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New Semi-empirical Approach to Handle Time-variable Boundary Conditions during Sterilisation of Non-conductive Heating Foods

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ABSTRACT

Semi-empirical methods for the prediction of time–temperature histories in conductive and non-conductive (convective and mixed mode) heating foods subjected to a time-variable processing temperature are proposed. Four alternatives are considered: (i) Hayakawa's method (Duhamel's theorem and Hayakawa's formulae); (ii) Duhamel's theorem with analytical solution; (iii) numerical solution with apparent time (time shift); (iv) numerical solution with apparent position. The incorporation of the empirical heating characteristics f *and* j *in conductive models was accomplished by evaluating the existing analogies with thermophysical properties in the solutions of the Fourier equation. Approaches using Duhamel's theorem or finite difference solutions were used to handle variable boundary conditions. The application of the models in the calculation of processing values for thermal processes with different come up times and different boundary conditions during come up time and thermal processes with process deviations is discussed. The numerical solution with apparent position was preferred because it combines accuracy and flexibility.*

NOTATION

a	Rate of change of the heating medium temperature (in eqns (13) and (14))
D	Time required to decrease the concentration by 90% (min)
f	Time required to reduce the difference between the heating medium temperature and the product temperature to one-tenth of its value (min)
F	Processing value (total lethality) (min)
j	Lag factor in heat penetration curves

J_0 Bessel's function of first kind of zero order
n Integer
N Number of micro-organisms or concentration of the quality factor
r Radial position (m)
R Characteristic length (radius for infinite cylinder and sphere, half thickness for infinite slab) (m)
R_1 First positive root of $J_0(x)=0$
t Time (s)
T Temperature (°C)
U Dimensionless temperature
z Temperature increment necessary for a ten-fold reduction of D (°C)

α Thermal diffusivity (m^2/s)
γ Integer
τ Duration of a transfer unit ($\tau = f/\ln(10)$) (min)
ψ Centre temperature response to a unit step variation at the surface
η, B, T_v Symbols used and defined in Table 1

Subscripts
0 Initial
1 Retort
c Cooling
cs Cold spot
h Holding, heating
i, k, n Integers
p Total process
ref Reference
s Surface
x, y Indices

INTRODUCTION

During thermal processing, food temperatures can deviate significantly from their design values because of process deviations. 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 standpoint only temperature drops are of concern) then several alternative solutions are possible: reprocessing the products, destruction of the product, holding of the product and 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 safety and the new retort temperature. The ideal case would be on-line control of the 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 coldest spot of a container, we need methods that allow the prediction of the temperature history at this location.

The first methods designed for the prediction of food temperature during thermal processing relied on the use of empirical formulae to describe, accurately, heat penetration curves (Ball & Olson, 1957; Hayakawa, 1970, 1977). The great advantage of these empirical methods is their simplicity and wide applicability independently of the mode of heat transfer involved. Today these methods are still widely applied for the design and evaluation of thermal processes. They were developed considering a constant heating medium temperature and cannot handle time-variable boundary conditions. Empirical rules (42% rule) have been suggested and used to handle different come up times (Ball, 1923). For pure conductive heating of foods where the heat transfer is described by Fourier's partial differential equation, several analytical solutions exist that allow the prediction of the transient temperature history for different geometries and boundary conditions. A more general approach to solve Fourier's equation is based on the use of numerical methods, mainly finite differences. Since the presentation of a computer implemented finite difference method for the determination of transient temperatures inside cylindrical cans (Teixeira *et al.*, 1969*a*), finite difference has been widely applied for the prediction of sterilising values and nutrient retention during the sterilisation of conduction heating of foods (Teixeira *et al.*, 1969*b*; Manson *et al.*, 1970; Teixeira *et al.*, 1975; Tandon & Bhowmik, 1986; Bhowmik & Shweta, 1987; Simpson *et al.*, 1989; Chau & Gaffney, 1990; Shin & Bhowmik, 1990; Tucker, 1991; Tucker & Holdsworth, 1991). The ease of incorporation of variable boundary conditions (variable external temperatures and/or external resistance to heat transfer) combined with a very simple computer implementation (for conduction heating in conventional shaped bodies) made finite differences a preferred tool for the design and evaluation of thermal processes. Several computer-based retort control strategies, based on finite differences for on-line correction of process deviations have been proposed (Teixeira & Manson, 1982; Datta *et al.*, 1986; Richardson & Holdsworth, 1988; Gill *et al.*, 1989).

