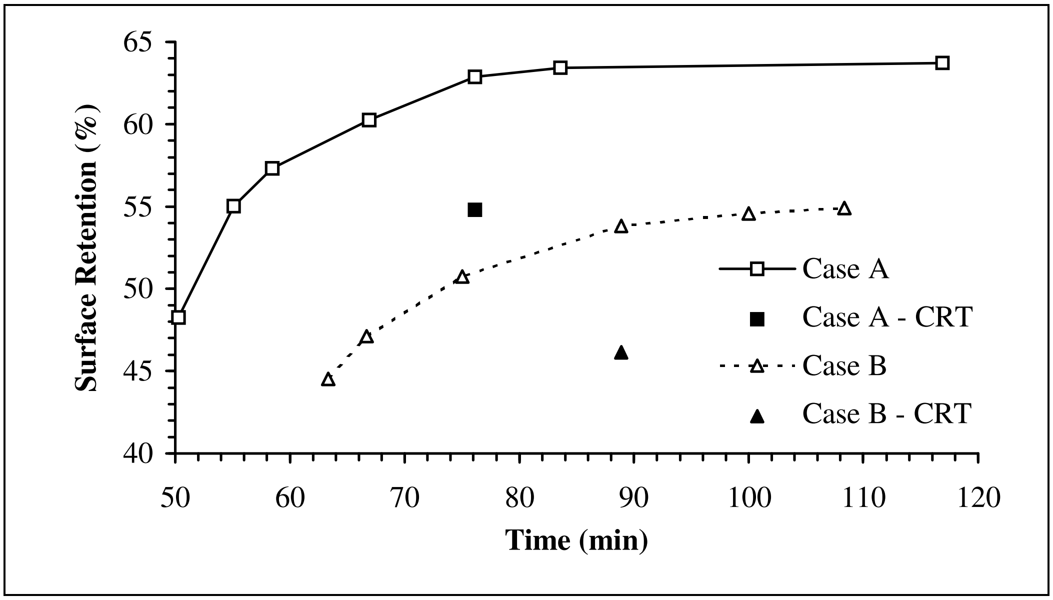

FIGURE 5.2 Surface retention versus process time for optimal VRT processes.
Case A - Slab, α =1.6E-07 (m^2/s), half thickness = 0.02 m, F^t = 9 min, z_q = 35°C.
Case B - Sphere , α =1.6E-07 (m^2/s), radius = 0.033 m, F^t = 9 min, z_q = 30°C.
The dark symbols represent the process time and surface retention of the corresponding optimum CRT profile.

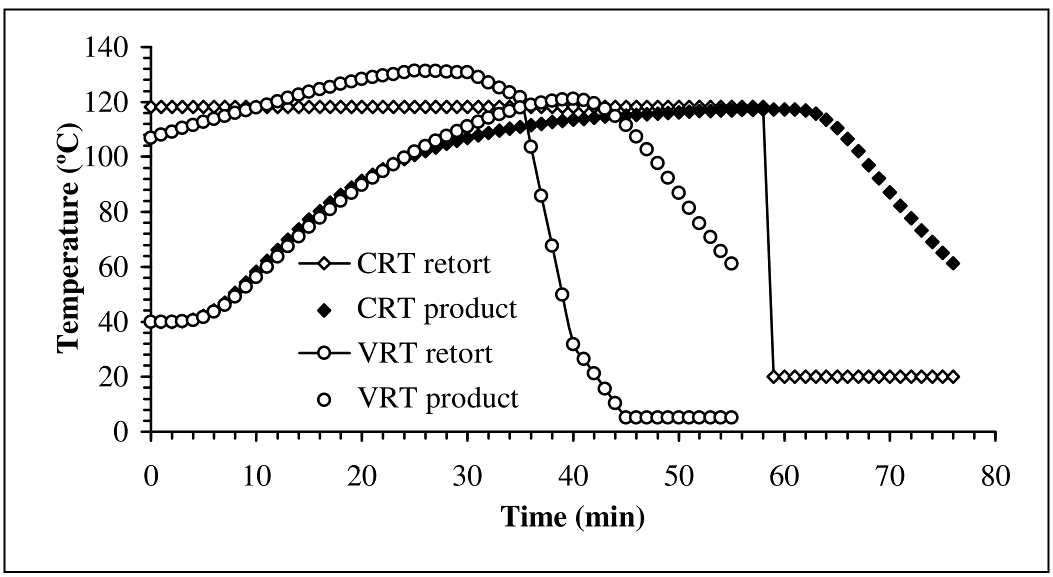

FIGURE 5.3 Optimum VRT and CRT profiles, and corresponding temperature profiles at the centre of the product, that show the same surface retention.

TABLE 5.6 Comparison, in terms of processing time, of the optimal CRT and the VRT with minimum process time resulting in the same quality retention. α = 1.6E-07 (m²/s), T_0 = 40°C.

Geom.	Radius/ Half thickness (m)	F_c^t (min)	z_q (°C)	RETS (%)	t_p (CRT) (min)	t_p (VRT) (min)*	gain (%)
cylinder	0.025	6.0	25	62.5	78.7	57	28
cylinder	0.025	12.0	30	52.4	71.6	52	27
cylinder	0.035	12.0	30	36.7	136.2	98	28
sphere	0.033	9.0	30	54.8	76.1	55	28
sphere	0.016	9.0	30	78.5	19.5	15	23
sphere	0.016	6.0	15	83.9	36.2	21	42
slab	0.020	9.0	35	46.2	88.9	65	27
slab	0.020	6.0	30	52.3	96.8	70	28
slab	0.020	12.0	15	61.1	193.2	110	43
slab	0.014	6.0	15	78.3	97.0	53	45
slab	0.014	6.0	25	68.1	54.6	38	30
slab	0.014	6.0	35	66.0	43.6	33	24

* interpolated values.

5.4. Generalisation of the variable retort temperature approach for the optimisation of the surface quality during the thermal processing of conductive heating foods

The method developed in the previous sections of this chapter for the determination of optimum variable retort temperature profiles maximising quality retention during sterilisation process has the disadvantage of using large computer facilities. The method is based on the approximation of the variable retort temperature profile by a set of linear pieces, so the dimension of the optimisation problem is directly related to the number of line pieces used. The reduction of the number of linear pieces allows the reduction of the complexity of the optimisation problem, as the number of variables to be optimised is reduced. However a minimum number of line pieces is necessary in order to define the VRT profiles, and the reduction of the number of line pieces cannot be performed indiscriminately.

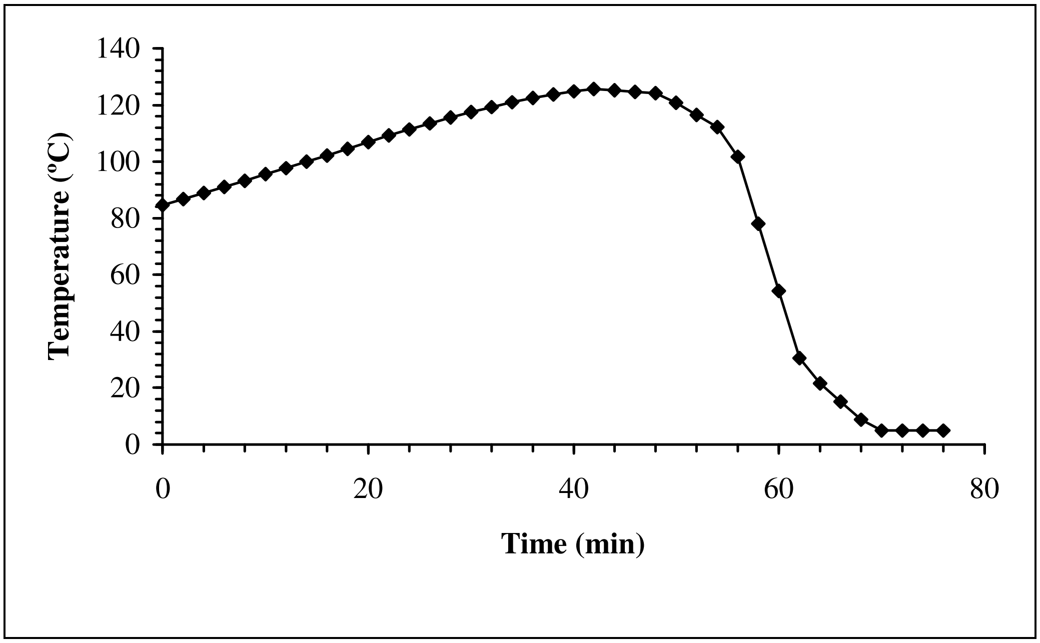

FIGURE 5.4 A typical variable retort temperature profile, showing the initial linear portion, followed from the fast cooling section.

To reduce the calculation efforts needed an attempt was made to develop an empirical equation able to describe the calculated optimum variable temperature profiles.

5.4.1. Development of an empirical equation for the description of the optimum VRT-profiles

The visual inspection of the calculated optimum VRT-profiles (approximately 100 cases) revealed that all the profiles presented a common set of characteristics. In all the optimal profiles we found (i) an initial rather slow, almost linear, increase of retort temperature from the initial retort temperature to a maximum process temperature, (ii) a relative short period close to the maximum temperature, and (iii) a rapid cooling of the heating medium so that the constraint on the final temperature in the centre of the product is respected (Fig. 5.4).

Using a trial and error approach the possibilities of several families of curves including polynomial, circular and exponential functions towards the description of the calculated VRT profiles were evaluated. Two simple equations (Eqs. 5.10 and 5.11) that could represent the principal characteristics of the calculated optimum VRT-profiles, were obtained,

$$T(t) = a_0 + a_1\, t - \exp(a_2\, t) \tag{5.10}$$

$$T(t) = a_0 + a_1\, t - a_3 \exp(a_2\, t) \tag{5.11}$$

When an appropriate low value for a_2 is considered the two proposed equations reduce to the equation of a straight line for small values of time. This agrees with the observed initial linear portion of the calculated VRT profiles. For longer times, the exponential term becomes predominant allowing to describe the fast cooling observed in the calculated optimum VRT profiles. The pre-exponential term a_3 in Eq. 5.11 increases the flexibility in fitting the optimum profiles. The only portion of the optimum VRT profiles which cannot be described by this equation is the constant cooling temperature at the end of the process but can be easily dealt with by considering a cut off value in the temperatures predicted by this equation, i.e. for temperatures below a given minimum retort temperature (*e.g.,* 15°C) this minimum value is considered.

In order to test the applicability of Eqs. 5.10 and 5.11 to describe the calculated optimum VRT-profiles, the parameters on these empirical equations that minimise the sum of squares between the calculated VRT-profiles and the profiles predicted by these empirical equations were estimated using the Levenberg-Marquardt method for non-linear regression (Myers, 1990). The points that define the constant final cooling temperature observed in the VRT-profiles were not considered in the non-linear regression, due to the reasons discussed above.

In Table 5.7 the statistics of the non-linear fitting of some selected VRT profiles using the two proposed equations are summarised. From the results presented it can be concluded that the four-parameter equation (Eq. 5.11) can describe accurately the considered optimum VRT profiles. In Fig. 5.5 the performance of the two considered equations in fitting the profiles is illustrated for two different case studies.

Based on the statistical data on Table 5.7 and on visual inspection of the fitted curves obtained, the four-parameter equation (Eq. 5.11) was chosen as a standard empirical equation for the subsequent description of the optimum VRT-profiles.

TABLE 5.7 Statistics of the non-linear fitting of some selected VRT profiles using Eqs. 5.10 and 5.11.

	$T(t) = a_0 + a_1\, t - a_3 \exp(a_2\, t)$				$T(t) = a_0 + a_1\, t - \exp(a_2\, t)$			
Case	R^2	Adjusted R^2	Std Error	F-statistic	R^2	Adjusted R^2	Std Error	F-statistic
1 a *	0.993	0.992	2.534	625.9	0.811	0.784	13.07	30.02
2	0.997	0.996	1.763	1369.0	0.822	0.797	13.01	32.34
3	0.997	0.996	1.819	969.1	0.904	0.887	9.306	52.04
4 b *	0.973	0.962	6.647	85.10	0.976	0.970	5.901	162.6
5	0.961	0.945	8.496	57.96	0.959	0.949	8.138	94.00
6	0.993	0.989	2.7916	264.61	0.936	0.918	7.6385	51.24
7	0.996	0.994	2.5321	505.42	0.897	0.867	12.172	30.43
8	0.999	0.998	1.0667	2559.4	0.975	0.969	5.0147	172.6
9	0.999	0.999	0.3730	18925	0.959	0.948	6.8617	82.34
10	0.997	0.996	1.8191	969.18	0.904	0.887	9.3064	52.04

* Cases a and b shown in Fig. 5.5

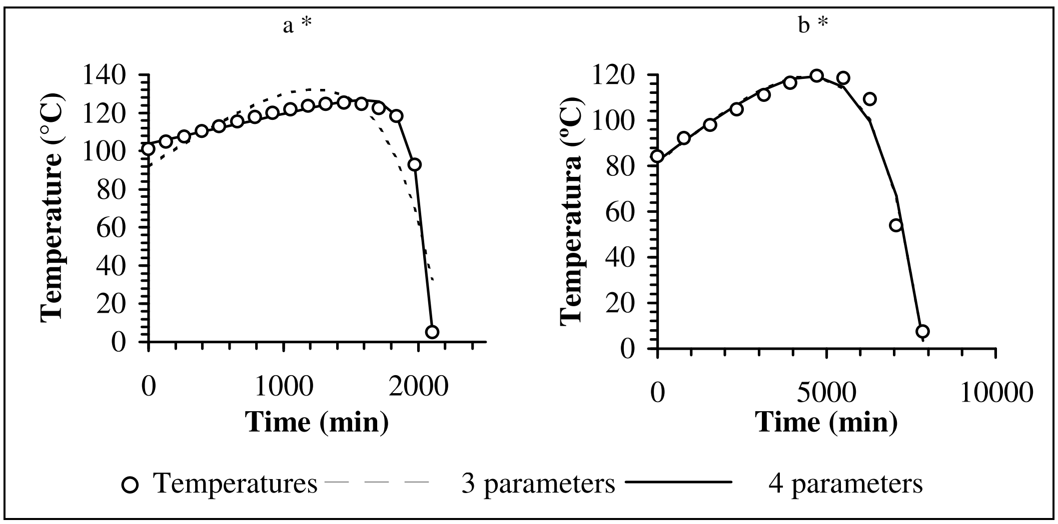

FIGURE 5.5 Non-linear fitting of selected VRT profiles using two different equations. 3 parameters - $T(t) = a_0 + a_1 \cdot t - \exp(a_2 \cdot t)$ and 4 parameters - $T(t) = a_0 + a_1 \cdot t - a_3 \cdot \exp(a_2 \cdot t)$. *a and *b are cases 1 and 4 in Table 5.7, respectively

5.4.2. Optimisation of the surface quality retention using VRT profiles defined using the developed equation

5.4.2.1. Formulation of the optimisation problem

According to the previous conclusions, the optimisation of the surface quality, for a fixed process time, using the VRT approach can be defined as the search of the parameters a_0 to a_3 in Eq. 5.11 that will minimise the surface quality degradation subjected to:

(i) A constraint in the final microbial sterility (Eq. 5.3)

(ii) A constraint in the final temperature at the centre of the product (Eq. 5.4)

5.4.2.2. Optimisation approach and algorithm

A computer program (Fig. 5.6) for the determination of the VRT (based on Eq. 5.11) profiles that minimise the surface quality degradation was developed.

For the determination of the parameters a_0 to a_3 in Eq. 5.11 that minimise the surface retention an optimisation method, the Complex method (Saguy 1983), was used. The Complex Method, is an optimisation method that evolves from the simplex method for unconstrained minimisation. The method is a sequential search technique which has been proved effective in solving problems with non-linear objective functions, subject to non-linear inequality constraints (Saguy 1983). The procedure tends to find the global extreme since the initial set of points is randomly scattered throughout the search region.

The complex method allows the incorporation of the constraints on final microbial sterility and final temperature at the centre of the product as implicit constraints. However the incorporation of the constraints as implicit constraints implies that the initial starting point for the optimisation is a feasible one, i.e., a point that complies with all the constraints. Due to the difficulties found in obtaining initial feasible starting points the constraints were incorporated by means of a penalty function (Eq. 5.7).

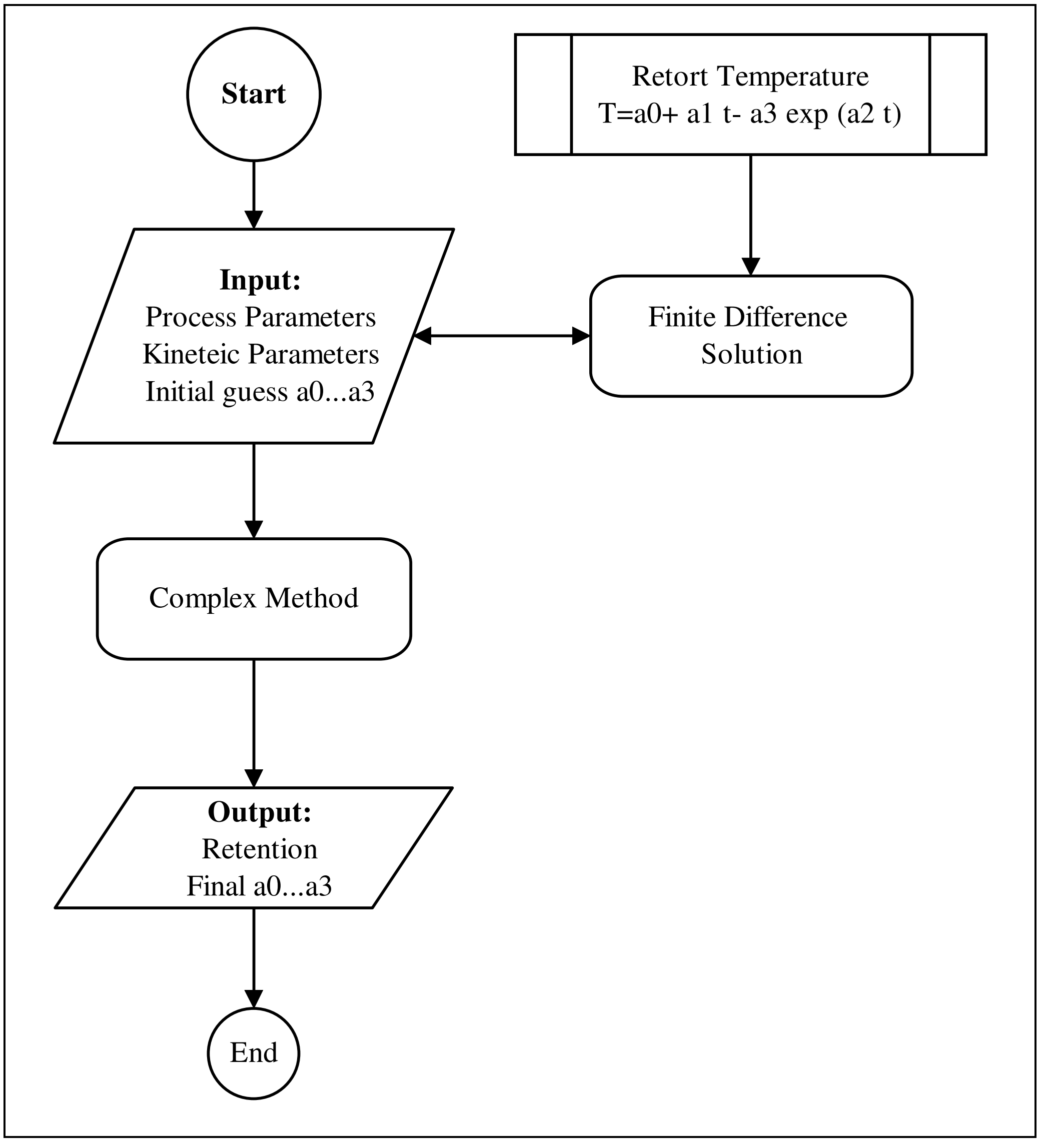

FIGURE 5.6 Flow diagram of the program used to calculate the parameters a_0 to a_3 in the empirical equation, $T(t) = a_0 + a_1\,t - a_3 \exp(a_2\,t)$, that maximise the surface retention.

5.4.3. Results and discussion

Eq. 5.11 was used for the calculation of some of the optimum VRT profiles calculated by the method described previously. It was found that after the optimisation of the 4 parameters of Eq. 5.11 it was possible to reach optimal surface retentions as high as those obtained using the previous, more time-consuming approach (Table 5.8). Moreover, when the profiles where compared in terms of the actual retort

TABLE 5.8 Comparison of the maximum surface retentions achieved using the line pieces approach and the 4 parameter equation for the description of the variable retort temperature profiles.

Geometry	R (m)	RF(E-04) (s^{-1})	F^t (min)	z_q (°C)	t_p (s)	RETS line pieces (%)	RETS 4 parameters (%)
Sphere	0.0100	6.00	6.0	30.0	1153	85.0	84.7
Sphere	0.0163	6.00	6.0	15.0	2173	87.0	87.3
Sphere	0.0327	1.50	9.0	30.0	4567	62.9	62.4
Cylinder	0.0250	2.60	6.0	25.0	4723	69.4	69.4
Cylinder	0.0250	2.60	12.0	30.0	7178	58.9	61.1
Cylinder	0.0394	9.95	16.0	25.0	10500	38.3	38.5
Slab	0.0200	4.00	6.0	15.0	11388	78.5	78.6
Slab	0.0140	8.16	6.0	35.0	3378	72.6	72.6
Slab	0.0200	4.00	12.0	35.0	5398	51.3	51.1

temperatures, a good agreement between the optimum profiles obtained by both optimisation schemes was observed.

The use of Eq. 5.11 reduces the number of parameters to be optimised to 4, allowing the reduction of the time necessary for the calculation of the optimum profiles.

In order to study the allowed tolerance in the optimised parameters a_0 to a_3 the same optimisation problem was run for 6 times with different initial guesses, and the optimum (minimum) C-values as well as the parameters calculated for each case (Table 5.9). It was found that it was possible to find in each case a minimum C-value, being all of the calculated C-values in a narrow range, around the optimum C-value calculated with the previous approach.

In Table 5.9 a large variability is observed for some of the calculated parameters (namely a_0 and a_2, in Eq. 5.11). This observed variability means that there is a region around the optimum profile where there is no large variation on the surface C-value, in other words there are a set of VRT profiles around the minimum that allow a quasi-optimum (minimum) C-value (Fig. 5.7), fact that in practical terms will mean that small variations around the calculated optimum VRT profiles will not lead to drastic reductions on the expected surface retentions.

TABLE 5.9 Variability observed in the determination of the optimum VRT profiles using Eq. 5.11

Run	Parameter			
	a_0	a_1	a_2	a_3
1	9.30E+01	1.20E-02	2.61E-03	-9.56E-04
2	8.46E+01	1.60E-02	2.24E-03	-5.38E-03
3	8.71E+01	1.45E-02	2.45E-03	-2.01E-03
4	9.10E+01	1.32E-02	2.49E-03	-1.77E-03
5	9.35E+01	1.22E-02	2.69E-03	-8.45E-04
6	8.08E+01	1.69E-02	2.49E-03	-1.84E-03
mean	8.83E+01	1.41E-02	2.50E-03	-2.13E-03
Standard deviation	5.06E+00	2.02E-03	1.54E-04	1.66E-03

Case Study - Infinite slab, α= 1.6E-07 m²/s, z_q =35°C, F^t =12 min, p_t = 5332 sec. In all the cases the same optimum surface retention (51%) was achieved.

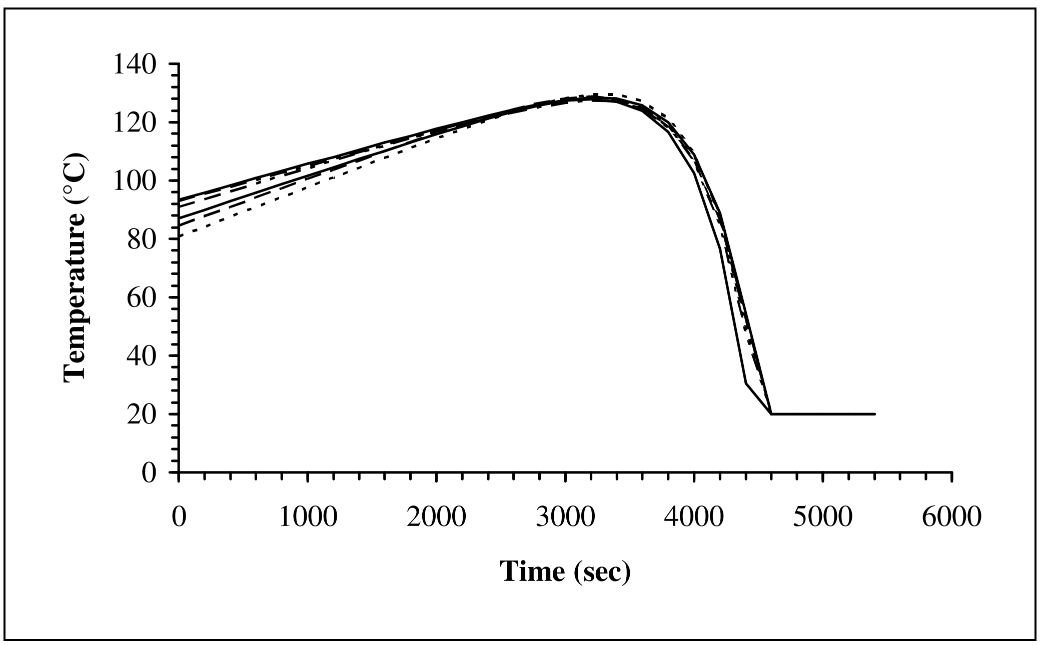

FIGURE 5.7 Variability observed in the calculation of the optimum VRT profiles using the four parameter equation. The different curves refer to the 6 cases reported in Table 5.9.
Case Study - Infinite slab, α= 1.6E-07 m²/s, z_q =35°C, F^t =12 min, p_t = 5332 sec. In all the cases the same optimum surface retention (51%) was achieved.

5.5. Conclusions

Optimal variable retort temperature profiles are a valuable policy for the optimisation of surface quality during the thermal processing of canned foods. Increases up to 20% in the surface quality can be achieved with VRT profiles in comparison with the optimal constant temperature profiles. When used for the minimisation of the process time VRT profiles allow decreases up to 45% in the process time while still providing the same surface quality of the correspondent CRT profiles.

The calculation effort necessary for the calculation of optimum VRT profiles could be reduced using an empirical equation able to describe accurately the VRT profiles. The equation was derived by analysing an extensive number of VRT profiles calculated for kinetic parameters for the quality factors and target lethality values covering the usual range of values found in practical situations.

Chapter 6. Simultaneous optimisation of surface quality during the sterilisation of foods using constant and variable retort temperature profiles

6.1. Introduction

In the previous chapters the optimisation of the surface quality retention for one single component using both the constant and variable retort temperature policies was considered. Here the possibilities of simultaneous optimisation of several surface quality factors will be considered.

As pointed out by Norback (1980) the maximisation of quality retention can only be done for one nutrient (or other quality attribute) during the process, since we can only optimise with respect to one objective function at a time. The optimum processing conditions for a single quality factor will depend on its inactivation kinetics (z_q value) (Silva *et al.* 1992a). However it is possible to reformulate the objective function in order to optimise more than one quality factor. The most straightforward approach is the maximisation of the sum of retentions of the considered quality attributes. A more elaborated approach would involve an evaluation of the relative importance of the different quality attributes (taking into account physical and chemical as well as sensory data) and the quantification of this information in terms of weight factors that would allow the construction of a well-balanced objective function.

The minimisation of the C-value has been used as a criterion when the minimisation of the degradation of a single quality factor is of interest (Ohlsson 1980d). For surface quality (single point), and taking into account that the cook value can be expressed as,

$$C = -D_{Tref,q} \log\left(\frac{N}{N_0}\right)$$

it is easily seen that the minimisation of the C-value is equivalent to the maximisation of the quality retention of a quality factor when a single component is considered, *i.e.*,

$$\min(C) \equiv \max\left(\frac{N}{N_0}\right)$$

When the maximisation of the quality retention for more than one component is of concern, the maximisation of the sum of the weighed retentions of the quality attributes is the criterion to be used. Considering the simple case of i components with the same relative importance, the objective function to be maximised can be formulated as,

$$\text{Objective Function} = \sum_i \frac{N^i}{N_0^i} \tag{6.1}$$

with $\dfrac{N^i}{N_0^i}$ representing the retention for the i[th] quality factor.

In this case the use of an objective function based on the sum of the cook values for each component,

$$\sum_i C_i = \sum_i -D_{T_{ref},q_i} \log\left(\frac{N^i}{N_0^i}\right) = \log \prod_i \left(\frac{N^i}{N_0^i}\right)^{-D_{T_{ref},q_i}} \tag{6.2}$$

would not lead to the minimisation of the objective function given by Eq. 6.1, but else, taken into account that,

$$\min \sum_i C_i \equiv \min \prod_i \left(\frac{N^i}{N_0^i}\right)^{-D_{T_{ref},q_i}} \tag{6.3}$$

to a product of retentions.

In the case where the simultaneous optimisation of different quality factors is of interest objective functions can not be formulated in terms of the sum of individual C values. They must be formulated considering sums of final retentions.

In order to investigate the possibilities of the simultaneous optimisation of surface quality for more than one quality factor, three case studies were considered. The first two case studies (System I and System II) refer to meals with three components in a single package. It is assumed that the components are separated inside the package thus presenting different heating rates (f_h-values). The third case study (System III) refer to a mixture of vegetables in a glass jar. In this case a single heat penetration rate is considered as the components are mixed.

These cases illustrate two situations found in the food industry: Convenient (microwavable) meals processed in retortable pouches where the different components are physically separated and vegetable mixes where the components are homogeneously mixed and packed in glass containers.

6.2. Material and methods

6.2.1. Modelling of temperature evolution

The calculation of the transient temperature history at the slowest heating point was performed using the APNS method, described in section 2.2.2.2. The surface temperature was considered to be equal to the heating medium temperature (infinite surface heat transfer coefficient).

6.2.2. Optimisation methods

For the optimisation of constant retort temperature profiles, the univariate search procedure of Davies-Swann-Campey (Saguy 1993) was used. For the determination of the optimum variable retort temperature profiles the method described in section (5.4.2.2.) was used.

6.2.3. Preparation of the vegetable mixture in glass jars

Commercially available frozen vegetables (frozen corn, broken green beans, peas and carrots slices) were used for the preparation of the vegetable mixture. The frozen vegetables were thawed in warm water for one minute. The excess of water was removed by letting the vegetables stand in a sieve for approximately one minute. The mixture was prepared by adding equal weights of the four vegetables. Glass Jars (600 ml; 127 mm x 40.5 mm; 2.6 mm average thickness, Carnaud-Giralt Laporta S.A., Spain) were filled with 400 g of the resulting mixture, 300 ml of distilled water were added to each glass jar. The glass jars were closed manually. Three glass jars were used per experimental run.

6.3. Results and discussion

6.3.1. System I (Chilli con Carne, White rice and Peach slices in syrup)

The parameters that characterise this system are presented in Table 6.1. The heating characteristics (f_h and j-values) refer to a meal-set consisting of 'chilli con carne', white rice and peach slices in syrup (Hayakawa *et al*. 1991). The z_q values chosen are in the range of z_q values normally found for quality factors.