While valid for any food, independently of the mode of heat transfer, the existing empirical methods for the prediction of temperatures are only valid for conditions of constant heating medium temperature. On the other hand the existing numerical solutions for the Fourier equation are limited to conduction heating foods. For mixed type heating foods, analytical or numerical solutions able to furnish a simple, straightforward solution for the time temperature history at the cold spot of the food, when subjected to a time-variable heating temperature are not available. While numerical simulation of natural convection heating in packaged foods was initiated by several authors using finite differences and finite elements to solve the partial differential equations that govern the heat and mass transfer in the system (Engelman & Sani, 1983; Kumar *et al.*, 1990; Datta & Teixeira, 1987, 1988), the complexity of the calculations involved and the large amount of CPU time necessary to perform the calculations together with the lack of accurate experimental data for the simulations do not allow the generalisation of such an approach for the general design and evaluation of thermal processes. In this context, particulated foods in agitated containers have not been considered yet.

One of the first attempts to deal with variable retort temperature was suggested by Ball (1923). Ball suggested that the time taken to bring a retort to processing temperature ('come up' time) should be considered as part of the process. According to the results of the experimental work carried out by this author, 42% of the come up time should be considered for the calculation of the process value. Since then several other researchers have derived relationships that allow the calculation of correction factors for the come up time based on the process variables (Gillespy, 1953; Uno & Hayakawa, 1980; Giannoni-Succar & Hayakawa, 1982; Berry & Bush, 1989). A tabular method using Duhamel's theorem to handle variable retort temperature was suggested by Gillespy (1951, 1953), while originally devised 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 process deviations during the processing of conduction heating foods. Hayakawa (1971) proposed the use of Duhamel's theorem, together with his experimental formulae for the prediction of the time–temperature relationship during the curvilinear portion of the heating curves (Hayakawa, 1970), for the prediction of the time–temperature history of a food subjected to a variable heating medium temperature. The modification of the basic conduction model of Teixeira *et al.* (1969*a*), to allow for the prediction of temperatures of mixed mode heating foods has been proposed (Teixeira *et al.*, 1992). This approach produces good estimates of temperature in the case of constant heating medium temperature. While suggested as valid for predicting temperatures under retort temperature deviations no results for variable heating medium temperatures were presented. For the particular case of perfectly mixed foods, formulae were developed that allow the prediction of the temperature history during the sterilisation when considering variable heating medium temperature (Bimbenet & Michiels, 1974).

The goal of this work is to develop semi-empirical procedures that allow the calculation of the time–temperature at the coldest spot of foods, for which heat penetration curves can be described using the classical f and j parameters, when subjected to a time-variable process temperature, thus allowing the evaluation of a deviant process in terms of the achieved F_0 value in the coldest spot of the container, and permitting the on-line correction of process deviations.

ALTERNATIVE METHODS FOR HANDLING PROCESS DEVIATIONS

Theoretical background

The processing value achieved in the coldest spot of the container (F_{cs}) can be calculated from the time–temperature history in the coldest spot using the following relationship,

$$F_{cs} = \int_0^{t_p} 10^{(T_{cs}(t) - T_{ref})/z} \mathrm{d}t \tag{1}$$

So to estimate properly a process deviation one must be in possession of physical mathematical methods that allow the calculation of the time–temperature history in the cold spot of the container, $T_{cs}(t)$.

Empirical methods

Ball (1923) proposed a simple formula for the description of the time–temperature behaviour of a food subjected to a constant ambient temperature,

$$\log\left(\frac{T_1 - T}{T_1 - T_0}\right) = \log j - \frac{t}{f} \qquad (2)$$

Ball's formula (2) 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 retort temperature is plotted against time. For the characterisation of the linear relationship observed, two parameters, f and j, are used. This equation does not describe the curvilinear portion observed at the beginning of the heating and cooling curves. Ball (1923) made the assumption that the lag portion of the cooling curve when plotted in Cartesian co-ordinates might be approximated by a hyperbola.

Hayakawa (1970, 1982) developed a set of experimental formulae (Table 1) for the description of the curvilinear portion of heat penetration curves with j values from 0·001 to 6500. These formulae allow accurate estimation of transient temperatures of foods at the beginning of the heating and cooling stages of the sterilisation processes.

TABLE 1
Formulae Proposed by Hayakawa to Describe the Curvilinear Portion of Heat Penetration Curves (Hayakawa, 1982; Lekwauwa & Hayakawa, 1986)

j value range	*Hayakawa's formulae*
$0{\cdot}001 \le j \le 0{\cdot}4$	$\begin{cases} U(t) = 1 - 10^{-\eta t/B} \\ \eta = ((tv/f) - \log_{10} j)/(tv/f) \\ tv = f(0{\cdot}3913 - 0{\cdot}3737 \log_{10} j) \\ B = tv\{(tv/f) - \log_{10} j\}^{\eta} \end{cases}$
$0{\cdot}4 \le j < 1$	$\begin{cases} U(t) = 1 - \Delta To^{\cot(Bt + \pi/4) - 1} \\ B = \frac{1}{tv}\left\{\arctan \frac{\log_{10}(\Delta To)}{[\log_{10}(j\Delta To) - tv/f]} - \pi/4\right\} \\ tv = 0{\cdot}9f(1 - j) \end{cases}$
$1 < j \le 5{\cdot}8$	$\begin{cases} U(t) = 1 - \Delta To^{\cos(Bt) - 1} \\ B = \frac{1}{tv} \arccos \frac{\log_{10}(j\Delta To - tv/f)}{\{\log_{10}\Delta To\}} \\ tv = 0{\cdot}7f(j - 1) \end{cases}$
$5{\cdot}8 < j \le 6500$	$\begin{cases} U(t) = 1 - \Delta To^{\cos(Bt) - 1} \\ B = \frac{1}{tv} \arccos \frac{\log_{10}(j\Delta To - tv/f)}{\{\log_{10}\Delta To\}} \\ tv = 1{\cdot}54f\log_{10}(j/1{\cdot}8) \end{cases}$