Both for the individual and simultaneous optimisation of quality factors an initial homogeneous temperature of the product of 30°C was considered. The temperature of the cooling medium for the calculation of the optimum CRT profiles was considered to be 15°C. The products were processed until an F value of 7.5 min was reached in the cold spot of the slowest heating component. The cooling phase was extended until the temperature of the slowest cooling product reached 60°C. The duration of the process was defined as the sum of the heating and cooling phase. A reference temperature of 121.1°C was considered both for the calculation of the F and the C-values. The product temperature evolution was calculated independently for each of the components, using the APNS method, due to the different heat penetration rates.

In Table 6.2 and Table 6.3 the results of the optimisation for both constant retort temperature and variable retort temperature policies are presented considering the individual and simultaneous optimisation, respectively. The VRT profiles were calculated for the same process time as the time of the optimum CRT profile.

For the optimal CRT-profiles the comparison between the retentions observed for optimisation of the individual components (Table 6.2) and the retentions observed when the simultaneous optimisation of the three components is performed (Table 6.3) shows a sensible decrease in the final retentions for the latter. However it should be taken into account that we are comparing the results of the simultaneous optimisation with the best possible results for each of the components and that a reduction should be expected. It is observed that two of the components show final processing values at the cold spot largely exceeding the set target value of 7.5. This is due to the fact that in the definition of the optimisation problem, a constraint on the minimum processing value was set in the product with the slowest heating rate.

TABLE 6.1 Parameters used for the optimisation of the surface quality for a three-component system.

Component	f_h (min)	j_h	z_q (°C)	D_{Tref} (min)
1 peach slices	18.32	1.17	15.0	200.0
2 white rice	28.30	1.38	25.0	200.0
3 chilli con carne	26.49	1.43	35.0	200.0

TABLE 6.2 Results from the individual optimisation for case I. F_{target} = 7.5 min, T_{end} (target)= 60°C

			CRT		VRT	
Component	T_{opt} (°C)	t_p (min)	RETS (%)	C-value (min)	RETS (%)	C-value (min)
1 peach slices	112.2	95.2	77.6	22.1	81.7	17.6
2 white rice	115.6	82.6	61.6	42.1	69.2	32.0
3 chilli con carne	118.7	80.4	54.7	53.3	60.3	44.0
Average	-	-	64.2	39.6	70.4	31.2

TABLE 6.3 Results from the simultaneous optimisation for case I. F_{target} = 7.5 min, T_{end} (target)= 60°C

	CRT(114°C/109 min)			VRT_1 (109 mine)			VRT_2 (79 min)		
Comp	Fc (min)	RETS * (%)	C (min)	Fc (min)	RETS * (%)	C (min)	Fc (min)	RETS * (%)	C-value (min)
1	12.9	69.9(-9.9)	31.1	15.0	73.7(-9.8)	26.5	30.72	58.6(-28.3)	46.4
2	9.7	57.5(-6.7)	48.1	10.4	66.0(-4.6)	36.1	14.45	59.8(-13.6)	44.6
3	7.5	51.3(-6.2)	58.0	7.5	60.6(+0.5)	43.6	7.5	59.0(-2.2)	45.8
Avg.	-	59.5	45.8	-	66.8	35.4	-	59.2	45.6

* Between brackets are the relative lost in relation to the optimum individual values.
1 VRT profile for the same process time as the optimum CRT profile
2 VRT profile showing approximately the same average retention as the optimum CRT profile

The fact that components 1 and 2 show a faster rate of heat transfer (smaller f_h values) explains the high processing values observed at the end of the process when comparing to the much lower value observed for the third component, that shows a slower rate of heat transfer (larger f_h value).

The simultaneous optimisation of the three quality factors using the VRT policy allowed a substantial increase in the individual quality retentions (5.4%, 14.8% and 18.1% for components 1, 2 and 3 respectively) when comparing with the results obtained from the simultaneous optimisation using the CRT policy. When the results of the simultaneous optimisation are compared with the individual optimisation, in terms of the achieved individual retentions, a decrease is found on the individual surface retentions for two of the components and a slight increase for the third component. However a direct comparison between these results cannot be performed due to the differences in process time between the different processes.

When considering the possibilities of the VRT profiles as a mean to reduce the process time and allow comparison with the CRT approach, one can use two different criteria. One can calculate the minimum process time below which one of the components shows a retention smaller than the retention achieved using the CRT profile, or as a second criterion one can calculate the process time below which the average of retentions shows a smaller value than the average retention for the optimum CRT profile calculated considering the three components simultaneously (Table 6.3). Using the first criterion and interpolating (see Fig. 6.1) it is possible to conclude that for processes approximately below 5500 seconds (92 min) the retention of the component with a z_q value of 15°C will be smaller than 69.9% (retention obtained using the optimum CRT profile). This means that using this criterion the process time could be reduced from 6510 to 5500 seconds (109 to 92 min, i.e., a reduction of about 15%. If the second criterion is used, it is possible to reduce the process time from 6510 seconds (109 min) to about 4555 seconds (76 min) (what represents a 30% reduction on the process time) and still achieve average retentions larger than those obtained using the CRT approach. Further inspection of Fig. 6.1 shows that the quality factor more sensible to temperature changes (component 1) suffers from a larger reduction in surface retention when the process time is reduced. This is due to the increase on the overall temperature observed when the process time

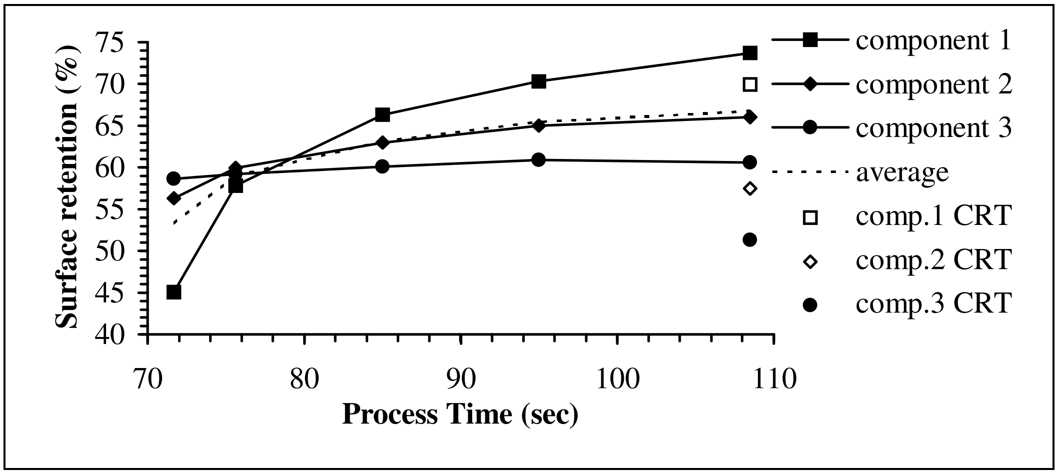

FIGURE 6.1 Graphical determination of the VRT profile that minimises the process time.

is decreased. Due to the constraint in the final target value at the centre of the container, a decrease in the process time will imply an increase on the heating medium temperature in order to comply with this constraint. So the component whose reaction rate of degradation is more sensible to changes on temperature will be the one showing a larger reduction on the surface quality with the reduction of the process time.

6.3.2. System II (Meat, potatoes and spinach)

The second system represents a meal-set consisting of three components. In Table 6.4 the parameters that characterise the system are given. The heating parameters are those of spinach, potatoes and meat in a pouch of 3 cm width. In all the considered simulations an initial homogeneous temperature of 40°C was assumed. The simulations were all performed considering a final lethality of 6.0 minutes. The cooling phase was extended until the temperature at the cold spot of the slowest heating component reached 60°C. The cooling medium temperature was set to 20°C for all the simulations.

TABLE 6.4 Parameters used for the optimisation of the surface quality for system II.

Component	f_h (min)	j	z_q (°C)	D_{Tref} (min)
1 meat	25.50	1.273	40.0	200.0
2 potatoes	28.20	1.273	30.0	200.0
3 spinach	32.80	1.273	20.0	200.0

TABLE 6.5 Results from the individual optimisation for case II.

Component	T_{opt} (°C)	t_p (min)	CRT RETS (%)	CRT C-value (min)	VRT RETS (%)	VRT C-value (min)
1 meat	120.3	63.2	63.1	40.0	68.2	33.2
2 potatoes	117.0	70.0	62.5	40.8	69.0	32.3
3 spinach	112.2	110.1	67.6	34.1	73.6	26.6
Average	-	-	64.4	38.3	70.3	30.7

TABLE 6.6 Results from the simultaneous for case II.

F_{target} = 6.0 min, T_{end} (target)= 60°C

	CRT(115.7°C/ 84 min)			VRT[1](84 min)			VRT[2] (63 min)		
Component	F_c (min)	RETS * (%)	C-value (min)	F_c (min)	RETS * (%)	C-value (min)	F_c (min)	RETS * (%)	C-value (min)
1 meat	8.7	56.3(-10.8)	50.0	9.7	62.8(-7.9)	40.4	14.7	61.8(-9.4)	41.8
2 potatoes	7.7	59.5(-4.8)	45.1	8.2	66.2(-4.1)	35.9	10.6	61.2(-11.3)	42.6
3 spinach	6.0	65.6(-3.0)	36.6	6.0	70.8(-3.8)	30.0	6.0	58.1(-21.1)	47.2
Average	-	60.4	43.9	-	66.6	35.4	-	60.4	43.8

* Between brackets are the relative lost in relation to the optimum individual values.
[1] VRT for the same process time as the optimum CRT profile
[2] VRT showing approximately the same average retention as the optimum CRT profile

In Tables 6.5 and 6.6 are the results for the optimisation of the surface quality using the constant and variable retort temperature profiles when the components are considered individually or simultaneously, respectively.

The individual surface retention values for the simultaneous optimisation (Table 6.6) show that in spite of the observed reduction of the quality for each of the quality factors the simultaneous optimisation was possible. It is worth to note that when the simultaneous optimisation is conducted using the VRT approach the individual surface retentions obtained (Table 6.6) are larger than the retentions obtained with the CRT approach when the surface quality is maximised individually (Table 6.5).

The use of a VRT profile allows a 25% reduction on the process time in relation to the optimum CRT profile without reductions in the average surface retention. The third component, with the lowest z_q value, is the one showing a larger decrease in surface quality when the process time is decreased.

6.3.3. System III - Mixture of four vegetables (green beans, peas, corn and carrots)

The third system consisted of a mixture of vegetables processed in glass jars. The mixture was prepared from individually frozen corn, broken green beans, peas and carrot slices. The heat penetration parameters were determined from a heat penetration run in water cascading mode (T_1=121°C, CUT=8 min). The APNS based method described in section 3.2.3. was used for the determination of the empirical heat penetration parameters. In Table 6.7 the heat penetration and kinetic parameters for this system are summarised. The kinetic parameters were taken from the literature (Villota and Hawkes 1986; Van Loey *et al*. 1994a)

In all the optimisations a final processing value of 6.0 min was targeted. The cooling water temperature was set at 15°C and the cooling phase extended until the temperature at the cold spot was below 60°C.

In this case study an objective function based on the sum of the average retentions for the different components is not appropriate due to large differences in the D values. This difference implies that the maximum RETS for the components will largely differ for the same F-target value.

TABLE 6.7 Parameters used for the optimisation of the surface quality for the vegetable mixture case.

Component	f_h (min)	j	z_q (°C)	D_{Tref} (min)
1 green beans	11.98	1.46	14.2	16.3
2 peas	11.98	1.46	32.0	61.0
3 corn	11.98	1.46	59.0	448.0
4 carrots	11.98	1.46	22.0	157.0

TABLE 6.8 Results from the individual optimisation for case III.

			CRT		VRT	
Component	T_{opt} (°C)	t_p (min)	RETS (%)	C-value (min)	RETS (%)	C-value (min)
1 green beans	112.2	70.8	12.0	15.0	19.0	11.8
2 peas	121.0	30.4	41.1	23.7	48.8	19.1
3 corn	129.4	22.4	89.5	21.6	90.7	18.8
4 carrots	117.3	39.0	72.4	22.0	77.7	17.2
Average	-	-	53.8	20.6	59.1	16.7

TABLE 6.9 Results from the simultaneous optimisation for case III.

F_{target} = 6.0 min, T_{end} (target)= 60°C

	CRT (115.5°C/46.7 min)		VRT[1] (46.7 min)		VRT[2] (26.7 min)	
Component	RETS (%)	C-value (min)	RETS (%)	C-value (min)	RETS (%)	C-value (min)
1 green beans	10.2(-15.0)	16.1	14.8(-22.1)	13.6	1.1(-94.2)	32.2
2 peas	36.4(-11.4)	26.9	47.8(-2.1)	19.7	47.0(-3.7)	20.2
3 corn	84.6(-5.5)	32.5	87.6(-3.4)	25.7	90.6(-0.1)	19.1
4 carrots	72.0(-0.6)	22.4	78.5(+1.3)	16.5	71.6(-7.9)	23.0
Average	50.8	24.5	57.2	18.9	52.6	23.6

* Between brackets are the relative lost in relation to the optimum individual values.
[1] VRT for the same process time as the optimum CRT profile
[2] VRT showing approximately the same average retention as the optimum CRT profile

In Table 6.8 the results of the optimal retentions achievable when the individual components are considered separately are presented. It can be seen that the first two components, with relatively lower D values, present an optimum surface retention much lower than the observed for the other two components (with much larger D values). If the simultaneous optimisation for the four parameters is performed using as a criterion the maximisation of the sum of the retention (as considered in system I and system II) the influence of the retention of component 1 (and 2 to a less extent) will be almost negligible and the optimum profiles obtained will be far from the optimum conditions for this component. The components more resistant to the heat destruction will be privileged in the optimisation. In order to avoid this fact a new objective function was considered that takes into account the relative heat sensitivity of the different components.

$$\text{Objective Function} = -\left(\sum_i \frac{RETS_i}{w_i} - P\right) \qquad (6.4)$$

where w_i are weighing factors chosen as the retentions achieved when the individual optimisation was performed, and P represents a penalty function (Eq. 5.7).

The weighing factors in the objective function (Eq. 6.4) have the role of transforming the contribution of each of the components into relative contributions based on the optimum (maximum) retentions possible to achieve for the component (the maximum retention when the component is considered individually). The optimum profiles calculated using this objective function will be profiles that minimise the sum of the deviations from the optimum conditions for each of the components.

The use of an optimised VRT (Table 6.9) profile allows the simultaneous optimisation of the quality retention without significant reductions on the individual retentions obtained when the quality retention for each of the components is maximised individually using the CRT approach.

A reduction from 46.7 min to 26.7 min in the process time , approximately 40%, is possible without reduction on the average quality observed in the optimum CRT profile. However with the reduction of the process time a dramatic decrease on the surface quality retention for component 1 is observed.

6.4. Conclusions

The simultaneous optimisation of more than one quality factor is possible. The main problem lies in a proper definition of the objective function to be optimised. While the most straightforward approach is to consider the optimisation of the sum of the surface retentions over the components, for practical optimisation problems the relative importance of the different components to be considered must be taken into account in the objective function by means of appropriate weighing factors.

The use of variable temperature profiles, allowed, as in the case of single quality factor, a decrease in the destruction of the quality factors during the sterilisation process when compared to the optimum constant retort temperature profile, and a decrease in the processing time without a reduction on the quality achieved using the constant retort temperature approach.

Optimisation using VRT profiles represent a valuable approach when the minimisation of quality degradation for more than one component is of interest. Using this approach it is possible to achieve in a single process surface retentions comparable (and sometimes slightly superior) to the maximum retentions possible with optimum CRT-profiles when the components are considered individually.

Chapter 7. Implementation of optimum variable retort temperature profiles

7.1. Introduction

In spite of the theoretical evidence that the use of variable retort temperature profiles can improve the surface quality retention and decrease the processing time during the heat sterilisation of foods, there are, to our best knowledge, no studies in available scientific literature on the practical implementation of such a kind of profiles.

In this chapter the possibilities of practical implementation of optimum variable retort temperature profiles in a pilot plant retort are investigated. Both the implementation of optimal VRT profiles for single and simultaneous optimisation of quality factors, as discussed in chapters 5 and 6 respectively, are considered in this chapter.

Three case studies are considered for the practical implementation of optimum variable retort temperature profiles: In the first study a model food system, a 5% bentonite suspension, was used and a hypothetical quality parameter with a z_q value of 25C° considered. In the second case study an actual food product, white beans, was considered. The maximisation of the quality appearance of white beans (z_q = 29.5 °C, Van Loey *et al*. 1994b) was taken as the optimisation criteria. In Table 7.2 a complete characterisation of the these two case studies is given. The third case study considered was the implementation of the optimum profiles for the simultaneous optimisation of the quality for four different components of the vegetable mixture discussed in section 6.3.3. For the three discussed cases both the optimum CRT and the correspondent VRT profiles that allow the maximisation of the quality retention and the minimisation of the process time were implemented.

7.2. Materials and methods

7.2.1. Preparation of the products

7.2.1.1. Bentonite suspensions in metal cans

Bentonite suspensions (5 %) were prepared as described in section 3.4.1.1.1. Three cans were used per experimental run.

7.2.1.2. White beans in glass jars

Glass jars filled with white beans were prepared as described in section 4.2.2.4. Three glass jars were used per experiment.

7.2.1.3. Vegetable mixture in glass jars

Glass jars with the vegetable mixture were prepared as described in section 6.2.3. Three glass jars were used per experiment.

7.2.2. Cold spot determination

Preliminary heat penetration tests were conducted for the determination of the slowest heating point. The determination of the cold spot was carried out by measuring the temperature evolution at different locations along the central axis of the container and selecting the cold spot as the point showing the slowest rate of heat penetration. For 5% bentonite suspensions the cold point was determined at 5 cm from the bottom of the can (the geometrical centre). For white beans in glass jars and for the vegetable mixture in glass jars the coldest point was located at 2 cm from the bottom of the jar. All subsequent temperature determinations were conducted at these locations.

7.2.3. Calculation of the optimum profiles

Optimal CRT profiles were determined using the Davies-Swann-Campey optimisation routine (Saguy 1983). For the calculation of the temperature evolution at the cold spot of the container the APNS method described in section (2.2.2.2.) was used. The method was used together with the empirical parameter, f_h and j_h, determined using the APNS based method described in section 3.2.3. As initial guesses the heating parameters determined using the graphical method described in section 3.2.1. were used.

Optimal VRT profiles for a fixed process time were calculated considering the method described in section (5.4.2.). The APNS method was used for the calculation of the temperature evolution under the variable retort temperature conditions. For the minimisation of the process time with a constraint in the quality level the search technique described in section 5.2.3.3. was used.

Surface cook-values were calculated using the general method. It was assumed that product temperature at the surface could be approximated by the heating medium temperature, i.e., the temperature gradient across the container wall discarded. This approximation was due as the APNS method used for the calculation of the centre temperature does not provide means for the calculation of the actual temperature at the surface.

7.2.4. Practical implementation of the optimum profiles

The optimum profiles were divided in a set of linear pieces in order to allow the programming of the retort controller. The obtained time-temperature pairs were used for the programming of the temperature evolution in the course of the sterilisation process. In Table 7.1 a typical example of a program use in the implementation of the VRT profiles is given.

7.2.5. Temperature measurement

For experiments with metal cans two thermocouples (see section 3.4.1.3.) were inserted in the can to allow to measure both the temperature in the coldest point and at a point in the product near to the surface (the tip of the thermocouple was placed as near as possible to the surface of the can without actually touching it). The ambient temperature was measured using copper-Constantan thermocouples (SSR-60020-G700-SF, Ellab, Denmark). For experiments with glass jars only the temperatures at the cold spot and the medium temperatures were collected. With the available thermocouples it was not feasible to measure the product temperature near to the surface of the glass jars.

TABLE 7.1 Program used for the implementation of an optimum variable retort temperature profile. Case study: Bentonite suspensions (5%) in metal cans processed in water cascading mode.

Step #	Medium #	Time * (min)	Temperature * (°C)	Pressure & (bar)
1	steam	0	40	0.5
2	steam	5	40	0.5
3	steam	0	85.8	1.5
4	steam	55	112	2.0
5	steam	10	116.1	2.0
6	steam	3.3	117.2	2.0
7	steam	5	118.4	2.0
8	steam	1.7	118.7	2.0
9	steam	1.7	119.0	2.0
10	steam	3.3	119.0	2.0
11	steam	1.7	118.8	2.0
12	steam	1.7	118.4	2.0
13	steam	3.3	116.8	2.0
14	steam	3.3	113.9	2.0
15	steam	3.3	109.2	2.0
16	water	3.3	101.7	2.0
17	water	3.3	90.4	1.6
18	water	3.3	73.8	0.5
19	water	60.0	ambient	

steam/water refer to the secondary heating/cooling medium, i.e., the fluid used to heat or cool the water that circulates in a closed circuit inside the retort.
* Duration of the time step. A programmed zero time means that the temperature programmed for the current time step will be reached as fast as possible. For a non-zero time the temperature will increase linearly during the programmed step from the temperature programmed for the previous step to the temperature programmed for the current step.
& A pressure profile is used to maintain container integrity by not allowing the build up of large pressure differences between the interior and exterior of the container

7.3. Results and discussion

The process parameters used for the calculation of the optimum CRT and VRT profiles for the 5% bentonite suspension processed in metal cans and for the white beans processed in metal jars can be found in Table 7.2. The process parameters and calculated optimum CRT and VRT profiles for the third case study, vegetable mixture in glass jar, can be found in section 6.3.3.

TABLE 7.2 Process parameters used for the calculation of the optimum profiles for 5% Bentonite suspension processed in glass jars and white beans processed in glass jars. Both processes in water cascading mode.

			Case 1 Bentonite 5%	Case 2 White Beans
Heat penetration data	f_h *	(min)	39.80	9.88
	j_h *		1.85	1.02
	T_0	(°C)	40.0	40.0
	T_c	(°C)	15.0	15.0
Kinetics Micro-organism	z_m	(C°)	10.0	10.0
	D_m	(min)	0.21	0.21
	$T_{ref,m}$	(°C)	121.1	121.1
Kinetics Quality Factor	z_q	(C°)	25.0 #	29.5 *
	D_q	(min)	178.6 #	53.61 *
	$T_{ref,q}$	(°C)	121.1	121.1
Constraints	F_t	(min)	5.0	5.0
	T_{end}	(°C)	60	60

Nadkarni and Hatton 1985; * Van Loey *et al*. 1994b.
* The heat penetration parameters were determined using the APNS based method described in section 3.2.3.

7.3.1. Bentonite processed in metal cans

The calculated optimum profiles for the 5% bentonite suspensions processed in metal cans are depicted in Fig. 7.1. In Table 7.3 the surface cook values and retentions for the calculated optimum profiles are presented. From these results it can be concluded that the use of the variable temperature approach would allow a 21% reduction of the surface cook value for the same process time as the optimum CRT profile or a reduction of 26% in the process time without losses on the surface quality. In Fig. 7.2 the results of the graphical optimisation for the determination the VRT profile that minimise the process time with a constraint in the surface quality profile (VRTa in Fig. 7.1) are presented.

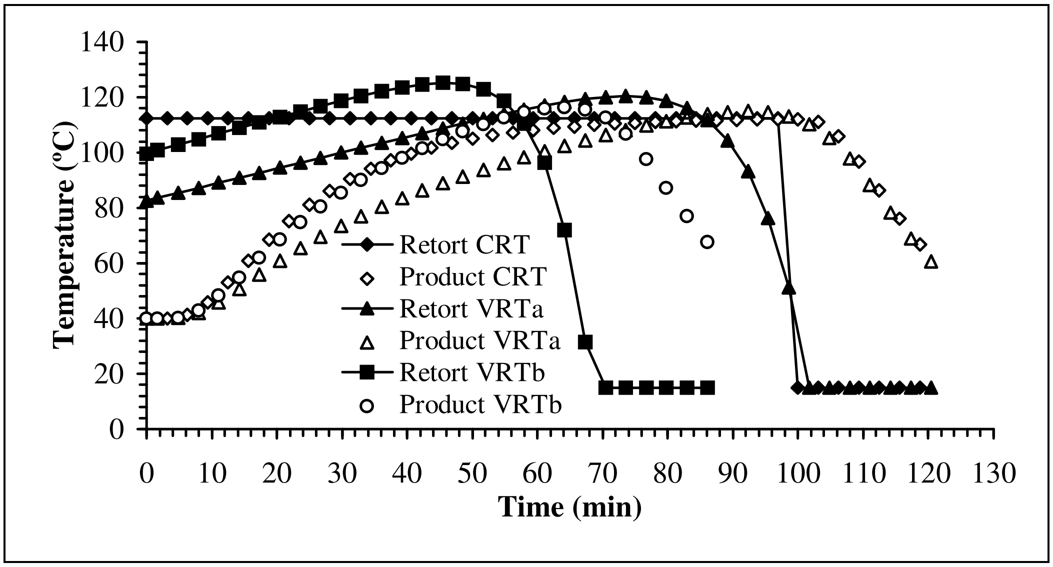

FIGURE 7.1 Calculated optimum CRT and VRT profiles and correspondent temperature evolution in the cold spot for the 5% bentonite suspensions processed in metal cans. VRT_a- Optimum VRT for the same process time as the CRT profile. VRT_b- VRT that minimises the process time.

TABLE 7.3 Surface cook values and retentions for the calculated optimum CRT and VRT profiles for 5% bentonite suspensions processed in metal cans

Profile	Process Time * (min)	F value (min)	Cook Value (min)	Retention (%)
CRT	121	5.0	44.0	56.7
VRT[a]	121	5.0	34.5	64.1
VRT[b]	89	5.0	43.8	56.8

* Including the cooling time.
[a] Optimum VRT profile for the same process time as the optimum CRT profile.
[b] VRT profile that shows the same retention as the optimum CRT profile

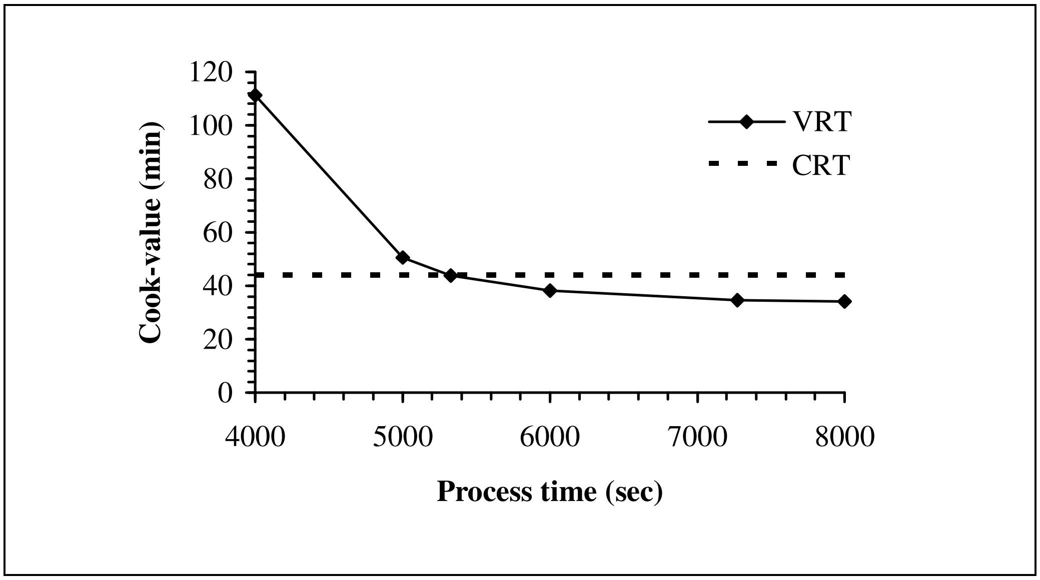

FIGURE 7.2 Surface cook value as a function of the process time. Graphical minimisation of the process time using the VRT approach for 5% bentonite suspensions processed in metal cans. The dotted line represents the Cook-value obtained for the optimum CRT profile, used as the constraint for the minimisation of the process time

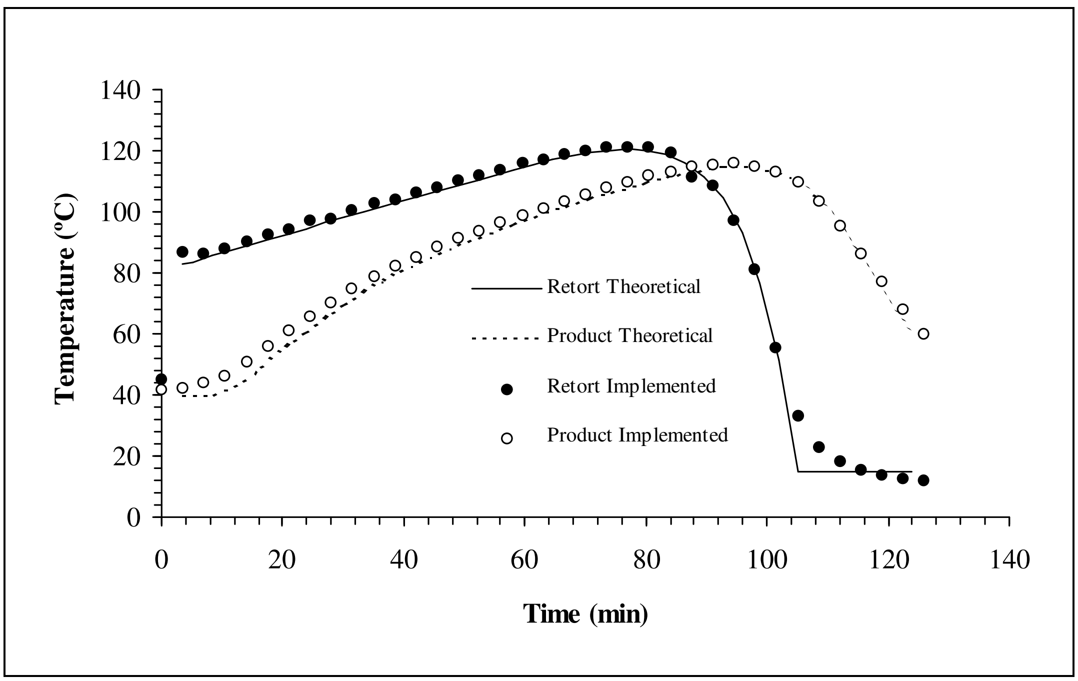

FIGURE 7.3 Theoretical optimum VRT profile with the same process time as the optimum CRT profile compared with the actual implemented profile. Case study: bentonite (5%) processed in metal cans. In this figure the theoretical profiles (both retort and product) were displaced in the time scale by the time taken in practice to achieve the initial calculated temperature for the optimum profile.

TABLE 7.4 Surface cook values and retentions for the implemented CRT and VRT profiles. Bentonite in can.

Profile	Process Time (min)	F_0 (min)	Retention * (%)	Cook-value * (min)	Retention # (%)	Cook-value # (min)
CRT	133	7.43	52.6	49.9	61.9	37.2
VRT[a]	129	6.28	61.2	38.1	69.3	28.4
VRT[b]	93	5.91	47.1	47.1	68.4	29.5

[a] Optimum VRT profile for the same process time as the optimum CRT profile.
[b] VRT profile that shows the same retention as the optimum CRT profile
* calculated based on the retort temperature; # calculated based on the measured surface temperature.

In Fig. 7.3 the implemented VRT profile with the same process time as the optimum CRT profile and correspondent product temperature profile for the 5% bentonite suspension processed in metal cans are compared with the correspondent optimum theoretical profiles. In Fig. 7.4 the same comparison in presented for the VRT profiles that allow the minimisation of the process time. From these figures it can be seen that, apart from the initial come-up-time necessary to achieve the programmed initial retort temperature (fact not taken into account in the calculation of the theoretical optimum profiles), a good agreement between the implemented and the calculated profiles could be achieved.