Theoretical solutions for conduction heating foods

For conduction heating foods the transient temperature history can be calculated using solutions of Fourier's second law. For geometries showing one dimensional heat transfer (infinite cylinder, infinite slab and sphere) Fourier's second law is given by eqn (3):

$$\frac{\partial T}{\partial t}=\frac{1}{r^{(\gamma-1)}\partial r}\left(a r^{(\gamma-1)}\frac{\partial T}{\partial r}\right) \tag{3}$$

where, $\gamma=1$, 2 and 3 respectively for an infinite slab, an infinite cylinder and a sphere.

The analytical solution of this differential eqn (3) for a conductive heating sphere with initial homogeneous temperature, subjected to a step change in the surface temperature, at time $t=0$, is given by eqn (4) (Carslaw & Jaeger, 1959):

$$U(r,t)=\begin{cases} 1+\dfrac{2R}{\pi r}\displaystyle\sum_{n=1}^{\infty}\dfrac{(-1)^n}{n}\sin\left(\dfrac{n\pi r}{R}\right)\exp\left(\dfrac{-an^2\pi^2 t}{R^2}\right) & \text{for } 0<r\leq R \\ 1+2\displaystyle\sum_{n=1}^{\infty}(-1)^n\exp\left(\dfrac{-an^2\pi^2 t}{R^2}\right) & \text{for } r=0 \end{cases} \tag{4}$$

where $U(r,t)$ represents a dimensionless temperature at radial position r at time t in a sphere of radius R. Considering the general case of a sphere at an initial uniform temperature T_0 subjected to a constant surface temperature T_1, the temperature $T(r,t)$ can be calculated using eqn (4) considering the following transformation,

$$U(r,t)=\frac{T_1-T(r,t)}{T_1-T_0} \tag{5}$$

Duhamel's theorem

Duhamel's theorem (Carlslaw & Jaeger, 1959; Myers, 1971) states that if $\psi(x,t)$ is the response of a system at 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 eqn (6):

$$T(x,t)=\int_0^t T_s(\tau)\frac{\partial\psi(x,t-\tau)}{\partial t}\,d\tau \tag{6}$$

Using Duhamel's theorem it is possible to derive analytical solutions for the case of variable surface temperature, however 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.

The empirical parameters f and j and the conduction model

For sufficiently large values of t, all terms in eqn (4) except the first will vanish. The temperature in the centre ($r=0$) is then given by,

$$U(t)=1-2\exp\left(\frac{-\alpha\pi^2 t}{R^2}\right) \quad (7)$$

Comparing eqns (2) and (7) we find that for a conductive heating sphere, initially at a uniform temperature and with constant surface temperature,

$$j=2{\cdot}0 \quad (8)$$

$$f=\frac{\ln(10)R^2}{\pi^2\alpha}=0{\cdot}233\,\frac{R^2}{\alpha} \quad (9)$$

Similar relationships can be obtained for other common regular geometries using a similar approach (Ball & Olson, 1957) (Table 2).

Methods for the calculation of transient temperatures during variable retort temperature

Hayakawa's method (HYK) (Hayakawa, 1971)

In this approach, previously presented by Hayakawa (1971), eqn (6) is solved numerically. To calculate the product temperature at time t, the time interval $[0, t]$ is divided into a set of n intervals of length $\Delta t = t/n$, and the retort temperature, $T_s(t)$, is approximated at each of the intervals, by the temperature at the middle of the interval. Based on this approximation the integral in eqn (6) is solved numerically as,

$$T(r,t)=T_0+\sum_{i=1}^{n}(T_s[(i-0{\cdot}5)\Delta t]-T_0)\Delta U(r)_{n-i+1} \quad (10)$$

with

$$\Delta U(r)_k = U(r,(k-1)\Delta t)-U(r,k\Delta t) \quad (11)$$

where $T_s[(i-0{\cdot}5)\Delta t]$ represents the surface temperature at $(i-0{\cdot}5)\Delta t$, the midpoint of the interval $[(i-1)\Delta t, i\Delta t]$, 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 formulae developed by Hayakawa (Table 1) were utilised for the prediction of the dimensionless temperature differences.