The results obtained when the optimal profiles were implemented in the pilot plant retort are presented in Table 7.4. From the observed differences between the surface retentions calculated from the measured temperatures at the internal surface of the can and the ones calculated from the ambient temperatures it is evident that the surface temperature is poorly estimated using the ambient temperature, i.e., the resistance of heat transfer through the can wall cannot be ignored, this fact is illustrated in Fig. 7.5 where the measured temperatures at the different locations are presented for one of the implemented optimum profiles. The high processing values obtained, larger than the expected 5.0 min, and the larger cook values calculated from the ambient temperature history, can be explained in one hand by the existence of a come-up-time in the implemented profiles not considered in the calculation of the optimum profiles an in the other hand by the fact that in the implemented profiles the retort temperature is slightly larger than the programmed temperatures, as it can be seen in Figs. 7.3 and 7.4.

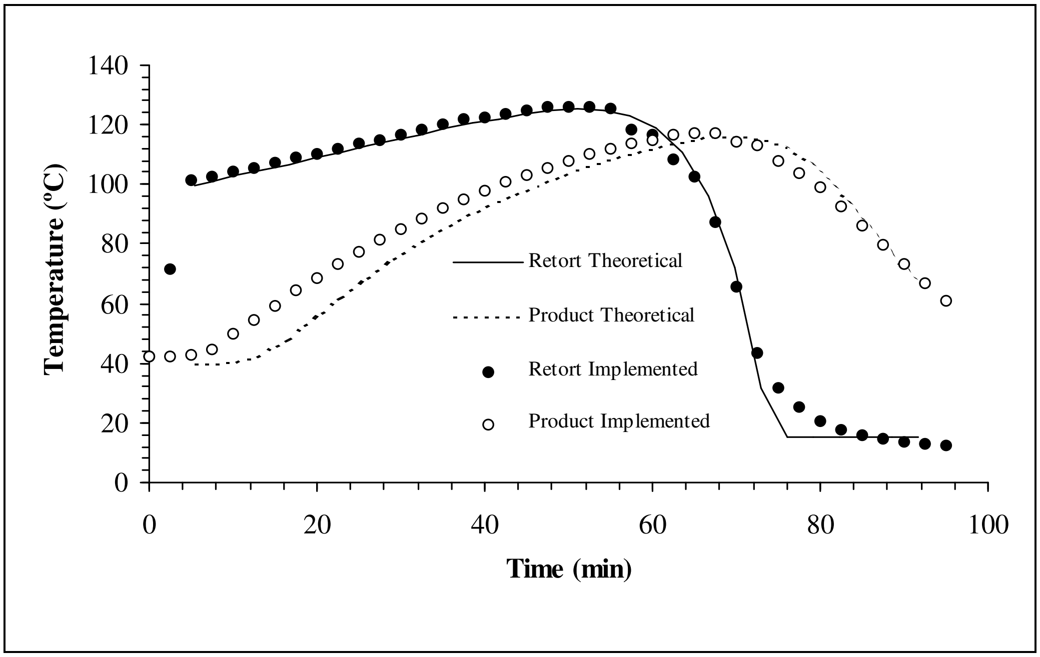

FIGURE 7.4 Theoretical VRT profile that minimises the process time with a constraint in the quality compared with the actual implemented profile. Case study Bentonite. Both the retort temperature and the temperature at the cold spot of the product are depicted. In this figure the theoretical profiles (both retort and product) were displaced in the time scale by the time taken in practice to achieve the initial calculated temperature for the optimum profile.

From the results in Table 7.4 it is apparent the use of a variable retort policy has some advantages over the use of constant retort temperature profiles. In one hand it was possible using an optimum variable retort temperature profile to increase the surface retention by 12%, when comparing the retentions calculated based on the measured surface temperatures, on the other hand it was possible to reduce the processing time of the optimum CRT profile by 30% without decreases in the surface quality retention. These results should not be considered in absolute terms but only as indicative of the possibilities of implementing optimum VRT profiles. The differences in processing value observed among the different processes does not allow for an absolute comparison in terms of achieved retentions.

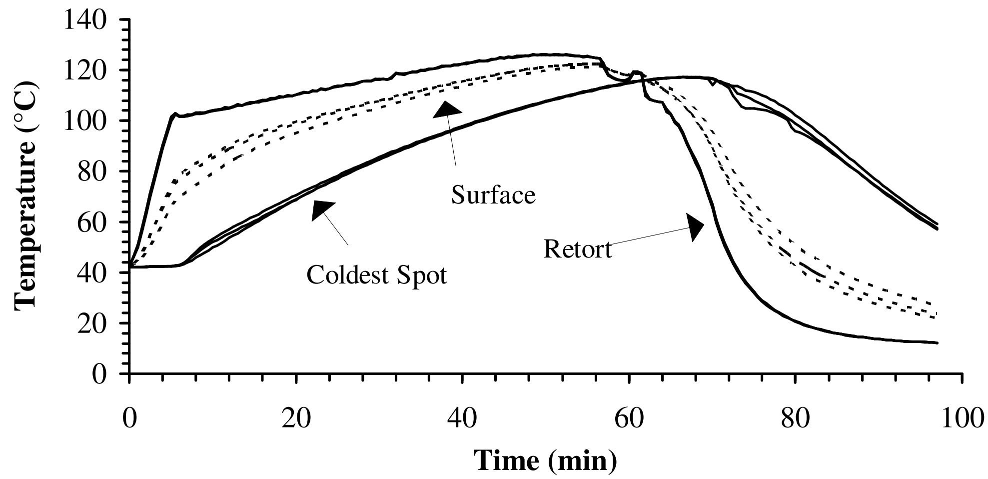

FIGURE 7.5 Measured experimental temperatures at the different locations, during the implementation of the optimal VRT profile that minimises the process time with a constraint on the surface quality retention. Case study: Bentonite processed in can. The results for three different cans processed simultaneously are presented.

TABLE 7.5 Surface cook values and retentions for the optimum CRT and VRT profiles. White beans processed in glass jars.

Profile	Process Time (min)	F_0 (min)	Cook Value (min)	Retention (%)
CRT	22.4	5.0	18.7	44.8
VRTa	22.4	5.0	14.6	53.4
VRTb	16.5	5.0	18.7	44.8

a- VRT profile with the same process time as the CRT profile
b-VRT profile with approximately the same retention as the optimum CRT profile

TABLE 7.6 Surface cook values and retentions for the implemented CRT and VRT profiles. White beans processed in glass jars.

Profile	Process Time (min)	F_0 (min)	Cook Value (min)	Retention (%)
CRT	42.5	10.4	21.8	39.2
VRT	35.5	6.9	16.0	50.2

7.3.2. White beans processed in glass jars

The optimal calculated profiles for the optimisation of the appearance of white beans processed in glass jars are show in Fig. 7.6, in Table 7.5 the correspondent optimal retentions and cook values are presented. The calculated optimum profiles show that the use of VRT profiles allows a significant reduction on the surface cook value (22%) and in the process time (26%) without reduction of the quality obtained using the more time consuming CRT approach.

In Fig. 7.7 the implemented optimum VRT profile for the same process time as the optimum CRT profile is compared with the theoretical VRT profile. In the heating phase, and by correcting for the time necessary for the retort to reach the programmed initial temperature, a good matching between the calculated and implemented retort profiles could be achieved. In the cooling region it was not possible to program the fast cooling observed in the calculated optimum profile due to the practical requirement of a slow cooling when processing products in glass jars in order to prevent the breaking of the containers due to thermal shock, this fact lead to implemented VRT profiles showing process times much larger than the calculated optimum profiles (Tables 7.5 and 7.6). The VRT profile that minimises the process time was not implemented as the calculated profile showed that processing temperatures above 130°C, the maximum allowed processing temperature with the available pilot plant steriliser, would be required.

The comparison of the cook values and retentions obtained for the implemented CRT and VRT profiles (Table 7.6), show that a reduction of the cook value (26%) could be achieved using the VRT policy. Here, due to the impossibility of measuring the temperature in the surface of the product, we only present cook values calculated from

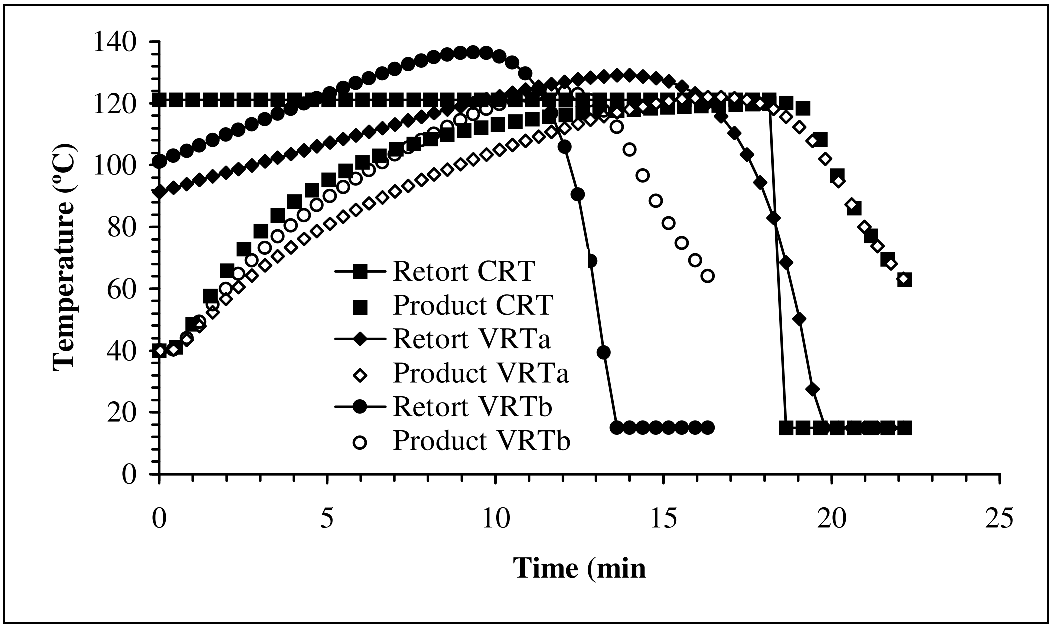

FIGURE 7.6 Calculated optimum CRT and VRT profiles and correspondent temperature evolution in the cold spot for the white beans processed in glass jars. VRTa- Optimum VRT for the same process time as the CRT profile. VRTb- VRT that minimises the process time.

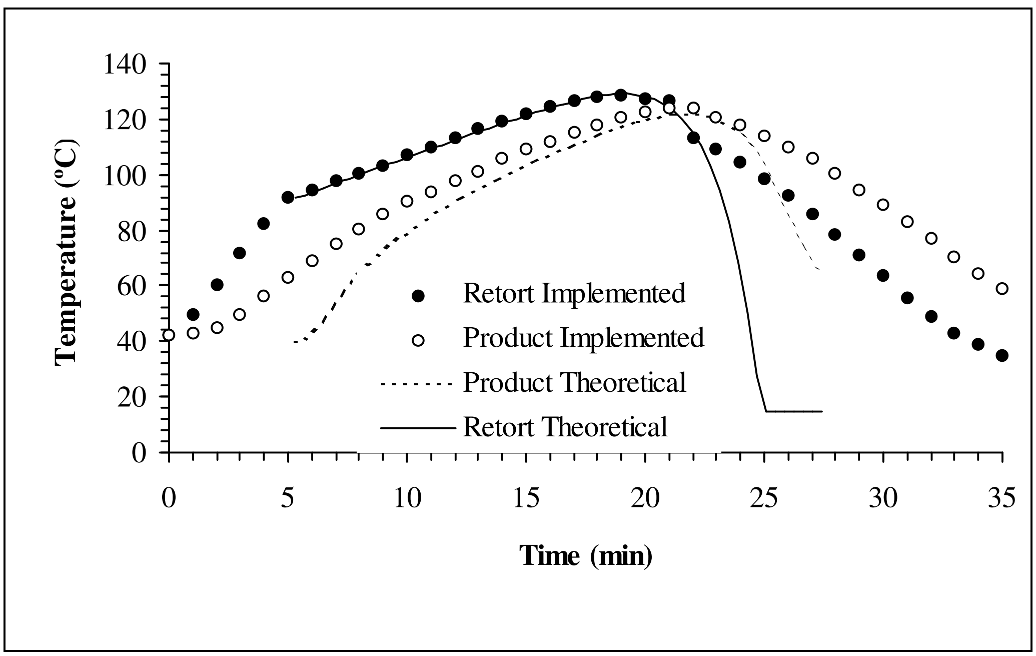

FIGURE 7.7 Theoretical optimum VRT profile with the same process time as the optimum CRT profile compared with the actual implemented profile. Case-study white beans in glass jars. Both the retort temperature and the temperature at the cold spot of the product are depicted. In this figure the theoretical profiles (both retort and product) were displaced in the time scale by the time taken in practice to achieve the initial calculated temperature for the optimum profile.

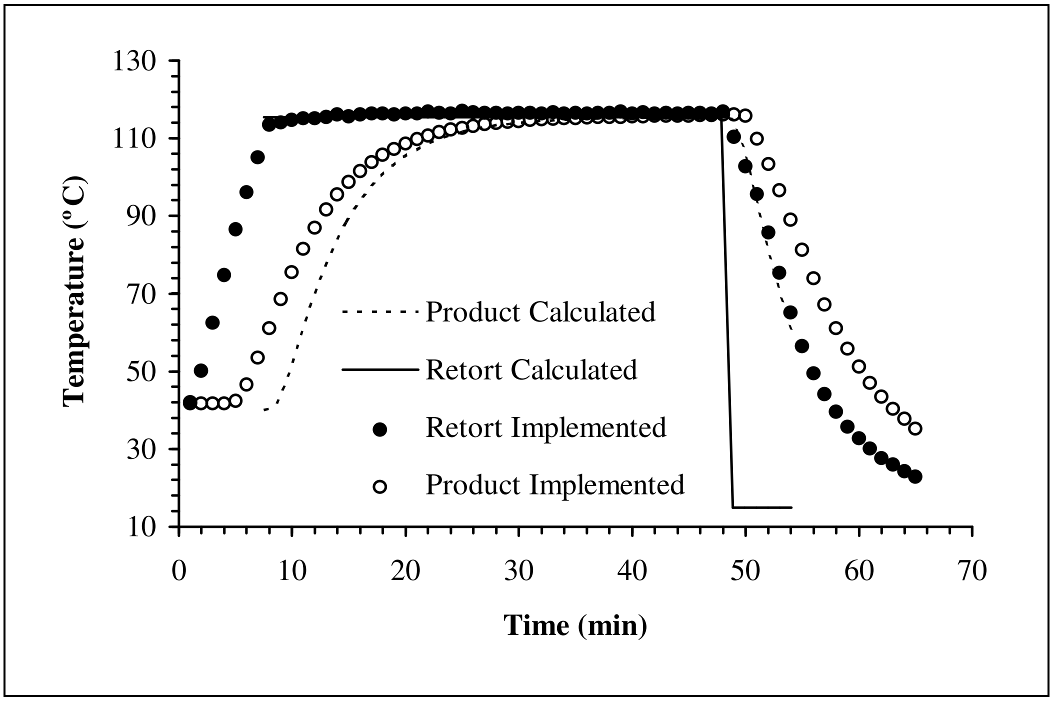

FIGURE 7.8 Implemented optimum CRT profile and experimental product temperature evolution compared with the theoretical calculated optimum CRT profile and associated product temperature. Case study: Vegetable mix. In this figure the theoretical profiles (both retort and product) were displaced in the time scale by the time taken in practice to achieve the calculated optimum processing temperature.

the ambient time-temperature history. These values should only be considered in relative terms, as the ambient temperature, from which the surface cook values and retentions were calculated, is not a good approximation of the temperature at the internal surface of the container due to the temperature gradient throughout the jar walls.