Analytical solution + Duhamel's theorem (ASDT)

As in the previously described approach, 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 former method empirical equations were used for the prediction of the dimensionless temperature differences in eqn (11), in this method the analytical solution of Fourier's second law for a sphere given by eqn (4) is applied.

In order to incorporate the empirical parameters f and j in the conduction model the previously discussed relationship between these empirical factors and r (radial position) and α were taken into account. The incorporation of the empirical f parameter in the conduction heating model was accomplished

TABLE 2
Theoretical Values of f and j Values of Various Objects when the Initial Temperature Distribution is Uniform (adapted from Ball & Olson, 1957)

Object	*f value*	*j at geometrical centre*	*j at any point in the object*
Sphere	$0{\cdot}233\,\frac{R^2}{\alpha}$	2·00000	$0{\cdot}63662\,\frac{R}{r}\sin\frac{\pi r}{R}$
Infinite cylinder	$0{\cdot}898\,\frac{R^2}{\alpha}$	1·60218	$1{\cdot}60128 J_0\left(\frac{R_1 r}{a}\right)$
Infinite slab	$0{\cdot}933\,\frac{R^2}{\alpha}$	1·27324	$1{\cdot}27324\cos\frac{\pi y}{2b}$
Finite cylinder	$\frac{0{\cdot}398}{\left(\frac{1}{a^2}+\frac{0{\cdot}427}{b^2}\right)\alpha}$	2·03970	$2{\cdot}03970 J_0\left(\frac{R_1 r}{a}\right)\cos\frac{\pi y}{2b}$
Brick	$\frac{0{\cdot}933}{\left(\frac{1}{a^2}+\frac{1}{b^2}+\frac{1}{c^2}\right)\alpha}$	2·06410	$2{\cdot}06410\cos\frac{\pi x}{2a}\cos\frac{\pi y}{2ab}\cos\frac{\pi z}{2c}$

considering the relationship, between the thermal diffusivity and the f value given by eqn (9). The incorporation of the j value was accomplished taking into account the theoretical variation of the j value inside a conductive heating sphere derived by Ball and Olson (1957) (Table 2). It is then possible to find for any food with empirical heating parameters f and j, an apparent position in a sphere (with unit radius) of thermal conductivity given by eqn (9), that shows the same heating parameters (j and f) as the considered food. For the apparent position and thermal diffusivity calculated in this way it is possible to use eqn (7) for the calculation of the dimensionless temperature history necessary for the numerical application of Duhamel's theorem using eqns (13) and (14). A sphere is chosen because it reflects the higher range of j values (0–2) for geometries where the heat transfer is one dimensional. The same approach can be applied using other geometries considering the appropriate analytical solution (Carlslaw & Jaeger, 1959) and taking into account the theoretical variation of the j value inside the chosen geometry (Table 2).

Numerical solutions

When there are changes in the heating characteristics of the product during the process, caused for example by changes in the f value in products that exhibit broken heating curves or changes in the surface transfer coefficients when moving from heating to cooling conditions, the Duhamel theorem is no longer applicable and consequently the methods described above cannot be applied. Numerical solutions for the transient heat transfer in conductive heating foods have been proved to be a fast and reliable way of dealing with the problem of heat conduction under variable retort profiles allowing changes to any of the variables, either separately or in combination (Tucker, 1991). An effort has been made to combine the flexibility of numerical solutions with the empirical description of heat penetration curves.

Apparent time concept (time delays) (ATNS). Teixeira *et al.* (1992) proposed the incorporation of the j value in the Teixeira *et al.* (1969*a*) finite difference algorithm for the calculation of the transient temperature of conductive heating foods. The procedure is based on the fact that two 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

$$\Delta t = f \times \log\left(\frac{j_x}{j_y}\right) \tag{12}$$

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 eqn (12)) in the calculations. The f value is implemented by considering an apparent thermal diffusivity.

Apparent position concept (APNS). This approach is a hybrid of the last two methods discussed, and combines the flexibility of finite differences with the empirical description of the heat penetration curves. The approach is different from Teixeira's (1992) one in the way it incorporates the empirical parameters in the conduction model. Here the incorporation of the empirical parameters is, as in the method that makes use of Duhamel's theorem together with the empirical solution of Fourier's equation, performed taking into account the existing analogies between the empirical description of the time–temperature curves and the first term approximate of the analytical solution of the Fourier's equation for a sphere discussed previously (Table 2). As in the referred method, a position inside a conductive sphere, where the j 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 (9).

CALCULATION RESULTS

Programs

A Pascal routine able to solve numerically eqn (6) was written based on the application of eqn (10) as had previously been proposed by Hayakawa (1971). Depending on the method being applied, HYK or ASDT, this routine was used together with a routine responsible for the calculation of the temperature history of a food initially at homogeneous temperature ($T_0 = 0$) subjected to a unitary step change in temperature at the surface, using Hayakawa's formulae (Table 1) or the analytical solution (eqn (4)) respectively.