7.3.3. Vegetable mixture

In Figs. 7.8 and Fig. 7.9 the implemented retort temperature profiles and the correspondent product temperature responses are compared with the theoretically ones for the optimum constant retort temperature profile and for the optimum VRT profile for the same process time as the optimum CRT profile, respectively.

TABLE 7.7 Retentions achieved in the implementation of the optimum variable retort temperature profile for the simultaneous optimisation of four quality attributes in a mixture of vegetables.

component #		CRT Theor.	CRT Exp.	VRT_1 Theor.	VRT_1 Exp.	VRT_2 Theor.	VRT_2 Exp.
1	(%)	10.2	6.5	14.8	10.0	1.1	0.4
2	(%)	36.4	31.5	47.8	44.8	47.0	42.9
3	(%)	84.6	82.2	87.6	86.8	90.6	89.4
4	(%)	72.0	68.5	78.5	76.2	71.6	68.0
F_0	(min)	6.0	7.5	6.0	4.8	6.0	5.6
process time	(min)	46.7	57.5	46.7	60.3	26.7	32.8

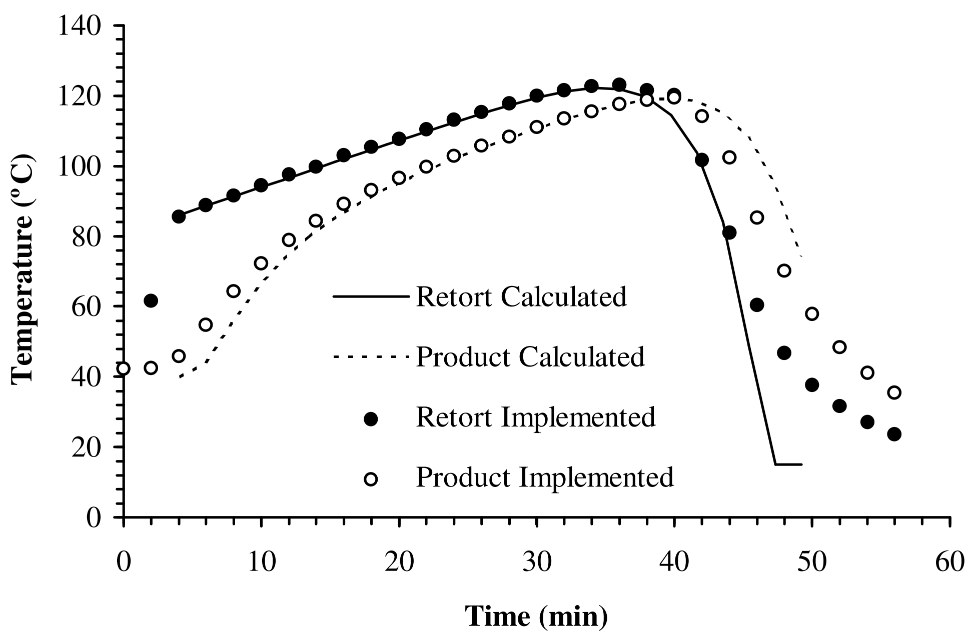

FIGURE 7.9 Theoretical optimum VRT profile with the same process time as the optimum CRT profile compared with the actual implemented profile and associated product temperature profiles. Case study: Vegetable mix. In this figure the theoretical profiles (both retort and product) were displaced in the time scale by the time taken in practice to achieve the initial calculated temperature for the optimum profile.

In Table 7.7 the retentions and processing values obtained for the three implemented profiles are presented and compared with the theoretically predicted results as calculated in section 6.3.3.

The fact that in the calculation of the optimum temperature profiles only one heating rate was considered, i.e. it was considered that the cooling rate (f_c-value) could be approximated by the heating rate (f_h-value) is the probable cause for the observed differences between the results expected from the calculated profiles and the results obtained from the experimental profiles.

7.4. Conclusions

When considering the practical implementation of optimal retort variable temperature profiles we can consider two different levels: The implementation of the profiles in pilot plant retorts and the use of this kind of profiles in industrial retorts.

The possibilities of implementation of optimal VRT profiles in a pilot plant retort were demonstrated in the present chapter. In spite of the problems associated with the presence of a come up period (not taken into account in the calculation of the optimum profiles) and the difficulties in controlling accurately the temperature in the cooling phase, it was possible to implement VRT profiles allowing increases in quality retention or decreases in processing time when compared to implemented constant retort temperature profiles.

Although it was possible to implement the variable retort temperature profiles in a pilot plant simulator, the implementation of this kind of profiles in industrial retorts will depend on the heat distribution characteristics of the retort. There is the need for a uniform heat distribution inside the retort for all the product to be subjected to the optimum variable retort temperature profile during the sterilisation process. The ability of maintaining a uniform temperature inside the retort while the temperature is changing with the time, accordingly to the calculated optimum profile, is the major constraint for the application of this kind of profiles in industrial retorts. In the pilot plant simulator used to carry out the experiments a good temperature distribution could be achieved, however when scaling-up for industrial sized retorts there are no guarantees of achieving an uniform temperature distribution, a case-by-case assessment of the temperature distribution inside the retort must by performed. The non-observance of a uniform temperature distribution will prevent the application of the VRT policy, as product at different locations in the retort would be subjected to different variable heating medium temperature profiles that will not necessarily be better than the more straightforward CRT approach.

Chapter 8. General Conclusions

In this thesis several issues relating to the design, evaluation and optimisation of quality during thermal processing of canned food have been addressed. In the first part of the thesis methods for the design and evaluation of thermal processes including the evaluation of deviations in the process have been proposed and validated for a range of food simulants. In the second part of the thesis the use of variable retort temperature control for the optimisation of surface quality has been investigated.

Design and evaluation of thermal processes including process deviations

A critical evaluation of the available methods for the design and evaluation of thermal processes was conducted, the possibilities and limitations of the presently available methodologies were discussed. The available methods allow the evaluation of thermal processes for constant heating and cooling medium temperature, however when the medium temperature changes with time the methods able to accommodate this change are only applicable to conduction heating foods. It was concluded that there is a need for simple and robust methods to the design and evaluation of thermal processes when the heating medium temperature changes with time applicable for other than pure conductive foods.

By combining the flexibility of numerical solutions of the conduction equation to handle variable heating medium temperature with the simplicity of the empirical description of heat transfer a new methodology for the design and evaluation of thermal processes was proposed: the APNS, Apparent Position Numerical Solution, method. This method allows the design and evaluation of thermal processes for conduction, convection and mixed mode heating foods subjected to a variable heating medium temperature, provided that the heat penetration curve of the product when plotted in log-linear co-ordinates can be described by a set of linear portions. The only parameters needed in this methodology are the empirical heat penetration parameters j and f_h calculated from a heat penetration curve plotted in a semi-log graph (or f_{h1} and f_{h2}, for the case of broken-heating curves).

An assessment of the method against theoretical solutions for conduction and perfectly mixed foods, showed that the proposed method could predict accurately the product temperature evolution when subjected to a variable heating medium temperature.

The nature of the proposed methodology makes necessary the use of empirical heat penetration parameters determined from heat penetration curves obtained under conditions of a step change in the heating medium temperature (no retort come up time). The fact that in batch type retorts there is a need to allow for a certain time to bring up the retort to the specified processing temperature makes impossible the direct measurement a heat penetration curves under the conditions required for the proper determination of the empirical parameters to be used with the proposed methodology.

In order to overcome this problem, a methodology was proposed for the determination of proper empirical heat penetration parameters from experimental data obtained when a come up time is present. It consisted of minimising the sum of the squared differences between the temperature profile predicted by the method for a certain experimental heating medium profile (boundary condition) and the experimental temperatures recorded at the coldest spot of the product when subjected to the same boundary conditions.

Using the parameters determined by the referred methodology, the method was tested for the evaluation of process deviations consisting of drops of the heating medium temperature. A good agreement between experimental and predicted temperatures could be found.

The proposed method for the evaluation of thermal processes was extended to handle broken-heating products. In order to accomplish this goal, the method was modified in such a way that it was possible to change the product heating rate at the moment the break (the change in the heating characteristics of the product) occurred. Means for the determination of appropriate heat penetration parameters from experimental data were also developed. The method was tested against experimental heating data for broken-heating products and a good agreement between experimental and predicted temperature could be found.

The method was used for the evaluation of a special type of process deviations consisting of drops in the rotational speed in processes which use rotation to increase the rates of heat transfer. A good agreement between experimental and predicted temperatures could be found. The type of experiments necessary for gathering heat penetration data for the determination of appropriate parameters to be used for the evaluation of this special case of process deviations will be dependent on the nature of the product.

Maximisation of surface quality retention

Variable retort temperature control was tested as a means of improving the surface quality retention during the thermal processing of conduction heating foods. Reductions up to 20% in the quality degradation and up to 45% in the process time could be theoretically predicted using VRT profiles.

A general formula able to describe the main characteristics of the optimum variable retort temperature profiles was developed. The use of such a formula allowed the reduction of the dimension of the optimisation problem allowing to reduce the calculation effort necessary for the calculation of optimum variable retort.

A theoretical assessment of the possibilities of using constant and variable retort profiles for the simultaneous optimisation of several quality indexes, showed that this was feasible. It was concluded that special care should be taken in formulating the objective function. For the simultaneous optimisation of quality factors the objective functions should be formulated in terms of maximising final retention and not, as in the case of single component optimisation, in terms of minimisation of cook values. The use of variable retort temperature profiles was shown to be particularly interesting for the simultaneous optimisation of more than one quality factor, as the final calculated retention compared well with the maximum retention achieved using individual calculated optimum constant retort temperature control for each of the components.

Experiments in a pilot water cascading retort showed that it was possible to implement the calculated optimum variable retort temperature profiles using the available technology. However in large systems is possible that non-homogeneous temperature distribution inside the system would prevent the successful application of such a kind of profiles.

Future work

During the development of the present work several themes for further research in the areas of design, evaluation and optimisation of thermal processing were identified:

- Need to determine clear quantitative relations between empirical heating parameters and product properties for cases other than pure conduction and perfectly mixing
- Study of the transferability of the empirical parameters for broken heating products between different processing conditions. Investigation and modelling of the mechanisms responsible for the break.
- Test the possibilities of practical implementation of calculated optimum variable retort profiles in commercially available equipment. Evaluate the possibilities of using this kind of approach taking into account the variability in product characteristics and the possibilities of control offered by the available equipment.
- Development of well balanced objective functions for the simultaneous optimisation of more than one quality factors that will take into account factors such as consumer acceptability of the product and energy consumption.

APPENDIX I - The Apparent Position Numerical Solution (APNS) method.

The empirical description of heat penetration curves using the empirical parameters f_h and j_h is given by the following equation,

$$\frac{T_1 - T(t)}{T_1 - T_0} = j_h 10^{-\frac{t}{f_h}}$$

On the other hand the analytical equation of Fourier's conduction equation for a sphere, initially at homogeneous temperature, subjected at time 0 to a step change in the surface temperature is given by,

$$\frac{T(r,t) - T_0}{T_1 - T_0} = \begin{cases} 1 + \dfrac{2R}{\pi r}\sum_{n=1}^{\infty}\dfrac{(-1)^n}{n}\sin\left(\dfrac{n\pi r}{R}\right)\exp\left(\dfrac{-n^2\pi^2\alpha t}{R^2}\right) & \text{for} \quad 0 < r < R \\ 1 + 2\sum_{n=1}^{\infty}(-1)^n \exp\left(\dfrac{-n^2\pi^2\alpha t}{R^2}\right) & \text{for} \quad r = 0 \end{cases}$$

For sufficiently large values of t, all terms in the above equation except the first will vanish. By comparison of the first approximation of the above equation with the empirical equation for the description of heat penetration, the following relationships are obtained,

$$f_h = 0.233\frac{R^2}{\alpha}$$

and,

$$j(r) = \begin{cases} 0.63662\dfrac{R}{r}\sin\left(\dfrac{\pi r}{R}\right) & \text{for } 0 < r < R \\ 2.0 & \text{for } r = 0 \end{cases}$$

Using the above equations it is possible to predict theoretically the f_h and j_h values for an heat penetration curve obtained in conditions of a step change in the surface temperature (i.e., no come up period) at any position of a conductive heating sphere of radius R and thermal diffusivity α. Inversely it is possible, for a given heat penetration curve characterised by a f_h and a j_h value, to calculate the thermal diffusivity and position inside a sphere of a given radius that will present the same heat penetration parameters. This constitutes the basic idea behind the APNS method.

In the APNS method the heat penetration parameters determined from heat penetration data are transformed in an apparent thermal difusivity and an apparent position inside a sphere using the discussed relationships. Using a finite-difference solution of the conduction equation for a sphere is then possible to calculate the temperature response at that point in the sphere to any variable external temperature evolution. The method combines the empirical description of heat penetration curves with the flexibility of numerical solutions to handle variable boundary conditions.

Bibliography

Anantheswaran, R.C. and Rao, M.A., 1985a. Heat transfer to model Newtonian liquid foods in cans during end-over-end rotation. Journal of Food Engineering, 4, 1-19.

Anantheswaran, R.C. and Rao, M.A., 1985b. Heat transfer to model non-Newtonian liquid foods in cans during end-over-end rotation. Journal of Food Engineering, 4, 21-35.

Anonymous, 1967. Calculation of thermal processes for canned foods. American Can Co., Research and Technical Dept., Maywood, IL, USA.

Ball, C.O., 1923. Thermal process time for canned foods. Bull. 37, Vol. 7, Part. 1. National Research council. Washington, D.C. USA.

Ball, C.O., 1928. Mathematical solutions of problems on thermal processing of canned food. Univ. of Cal. Pub. in Pub. Health 1, No. 2, 15-245.

Ball, C.O. and Olson, F.C.W., 1957. Sterilization in Food Technology. Theory Practice and Calculation. McGraw-Hill Book Co., New York.

Banga, J.R.; Perez-Martin, R.I.; Gallardo, J.M. and Casares, J.J., 1991. Optimisation of the thermal processing of conduction-heated foods: study of several objective functions. Journal of Food Engineering 14, 25-31.

Banga, J.R.; Alonso, A.A.; Gallardo, J.M. and Perez-Martin, R.J., 1993. Mathematical modelling and simulation of the thermal processing of anisotropic and non-homogeneous conduction heated canned foods: Application to canned tuna. Journal of Food Engineering, 18, 369-387.

Barreiro, J.A.; Guariguata, C. and Salas, G.R., 1984a. A manual method for predicting nutrient retention during thermal processing of conduction-heating foods in rectangular containers. Journal of Food Science, 49, 2, 478-481, 492.

Bera, F.; Deltour, J. and Deroanne, C., 1987. Mesure de l'importance relative des phénomenènes de conduction et de convection dans les transferts de chaleur lors de la sterilisation des boîtes de conserve. Lebensm.-Wiss. u.- Technol., 20, 1-7.

Berry, M.R., 1983. Prediction of come-up time correction factors for batch-type agitating and still retorts and the influence on thermal process calculations. Journal of Food Science, 48, 1293-1299.

Berry, M.R. and Bush, R.C., 1987. Establishing thermal processes for products with broken-heating curves from data taken at other retort and initial temperatures. Journal of Food Science, 52, 4, 958-961.

Bhowmik, S.R. and Tandon, S., 1987. A method for thermal evaluation of conduction heated foods in retortable pouches. Journal of Food Science, 52,1, 202-209.

Bhowmik, S.R. and Hayakawa, K., 1989. Quality retention and steam consumption of selected thermal processes. Lebensmittel Wissenshaft und Technologie, 21, 13-19.

Bichier, J.G. and Teixeira, A.A., 1993. Thermal processing of canned foods under mechanical agitation. HTD-Vol.254, Heat transfer in Food Processing, Editors: Karwe, M.V., Bergman, T.L. and Paolucci, S., Book No. G00811. The American Society of Mechanical Engineers.