A finite difference conduction model described elsewhere (Chau & Gaffney, 1990; Silva *et al.*, 1992) has been modified in such a way that the empirical parameters f and j could be incorporated. To perform this incorporation a 'pseudo' thermal diffusivity was calculated from the f value using eqn (9) considering a sphere of unit length. The position inside the sphere showing the target j value was calculated using the equations in Table 2 and a repeated linear interpolation scheme (Dorn & McCracken, 1972) was used to determine the temperature at this exact location inside the sphere from the temperatures calculated for each time step for adjacent nodes (three nodes) of the finite differences grid.

A program was written to calculate the time–temperature history of 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 eqn (12). The shifting in time was only performed once at the start of the process (time = 0).

RESULTS AND DISCUSSION

The four methods described above were validated for both conduction heating and perfectly mixed products by comparing their time–temperature predictions with those of the finite difference (conduction) or Bimbenet and Michiel's method (perfectly mixed). For conduction heating data were generated using finite difference models for various regular geometries (infinite slabs, infinite cylinders, sphere, finite cylinder, bricks), (Chau & Gaffney, 1990; Silva *et al.*, 1992), from which the theoretical *j* values can be derived from analogy between the Ball eqn (2) and the first term approximation of the analytical solutions of the second Fourier equation for each of the geometries (Ball & Olson, 1957) (Table 2).

For the generation of the temperature history for perfectly mixed products subjected to a variable heating temperature, Bimbenet and Michiel's (1974) method (13), valid when the variable external temperature can be approximated by a set of linear pieces, was used:

$$T(t) = T_{1,0} + a(t-\tau) + (T_0 - T_{1,0} + a\tau)\exp\left(-\frac{t}{\tau}\right) \tag{13}$$

where the retort temperature varies linearly according to,

$$T_1(t) = T_{1,0} + at \tag{14}$$

and where τ, the duration of a transfer unit, is defined as,

$$\tau = f/\ln(10) \tag{15}$$

For each of the geometries different types of processing conditions were considered: (i) constant retort temperature, (ii) a linear come up behaviour, (iii) constant heating temperature followed by constant cooling temperature and (iv) different process deviations during the holding phase (Table 3) and the predicted temperature response, using the different methods, calculated. The predicted product temperature response was compared with the reference method, 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 $z = 10$°C. All the reported F_0 values were calculated by numerical integration of eqn (1), using Simpson's rule (Carnahan *et al.*, 1969).

In Tables 4–7 the processing values calculated from the time–temperature history determined for each of the described methods are presented, and the

TABLE 3
Retort Temperature Profiles Considered for the Simulations

No.	*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

TABLE 4

Process Values (min) Calculated from the Time–Temperature Profiles Predicted Using the Different Models, as Compared with the Process Values Calculated Using the Finite Difference Solution. Case Study: Infinite Cylinder, $fh = 20$ min, $jh = 1{\cdot}6018$. See Table 3 for definition of process. Error $= (F_0^{method} - F_0^{FD})/F^{FD} \times 100\%$

No.	*FD*	*HYK*	*Error (%)*	*ATNS*	*Error (%)*	*ASDT*	*Error (%)*	*APNS*	*Error (%)*
1	25·49	25·74	0·98	25·53	0·16	25·69	0·78	25·63	**0·55**
2	16·01	16·21	**1·25**	14·52	−9·31	16·18	1·06	16·09	0·50
3	13·68	13·77	0·66	13·66	−0·15	13·79	0·80	13·71	0·22
4	18·98	18·47	−2·68	20·19	6·38	19·04	0·32	18·89	−0·47
5	8·06	8·08	0·25	9·06	**12·41**	8·11	0·62	8·05	−0·12
6	11·64	11·76	1·03	10·99	−5·58	11·77	**1·12**	11·66	0·17
7	10·46	10·56	0·96	10·18	−2·68	10·53	0·67	10·45	−0·10
8	6·54	6·60	0·92	6·83	4·43	6·59	0·76	6·55	0·15

FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.

TABLE 5

Process Values (min) Calculated from the Time–Temperature Profiles Predicted Using the Different Models, as Compared with the Process Values Calculated Using the Finite Difference Solution. Case Study: Infinite Slab, $fh = 20$ min, $jh = 1{\cdot}27324$. See Table 3 for definition of process. Error $= (F_0^{method} - F_0^{FD})/F^{FD} \times 100\%$