Bigelow, W.D.; Bohart, G.S.; Richardson, A.C. and Ball, C.O., 1920. Heat penetration in processing canned foods. Bull. No 16-L, August, 1920. Research Laboratory. National Canners Association. Washington, D.C.

Bimbenet, J.J. and Duquenoy, A., 1974. Simulation mathématique de phénomenes intéressant les industries alimentaires. I. Transferts de chaleur au cours de la stérilisation. Industries Alimentaires et Agricoles, 4, 359-365.

Bimbenet, J.J. and Michiels, L., 1974. Convective heat transfer in caning process. Transferts de chaleur par convection au cours de la stérilisation des conserves. Proceedings. IV Int. Congress Food Science and Technology. Vol. IV, 361-379.

Bird, R.B., Stewart, W.E. and Lightfoot, E.N., 1960. Transport Phenomena, Wiley, New York.

Carnahan, B; Luther, H.A. and Wilkes, J.O., 1969. 'Applied Numerical Methods'. John Wiley & Sons, Inc., New York.

Carslaw, H.S. and Jaeger, J.C., 1959. 'Conduction of Heat in Solids'. Oxford University Press, London, UK.

Cass, G.V., 1947. A note on the use of Schultz and Olson lethal-rate paper for calculation of thermal processes for food products in tin containers. Food Research, 12, 24-26.

Chau, V. and Gaffney, J.J., 1990. A finite-difference model for heat and mass transfer in products with internal heat generation and transpiration. Journal of Food Science, 55, 2, 484-487.

Clark, J.P., 1978. Mathematical modelling in sterilisation processes. Food Technology, March, 1978, 73-75.

Clifcorn, L.E.; Peterson, G.T.; Boyd, J.M. and O' Neil, J.H., 1950. A new principle for agitating in processing of canned foods. Food Technology, 4, 11, 450-457.

Cohen, J.S. and Wall, M.A., 1971. A method of calculating average sterilizing value in cylindrical containers. Transactions of the ASAE, 14, 2, 329-333.

Datta, A.K., 1990. On the theoretical basis of the asymptotic semilogarithmic heat penetration curves used in food processing. Journal of Food Engineering, 12, 177-190.

Datta, A.K.; Teixeira, A.A. and Manson, J.E., 1986. Computer-based retort control logic for on-line correction of process deviations. Journal of Food Science, 51, 2, 480-483, 507.

Datta, A.K. and Teixeira, A.A., 1987. Numerical modelling of natural convection heating in canned liquid foods. Transactions of the ASAE, 30, 5, 1542-1551.

Datta, A.K. and Teixeira, A.A., 1988. Numerically predicted transient temperature and velocity profiles during natural convection heating of canned liquid foods. Journal of Food Science, 53,1, 191-195.

De Baerdemaeker, J.; Singh, R.P. and Segerlind, L.J., 1977. Modelling heat transfer in foods using the finite-elements method. Journal of Food Engineering, 1, 37-50.

De Cordt, S., 1994. Feasibility of development of protein-based time-temperature-integrators for heat process evaluation. Doctoral dissertation Nr. 254, Faculty of Agricultural and Applied Biological Sciences, K.U. Leuven, Belgium.

De Cordt, S.; Hendrickx, M.; Maesmans, G. and Tobback, P., 1992. Immobilized α-amylase from Bacillus licheniformis: a potential enzymic time-temperature integrator for thermal processing. International Journal of Food Science and Technology, 27, 661-673.

Dobie, P.A.P., Tucker, G.S. and Williams, A., 1994. The use of the 'CTemp' model to assess the effects of process deviations in reel and spiral cooker coolers.

Technical Memorandum, No. 697, Campden Food and Drink Research Association, January 1994.

Dorn, W.S. and McCracken, D.D., 1972. 'Numerical Methods with FORTRAN IV Case Studies'. John Wiley & Sons, Inc. New York.

Downes, T.W. and Hayakawa, K., 1977. A procedure for estimating the retention of components of thermally conductive processed foods. Lebensmittel Wissenshaft und Technologie, 10, 256-259.

Engelman, M.S. and Sani, R.L., 1983. Finite-elements simulation of an in-package pasteurization process. Numerical Heat Transfer, 6, 41-54.

Esty, J.R. and Meyer, K.F., 1922. The heat resistance of the spores of B. Botulinum and allied anaerobes. Journal of Infectious Diseases, 34, 1, 650-663.

Fagerson, I.S. and Esselen Jr., W.B., 1950. Heat transfer in commercial glass containers during thermal processing. Food Technology, 4, 411-415.

Flambert, F. and Deltour, J., 1972. Exact lethality calculation for sterilizing process. I. Principles of the method. Lebensmittel Wissenshaft und Technologie, 5, 2, 72-73.

George, R.M., 1990. A literature survey of thermal diffusivity of food products. TechniCal Bulletin No. 73, Campden Food & Drink Research Association, Chipping Campden, Gloucestershire, UK.

Gill, T.A., Thompson, J.W. and LeBlank, G., 1989. Computerized control strategies for a steam retort. Journal of Food Engineering, 10,135-154.

Gillespy, T.G., 1951. Estimation of sterilising values of processes as applied to canned foods. I. Packs heating by conduction. J. Sci. Food Agric., 2, March, 1951, 107-125.

Gillespy, T.G., 1953. Estimation of sterilising values of processes as applied to canned foods. II. Packs heating by conduction: complex processing conditions and the value of coming-up time of retort. J. Sci. Food Agric., 4, December, 1953, 553-565.

Goldblith, S.A.; Joslyn, M.A. and Nickerson, J.T.R., 1961. 'An Introduction to the Thermal Processing of Foods', The Avi Publishing Company, Inc. Westport, Connecticut.

Griffin, R.C.; Herndon, D.H. and Ball, C.O., 1969. Use of computer-derived tables to calculate sterilizing processes for packaged foods. 2. Application to broken-line heating curves. Food Technology, 23, 519-523.

Griffin, R.C.; Herndon, D.H. and Ball, C.O., 1971. Use of computer-derived tables to calculate sterilizing processes for packaged foods. 3. Application to cooling curves. Food Technology, 25, 134-143.

Hayakawa, K., 1968. A procedure for calculating sterilizing value of a thermal process. Food Technology 22, 905-907.

Hayakawa, K., 1969. Estimating the central temperature of canned food during the initial heating and cooling period of heat process. Food Technology, 23, 1473-1477.

Hayakawa, K., 1970. Experimental formulas for accurate estimation of transient temperature of food and their application to thermal process evaluation. Food Technology 24, 1407-1418.

Hayakawa, K., 1971. Estimating food temperatures during various processing or handling treatments. Journal of Food Science. 36, 378-385.

Hayakawa, K., 1973. Modified lethal rate paper technique for thermal process evaluation. J. Inst. Can. Sci. Technol. Aliment., 6, 4, 295-297.

Hayakawa, K., 1977a. Mathematical methods for estimating proper thermal processes and their computer implementation in 'Advances in Food Research', vol. 23, 75, Academic Press, New York.

Hayakawa, K., 1977b. Review on computerized prediction of nutrients in thermally processed canned foods. Journal of the AOAC, 60, 6, 1243-1247.

Hayakawa, K., 1978. A critical review of mathematical procedures for determining proper heat sterilisation processes. Food Technology, 32, 3, 59-65.

Hayakawa, K., 1982. Empirical formulae for estimating non-linear survivor curves of thermally vulnerable factors. Canadian Institute of Food Science and Technology. Journal. 15, 2, 116-119.

Hayakawa, K. and Ball, C.O., 1971. Theoretical formulas for temperature in cans of solid food and evaluating various heating process. Journal of Food Science 36:299-306.

Hayakawa, K. and Timbers, G.E., 1977. Influence of heat treatment on the quality of vegetables: changes in visual green colour. Journal of Food Science, 42, 2, 778-781.

Hayakawa, K.; Wang, J. and Gilbert, S.G., 1991. Simultaneous heat processing of high and low acid foods in semirigid containers - A theoretical analysis. Journal of Food Science, 56, 6, 1714-1717.

Hendrickx, M; Van Genechten, K. and Tobback, P., 1990. Optimizing quality attributes of conduction heated foods, a simulation approach. In Engineering and Food :Preservation Processes and Related Techniques, vol. 2, Ed. Spess, W.E.L. and Shubert, H., Elsevier Applied Science, London, New-York, 167-176.

Hendrickx, M.; Silva, C.; Oliveira, F. and Tobback, P., 1991a. Generalized (semi)-empirical formulas for optimal sterilization temperatures of conduction heated foods with infinite surface heat transfer coefficients. Journal of Food Engineering, in press.

Hendrickx, M.; Silva, C.; Oliveira, F. and Tobback, P., 1991b. Optimal sterilization temperatures as a function of processing variables for conduction heated foods. Poster presented at the 8th World Congress of Food Science and Technology, September 29-October 4, Toronto, Canada.

Hendrickx, M.; Silva, C.; Oliveira, F. and Tobback, P., 1991c. Optimizing thermal processes of conduction heated foods: generalized equations for optimal processing temperatures. Paper presented at 'Food Engineering in a Computer Climate Design and Control in Food Production Processes'. March 30 - April 1, St. John's College, Cambridge, UK.

Hendrickx, M.; Weng, Z.; Maesmans, G. and Tobback, P., 1992a. Validation of a time-temperature-integrator for thermal processing of food under pasteurization conditions. International Journal of Food Science and Technology, 27, 21-31.

Hendrickx, M.E.; Silva, C.L.; Oliveira, F.A. and Tobback, P., 1992b. Optimization of heat transfer in thermal processing of conduction heated foods. In 'Advances in Food Engineering', Ed. Singh, R.P and Wirakartakusumah, A., CRC Press, Florida, USA.

Hendrickx, M.; Maesmans, G., De Cordt, S.; Noronha, J.; Van Loey, A. and Tobback, P., 1995. The evaluation of the integrated time-temperature effect in thermal processing of foods. Critical Reviews in Food Science and Nutrition, 35, 1. In press.

Herndon, D.H.; Griffin Jr., R.C.; Ball, C.O., 1968. Use of computer-derived tables to calculate sterilizing processes for packaged foods. Food Technology, 22, 4, 473-478, 480, 482, 484.

Hiddink, J., 1975. Natural convection heating of liquids, with reference to sterilization of canned food. Doctoral Thesis. Center for Agricultural Publishing and Documentation. Wageningen, The Nederlands.

Holdsworth, S.D., 1985, Optimisation of thermal processing - a review. Journal of Food Engineering, 4, 89-116.

Jakobsen, F., 1954. Notes on process evaluation. Food Research, 19, 66-79.

Javier, R.A.; Naveh, D.; Perlstein, T. and Kopelman, I.J., 1985. Convective heating rate parameters of model solutions in an agitating retort simulator. Lebensmittel Wissenshaft und Technologie, 18, 311-315.

Jen, Y., Manson, J.E., Stumbo, C.R., and Zahradnik, J.W., 1971. A procedure for estimating sterilization and quality factor degradation in thermally processed foods. Journal of Food Science 36, 692-698.

Kao, J.; Naveh, D.; Kopelman, I.J. and Pflug, I.J., 1981. Thermal process calculations for different z and j_c-values using a hand-held calculator. Journal of Food Science, 47, 1, 193-197.

Kopelman, I.J.; Naveh, D. and Pflug, I.J., 1982. Overshooting of thermal processes due to temperature distribution at steam-off. Journal of Food Technology, 17, 441-449.

Kumar, A.; Bhattacharya, M. and Blaylock, J., 1990. Numerical simulation of natural convection heating of canned thick viscous liquid food products. Journal of Food Science, 55, 5, 1403-1411 & 1420.

Larkin, J.W. and Berry, M.R., 1991. Estimating cooling process lethality for different cooling j-values. Journal of Food Science, 56, 4, 1063-1067.

Lekwauwa, A.N. and Hayakawa, K., 1986. Computerized model for the prediction of thermal responses of packaged solid-liquid food mixture undergoing thermal processes. Journal of Food. Science. 51, 4, 1042-1049, 1056.

Lenz, M.K. and Lund, D.B., 1977a. The lethality-Fourier number method: Experimental verification of a model for calculating temperature profiles and lethality in conduction-heating canned foods. Journal of Food Science, 42, 4, 989-996, 1001.

Lenz, M.K. and Lund, D.B., 1977b. The lethality-Fourier number method: Experimental verification of a model for calculating average quality factor retention in conduction-heating canned foods. Journal of Food Science, 42, 4, 997-1001.

Leonhardt, G.F., 1978. A general lethal-paper for the graphical calculation of processing times- A research note. Journal of Food Science, 43, 660.

Lopez, A., 1987. ‘A Complete Course in Canning and Related Processes’ 12th ed. The Canning Trade Inc., Baltimore, MD, USA.

Lund, D.B., 1975. Heat Processing. In ‘Principles of Food Science. Part II - Physical Principles of Food Preservation’; Ed. Karel, M; Fennema, O.R. and Lund, D.B., Marcel Dekker, Inc., New York.

Lund, D.B., 1977. Design of thermal processes for maximizing nutrient retention. Food Technology, 31, 2, 71-78.

Lund, D.B., 1982, Applications of optimization in heat processing. Food Technology, 36, 7, 97-100.

Lynt, R.K., Solomon, H.M., Lilly, T. and Kautter, D.A., 1977. Thermal death time of Clostridium botulinum type E in meat of the blue crab. Journal of Food Science, 42, 4, 1022-1025, 1037.

Maesmans, G., 1993. Possibilities and limitations of thermal process evaluation techniques based on time-temperature integrators. Doctoral dissertation Nr. 240, K. U. Leuven, Belgium.

Maesmans, G., Hendrickx, M., Zhijun Weng, Keteleer, A. and Tobback, P., 1990. Endpoint definition, determination and evaluation of thermal processes in food preservation. Belgian Journal of Food Chemistry and Biotechnology, 45, 5, 179-192.

Maesmans, G.; Hendrickx, M.; De Cordt, S. and Tobback, P., 1993. Theoretical considerations on design of multicomponent time-temperature integrators in evaluation of thermal processes. Journal of Food Processing and Preservation 17, 369-389.

Manji, B. and Van De Voort, F.R., 1985. Comparison of two models for process holding time calculations: Convection system. Journal of Food Protection, 48, 4, 359-363.

Manson, J.E., 1991. Limitations and pitfalls in the use of different calculation methods - Numerical Methods. Tech Knowledge, Bulletin #200, Metaire, LA, USA.

Manson, J.E., 1992. A new approach to determining product heating factors from heat penetration data. Tech Knowledge, Bulletin #201, Metaire, LA, USA.

Manson, J.E.; Zahradnik, J.W. and Stumbo, C.R., 1970. Evaluation of lethality and nutrient retention in conduction-heating foods in rectangular containers. Food Technology, 24, 11, 109-113.

Martens, T., 1980. Mathematical Model of Heat Processing in Flat Containers. Ph.D. Thesis, Catholic University of Leuven, Belgium.

McGinnis, D.S., 1986. Prediction of transient conduction heat transfer in foods packaged in flexible retort pouches. Canadian Institute Food Science and Technology Journal, 19, 4, 148-157.

Merson, R.L., Singh, R.P. and Carroad, P.A., 1978. An evaluation of Ball's formula method of thermal process calculations. Food Technology, 32, 3, 66-72.

Moats, W.A.; Dabbah, R. and Edwards, V.M., 1971. Interpretation of non logarithmic survivor curves of heated bacteria. Journal of Food Science, 36, 3, 523-526.

Mulley, E.A.; Stumbo, C.R. and Hunting, W.N., 1975. Thiamin: A chemical index of the sterilization efficacy of thermal processing. Journal of Food Science, 40, 993-996.

Myers, G.E., 1971. Analytical methods in conduction heat transfer. McGraw-Hill Book Company, New York.

Myers, R.H., 1990. Classical and modern regression with applications. 2nd Ed. PWS-KENT Publishing Company, Boston, USA.