No.	*FD*	*HYK*	*Error (%)*	*ATNS*	*Error (%)*	*ASDT*	*Error (%)*	*APNS*	*Error (%)*
1	27·53	27·68	0·54	27·53	0·00	27·64	0·40	27·57	**0·15**
2	17·92	18·04	0·67	14·54	−18·86	18·01	0·50	17·91	−0·06
3	15·33	15·43	0·65	15·23	−0·65	15·41	0·52	15·33	0·00
4	19·89	19·73	−0·80	22·20	11·61	20·03	0·7	19·88	−0·05
5	8·48	8·51	0·35	10·60	**25·00**	8·54	**0·71**	8·49	0·12
6	13·27	13·37	**0·75**	11·98	−9·72	13·36	0·68	13·25	−0·15
7	11·96	12·05	**0·75**	11·40	−4·68	12·00	0·33	11·91	−0·42
8	7·08	7·12	0·56	7·77	9·75	7·12	0·56	7·07	−0·14

FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.

values compared with processing values calculated from the time–temperature history calculated 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 percentage error is outlined using bold type to enable an easy comparison between the accuracy of the different methods. From these results it is easily

TABLE 6
Process Values (min) Calculated from the Time–Temperature Profiles Predicted Using the Different Models, as Compared with the Process Values Calculated Using the Finite Difference Solution. Case Study: Infinite Cylinder, $fh = 10$ min, $jh = 1{\cdot}60218$. See Table 3 for definition of process. Error $= (F_0^{\text{method}} - F_0^{\text{FD}})/F^{\text{FD}} \times 100\%$

No.	*FD*	*HYK*	*Error (%)*	*ATNS*	*Error (%)*	*ASDT*	*Error (%)*	*APNS*	*Error (%)*
1	42·61	42·74	0·31	42·65	0·09	42·72	0·26	42·67	0·14
2	30·50	30·61	0·36	29·64	−2·82	30·60	0·33	30·57	**0·23**
3	29·06	29·12	0·21	29·02	−0·14	29·14	0·28	29·09	0·10
4	34·20	33·93	−0·79	34·85	1·90	34·19	−0·03	34·15	−0·15
5	18·70	18·71	0·05	19·44	**3·96**	18·72	0·11	18·70	0·00
6	24·08	24·16	0·33	23·97	−0·46	24·17	0·37	24·09	0·04
7	23·70	23·79	**0·38**	23·65	−0·21	23·79	**0·38**	23·70	0·00
8	13·91	13·93	0·14	14·44	3·81	13·94	0·22	13·90	−0·07

FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.

TABLE 7
Process Values (min) Calculated from the Time–Temperature Profiles Predicted Using the Different Models, as Compared with the Process Values Calculated Using the Finite Difference Solution. Case Study: Infinite Slab, $fh = 10$ min, $jh = 1{\cdot}27324$. See Table 3 for definition of process. Error $= (F_0^{\text{method}} - F_0^{\text{FD}})/F^{\text{FD}} \times 100\%$

No.	*FD*	*HYK*	*Error (%)*	*ATNS*	*Error (%)*	*ASDT*	*Error (%)*	*APNS*	*Error (%)*
1	43·68	43·74	0·14	43·67	−0·02	43·72	0·09	43·67	−0·02
2	31·55	31·60	0·16	29·60	−6·18	31·58	0·10	31·56	**0·03**
3	30·23	30·28	0·17	30·01	−0·73	30·28	0·17	30·22	−0·03
4	34·69	34·60	−0·26	35·89	3·46	34·74	0·14	34·69	0·00
5	19·00	19·02	0·11	20·46	**7·68**	19·03	0·16	19·00	0·00
6	25·23	25·28	**0·20**	24·84	−1·55	25·28	**0·20**	25·20	−0·12
7	24·83	24·88	**0·20**	24·58	−1·01	24·87	0·16	24·79	−0·16
8	14·34	14·36	0·14	15·35	7·04	14·36	0·14	14·32	−0·14

FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.

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%. When the method based on the application of the apparent time concept is applied process values 25% bigger (overestimation) than the predicted with finite differences can be found.

In Figs 1–4 the time–temperature curves obtained with different methods 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 (at time 0 the retort temperature is suddenly raised to processing temperature) (Fig. 1) all the methods are able to predict accurately the transient temperature history. It can also be observed that in the first line of Tables 3–6 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) 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 differences 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 (process no. 5 in Tables 3–6), where, as it could be expected from the temperature overestimation during the cooling section, this method overestimates the processing value. For the other examples (Figs 3 and 4) there is close agreement between the temperatures predicted by the different methods when compared to the finite difference solution, again with the exception of the method using the time delay concept. For this method it was observed that when the external (retort) temperature suddenly changes (Figs 2 and 4) or gradually changes (Fig. 3) the method is not a good predictor of the product