Nadkarni, N.M. and Hatton, T.A., 1985. Optimal nutrient retention during the thermal processing of conduction-heated canned foods: Application of the distributed minimum principle. Journal of Food Science, 50, 1312-1321.

NAG (Numerical Algorithms Group), 1983. E04JBF- NAG FORTRAN Library Routine Document, Mark, 11, Oxford, UK.

Naveh, D.; Kopelman, I.J.; Zechman, L. and Pflug, I.J., 1983. Transient cooling of conduction heating products during sterilisation: Temperature histories. Journal of Food Processing and Preservation, 7, 259-273.

Naveh, D.; Pflug, I.J. and Kopelman, I.J., 1984. Sterilization of food in container with an end flat against a retort bottom: Numerical analysis and experimental measurements. Journal of Food Science, 49, 461-467.

Nicolaï, B.M. and De Baerdemaeker, J., 1992. Simulation of heat transfer on foods with stochastic initial and boundary conditions. Trans. IChemE, Vol. 70, part C, June 1992. 78-82.

Nicolaï, B., 1984. Modeling and uncertainty propagation analysis of thermal food processes. Doctoral dissertation Nr. 264, Faculty of Agriculture and Applied Biological Sciences, K. U. Leuven, Belgium.

Nicolaï, B.M. and De Baerdemaeker, J., 1993. Computation of heat conduction in materials with random variable thermophysical properties. Int. Journal for Numerical methods in Engineering, 36, 523-536.

Niekamp, A.; Unklesbay, K.; Unklesbay, N. and Ellersieck, M., 1984. Thermal properties of water dispersions used for modeling foods. Journal of Food Science, 49, 1, 28-31.

Norback, J.P., 1980. Techniques for optimization of food processes. Food Technology, 34, 2, 86-88.

Noronha, J.; Hendrickx, M.; Suys, J. and Tobback, P.,1993. Optimization of surface quality retention during thermal processing of conduction heated foods using variable temperature retort profiles. Journal of Food Processing and Preservation, 17, 2, 75-91.

Nunes, R.V. and Swartzel, K.R., 1990. Modeling thermal processes using the equivalent point method. Journal of Food Engineering, 11, 103-107.

Ohlsson, T., 1980a, Optimisation of heat sterilisation using C-values. In: 'Food Process Engineering', vol. 1, paper 14, 137-145, Eds. Linko, P., Applied Science Publishers, UK.

Ohlsson, T., 1980b. Optimal sterilization temperatures for flat containers. Journal of Food Science, 45, 848-852.

Ohlsson, T., 1980c. Optimal sterilization temperatures for sensory quality in cylindrical containers. Journal of Food Science, 45, 1517-1521.

Ohlsson, T., 1980d. Temperature dependence of sensory quality changes during thermal processing. Journal of Food Science, 45, 836-839, 847.

Olson, F.C.W. and Stevens, H.P., 1939. Thermal processing of foods in tin containers. II. Nomograms for graphic calculation of thermal processes for non-acid canned foods exhibiting straight-line semi-logarithmic heating curves. Food Research, 4, 1, 1-20.

Patashanik, M., 1953. A simplified procedure for thermal process evaluation. Food Technology, 7, 1-6.

Pflug, I.J., 1987a. Determining the preservation requirements of processes designated to eliminate viable microorganisms from products and objects in 'Textbook for an Introductory Course in the Microbiology and Engineering of Sterilization processes', Sixth Edition. Environmental Sterilization Laboratory, Minneapolis, MN, USA.

Pflug, I.J., 1987b. Using the straight-line semilogarithmic microbial destruction model as an engineering design model for determining the F-value for heat processes. Journal of Food Protection, 50, 4, 342-346.

Pflug, I.J., 1987c. Endpoint of a preservation process. Journal of Food Protection, 50, 4, 347-351.

Pflug, I.J. and Odlaug, T.E., 1978. A review of z and F values used to ensure the safety of low-acid canned foods. Food Technology, 32, 6, 63-70.

Pham, Q.T., 1987. Calculation of thermal process lethality for conduction-heated canned foods. Journal of Food Science, 52, 4, 967-974.

Pham, Q.T., 1990. Lethality calculation for thermal process lethality with different heating and cooling rates. International Journal of Food Science and Technology, 25, 148-156.

Pinheiro-Torres, A.; Oliveira, F.A.R.; Silva, C.L.M. and Fortuna, S.P., 1994. The influence of pH on the kinetics of acid hydrolysis of sucrose. Journal of Food Processing Engineering, in press.

Puri, V.M. and Anantheswaran, R.C., 1993. The finite-elements method in food processing: a review. Journal of Food Engineering, 19, 247-274.

Purohit, K.S. and Stumbo, C.R., 1973. Refinement and extension of fh/U:g parameters for process calculation. Journal of Food Science, 38, 726-728.

Rao, M.A.; Cooley, H.J.; Anantheswaran, R.C. and Ennis, R.W., 1985. Convective heat transfer to canned liquid foods in a steritort. Journal of Food Science, 50, 150-154.

Rao, M.A.; Anantheswaran, R.C. and Ennis, R.W., 1988. Convective heat transfer to fluid foods in cans. in 'Advances in Food Research', Vol. 32, 40-48, Eds. Chichester, C.D. and Schweigert, B.S., Academic Press, Inc., London, UK.

Richardson, P.S. and Holdsworth, S.D., 1988. Mathematical modelling and control of sterilisation process. In Field, R.W. and Howell (Eds.), 'Process Engineering in the Food Industry - Developments and Opportunities', Elsevier Applies Science, London, UK.

Rotstein, E.; Saguy, I. and Valentas, K., 1988. Heat processing of viscous materials in axially rotating cans. An engineering model. in 'Proceedings of the International Symposium on Progress of Food Preservation', vol. 1, CERIA, Brussels, Belgium.

Saguy, I. and Karel, M., 1980. Modeling of quality deterioration during food processing and storage. Food Technology, 34, 2, 78-85.

Saguy, I., 1983. Optimization Methods and Applications. In: Computer-Aided Techniques in Food Technology. Ed. Saguy, I., Marcel Dekker, New York, 263-320.

Saguy, I. and Karel, M., 1979. Optimal retort temperature profile in optimizing thiamin retention in conduction-type heating of canned foods. Journal of Food Science, 44, 1485-1490.

SAS Institute Inc., 1982. SAS user's guide: Statistics, 1982 Edition. SAS Institute Inc., Cary, NC, USA.

Saraiva, J.; De Cordt, S.; Hendrickx, M.; Oliveira, J. and Tobback, P., 1993. Inactivation of α-amylase from Bacillus amyloliquefaciens at low moisture contents. In: Van den Twell, W.J.J.; Harder, A. and Buitelaar, R.M. (Ed.), Stability and Stabilization of enzymes. Elsevier Science Publishers, Amsterdam.

Sastry, S.R.; Odlaugh, T.E. and Christenses, R., 1985. A three dimensional finite element model for thermally induced changes in foods: Application to agaritine in canned mushrooms. Journal of Food Science, 50, 1293.

Schultz, O.T. and Olson, F.C.W., 1938. Thermal processing of canned foods in tin containers. I. Variation of heating rate with can size for products heating by convection. Food Res., 3, 647-651.

Schultz, O.T. and Olson, F.C.W., 1940. Thermal processing of canned foods in tin containers. III. Recent improvements in the general method of thermal process calculations - A special co-ordinate paper and methods of converting initial and retort temperatures. Food Res., 5, 399-407.

Shin, S. and Bhowmik, S.R., 1990. Computer simulation to evaluate thermal processing of food in cylindrical plastic cans. Journal of Food Engineering, 12, 117-131.

Silva, C.; Hendrickx, M; Oliveira, F. and Tobback, P., 1992a. Optimal temperatures for conduction heating foods considering finite surface heat transfer coefficients. Journal. Food Science 57, 3, 743-748.

Silva, C.; Hendrickx, M; Oliveira, F. and Tobback, P, 1992b. Critical review of commonly used objective functions to optimize overall quality and nutrient retention of heat preserved foods. Journal of Food Engineering, 17, 241-258.

Silva, C.L.; Oliveira, C.L. and Hendrickx, M., 1993. Modeling optimum processing conditions for the sterilization of prepackaged foods. Food Control, 4, 2, 67-78.

Simpson, R; Aris, I. and Torres, J.A., 1989. Sterilization of conduction-heated foods in oval-shaped containers. Journal of Food Science, 54, 5, 1327-1331 & 1363.

Simpson, R; Almonacid, S. and Torres, J.A., 1990. Computer control of batch retort process operations. Proceedings from the Food Processing Automation Conference, FPEI, ASAE, Kentucky, USA.

Singh, R.P. and Segerlind, 1974. The finite element method in food engineering. ASAE paper No 74-6015.

Soulé, C.L. and Merson, R.L, 1985. Heat transfer coefficients to Newtonian liquids in axially rotated cans. Journal of Food Engineering, 8, 33-36.

Sperber, R.M., 1989. Advanced modeling software optimizes thermal processing. Food Processing, 50, 11, 84-85.

Steele, R.J. and Board, PAW., 1979. Thermal process calculations using sterilizing ratios. Journal of Food Technology, 14, 227-235.

Stoforos, N.G.; Noronha, J.; Hendrickx, M. and Tobback, P., 1994. A critical analysis of mathematical procedures for the evaluation and design of thermal processes for foods. Submitted for publication.

Stumbo, C.R., 1953. New procedures for evaluating thermal processes for foods in cylindrical containers. Food Technology, 7, 309-315.

Stumbo, C.R., 1973. 'Thermobacteriology in Food Processing', 2nd. Ed. Academic Press, New York.

Stumbo, C.R.; Murphy, J.R. and Cochran, J., 1950. Nature of thermal death time curves for P.A. 3679 and Clostridium botulinum. Food Technology, 4, 321-326.

Stumbo, C.R. and Longley, R.E., 1966. New parameters for process calculation. Food Technology, 20, 3, 341-345.

Succar, J. and Hayakawa, K., 1982. Prediction of time correction factor for come-up heating of packaged liquid foods. Journal of Food Science, 47, 2, 614-618.

Swartzel, K.R., 1982. Arrhenius kinetics as applied to product constituent losses in ultra high temperature processing. Journal Food Science, 47, 6, 1886-1891.

Swientek, R.J., 1986. Specialized software programs speed thermal process studies. Food Processing, June 1986.

Tandon, S. and Bhowmik, S.R., 1986. Evaluation of thermal processing of retortable pouches filled with conduction heated foods considering their actual shapes. Journal of Food Science, 51,3, 709-714.

Taoukis, P.S. and Labuza, T.P., 1989. Applicability of time-temperature indicators as shelf life monitors of food products. Journal of Food Science, 54, 4, 783-788.

Teixeira, A.A.; Dixon, J.R.; Zahradnik, J.W. and Zinmeister, G.E., 1969a. Computer determination of spore survival distributions in thermally processed conduction foods. Food Technology 23, 3, 78-80.

Teixeira, A.A.; Dixon, J.R.; Zahradnik, J.W. and Zinmeister, G.E., 1969b Computer optimization of nutrient retention in the thermal processing of conduction-heated foods. Food Technology 23, 6, 137-142.

Teixeira, A.A.; Stumbo, C.R. and Zahradnik, J.W., 1975a. Experimental evaluation of mathematical and computer models for thermal process evaluation. Journal of Food Science, 40, 653-655.

Teixeira, A.A.; Zinmeister, G.E. and Zahradnik, J.W., 1975b Computer simulation of variable retort control and container geometry as a possible means of improving thiamin retention in thermally processed foods. Journal of Food Science, 40, 656-659.

Teixeira, A.A. and Manson, J.E., 1982. Computer control of batch retort operations with on-line correction of process deviations. Food Technology, 36, 4, 85-90.

Teixeira, A.A.; Tucker, G.S.; Balaban, M.O. and Bichier, J., 1992. Innovations in conduction-heating models for on-line retort control of canned foods with any j-value. In, ‘Advances in Food Engineering’, Ed. Singh, R.P and Wirakartakusumah, A., CRC Press, Florida, USA.

Thijssen, H.A.C.; Kerkhof, P.J.A.M. and Liefkens, A.A.A., 1978. Short-cut method for the calculation of sterilization conditions yielding optimum quality retention for conduction-type heating of packaged foods. Journal of Food Science, 43,1099-1101.

Thijssen, H.A.C. and Kochen, L.H.P.J.M., 1980. Calculation of optimum sterilization conditions for packed conduction-type foods. Journal of Food Science, 45, 1267-1292.

Thompson, G.E., 1919. Temperature-time relations in canned foods during sterilisation. J. Ind. and Eng. Chem., 11, 7, 657-664.

Timbers, G.E. and Hayakawa, K., 1967. Calculation by digital computer: Mass average sterilizing value. Food Technology, 21, 1069, 1072-1073, 1076.

Tucker, G.S. and Clark, P., 1990. Modeling the cooling phase of heat sterilization processes, using heat transfer coefficients. Journal of Food Science and Technology, 25, 668-681.

Tucker, G.S. and Holdsworth, S.D., 1991. Mathematical modelling of sterilisation and cooking processes for heat preserved foods, applications of a new heat transfer model. Trans. IChemE, 69, C, 5-12.

Tucker, G.S., 1991. Development and use of numerical techniques for improved thermal process calculations and control. Food Control, January 1991, 15-19.

Tung, M.A. and Garland, T.D., 1978. Computer calculations of thermal processes. Journal of Food Science, 43, 365-369

Uno, J. and Hayakawa, K., 1980. Correction factor of come-up heating based on critical point in a cylindrical can of heat conduction food. Journal of Food Science, 45, 853-859.

Uno, J. and Hayakawa, K., 1981. Correction factor of come-up heating based on mass average survivor concentration in a cylindrical can of heat conduction food. Journal of Food Science, 46, 5, 1484-1487.

Van Loey, A.; Fransis, A.; Hendrickx, M.; Maesmans, G. and Tobback, P., 1994a. Kinetics of quality changes of green peas and white beans during thermal processing. Journal of Food Engineering. In press.

Van Loey, A.; Fransis, A.; Hendrickx, M.; Maesmans, G.; Noronha, J. and Tobback, P., 1994b. Optimizing thermal process for canned beans in water cascading retorts. Journal of Food Science, 59, 4, 828-832.

Villota, R. and Hawkes, J.G, 1986. Kinetics of nutrients and organoleptic changes in foods during processing. In 'Physical and Chemical Properties of Foods', Ed., Okos, M.R., American Society of Agricultural Engineering, St. Joseph, Michigan, USA.

Vinters, J.E.; Patel, R.H. and Halaby, G.A., 1975. Thermal process evaluation by programmable computer calculation. Food Technology, March 1975, 42-48.

Wen Chin, L., 1977. Disaccharide hydrolysis as a predictive measurement for the efficacy of heat sterilization in canned foods. Ph.D. thesis, Department of Food Science and Nutrition, University of Massachusetts, USA.

Weng, Z.; Hendrickx, M.; Maesmans, G. and Tobback, P., 1991. Immobilized peroxidase: a potential bioindicator for evaluation of thermal processes. Journal of Food Science, 56, 2, 567-570.

Whitaker, J.R., 1991. Enzymes: monitors of food stability and quality. Trends in Food Science & Technology, April 1991, 94-97.

Wiese, K.L. and Wiese, K.F., 1992. A comparison of numerical techniques to calculate broken line heating factors of a thermal process. Journal of Food Processing an Preservation, 16, 301-312.

Witonsky, R.J., 1977. A new tool for the validation of the sterilization of parentals. Bulletin of the Parental Drug Association, 31, 6, 274-281.

Yawger, E.S., 1978. Bacteriological evaluation for thermal design. Food Technology, 32, 6, 59-62.

Young, K.E.; Steffe, J.F. and Larkin, J.W., 1983. Product temperature prediction in hydrostatic retorts. Transactions of the ASAE, 26, 1, 316-320.