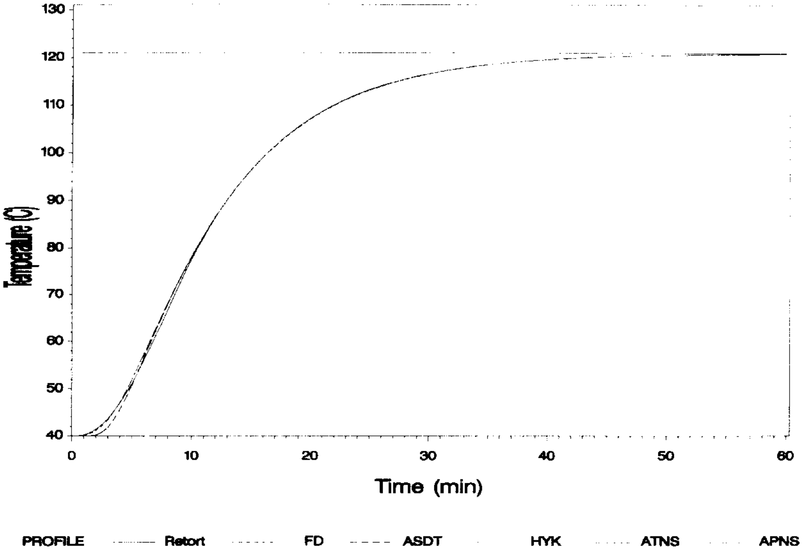

Fig. 1. Time–temperature profiles predicted using the different methods compared with the finite difference solution. Case study infinite cylinder $fh = 20$ min. Some of the curves are partially superimposed. (FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.)

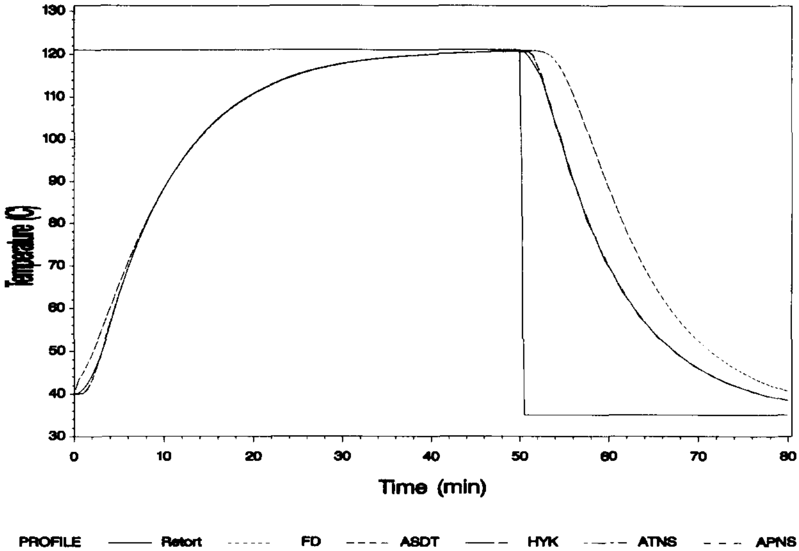

Fig. 2. Time–temperature profiles predicted using the different methods compared with the finite difference solution. Case study infinite slab *fh* = 20 min. Some of the curves are partially superimposed. (FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.)

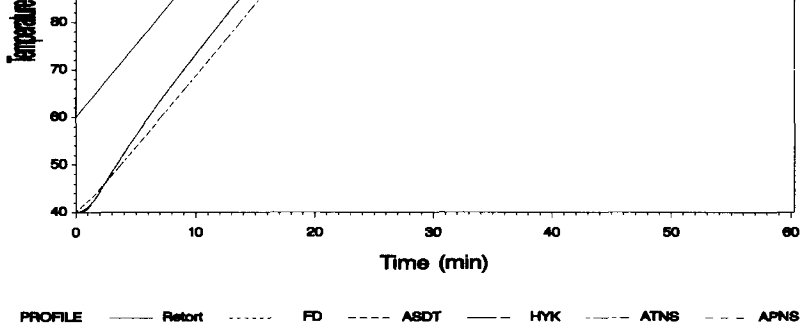

Fig. 3. Time–temperature profiles predicted using the different methods compared with the finite difference solution. Case study infinite slab *fh* = 10 min. Some of the curves are partially superimposed. (FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.)

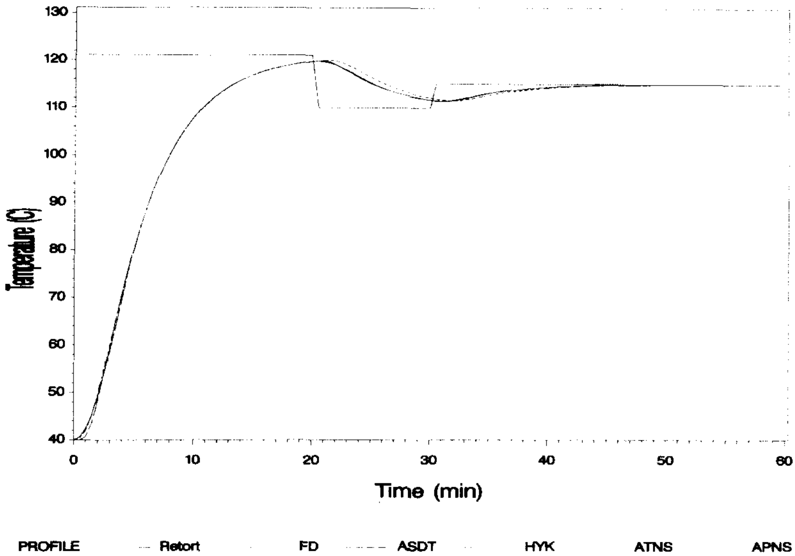

Fig. 4. Time–temperature profiles predicted using the different methods compared with the finite difference solution. Case study infinite cylinder *fh* = 10 min. Some of the curves are partially superimposed. (FD, finite differences; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.)

time–temperature course. Lower or higher temperatures 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 model for taking into account the *j* value. Each time that the boundary condition changes there is a lag period before the coldest spot temperature responds to these changes, which is reflected by the *j* 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* 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* value of the system at the moment the boundary condition changes. Since temperature gradients exist during the process, *j* values cannot be predicted. This problem is overcome by the use of an apparent position concept.

In Table 8 the results obtained for the four alternatives are compared with results obtained using the formulae of Bimbenet and Michiels (1974) (see Fig. 5) for the calculation of the transient temperature of perfectly mixed liquids with *j* values equal to 1. In the case of perfectly mixed liquids Hayakawa's method (1971) produced the best results. In this method Hayakawa's empirical formulae 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 formulae were developed considering heat penetration

TABLE 8

Process Values (min) Calculated from the Time–Temperature Profiles Predicted Using the Different Models, as Compared with the Process Values Calculated Using the Temperatures Calculated According to Bimbenet and Michiel's Method: $fh = 10$ min, $j = 1{\cdot}0$. See Table 3 for definition of process. Error $= (F_0^{\text{method}} - F_0^{\text{FD}})/F^{\text{FD}} \times 100\%$

No.	*BIM*	*HYK*	*Error (%)*	*ATNS*	*Error (%)*	*ASDT*	*Error (%)*	*APNS*	*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 Michiels' method; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.

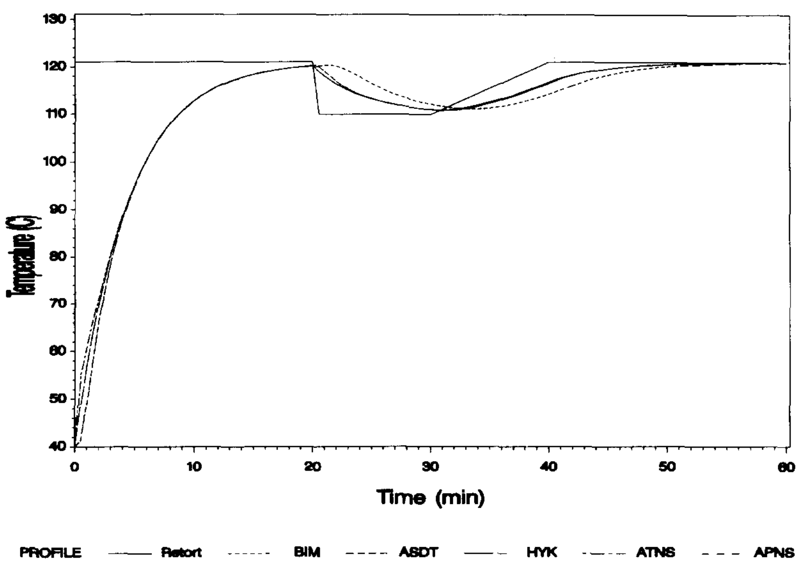

Fig. 5. Time–temperature profiles predicted using the different methods compared with the results obtained using Bimbenet and Michiel's method. Case study $fh = 10$ min. Some of the curves are partially superimposed. (BIM, Bimbenet and Michiels' method; HYK, Hayakawa's method; ASDT, analytical solution Duhamel's theorem; ATNS, apparent time numerical solution; APNS, apparent position numerical solution.)

data from products covering a wide range of j 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 1·5%. As in the case of conduction heating foods the use of the apparent time concept leads to higher deviations, in our case studies up to 12% compared to the method of Bimbenet and Michiels.

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.

It was observed for the cases studied that three of the proposed methods (HYK, ASDT and APNS) allow good prediction of the temperature history in the coldest spot of the product when compared to theoretical solutions. 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 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, homogeneous, 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.

CONCLUSIONS

The proposed methods allow the evaluation of deviant processes, requiring as input merely the heat penetration parameters (f and j) obtained from heat penetration tests together with the retort temperature profile. The methods should be used with caution because they are empirical in nature and are not intended to simulate the heat transfer mechanisms during the sterilisation and rely on a correct determination of the heat penetration parameters (f and j) under the same conditions (viscosity, head space, agitation,...) expected during the actual sterilisation process. Because it combines accuracy with superior flexibility the numerical solution with the apparent position concept is preferred. Extensive experimental work is needed to validate the proposed methods.

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