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Characterising the Detachment of Thermal and Geometric Centres in a Parallelepipedic Frozen Food Subjected to a Fluctuation in Storage Temperature

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ABSTRACT

The three-dimensional transient heat transfer phenomenon occurring in a rectangular brick-shaped frozen food when subjected to diverse functional forms of variation in the storage temperature is solved by computer simulation in order to analyse the behaviour of the thermal centre in comparison with that of the geometric centre, characterisation being made through the evolution of two dimensionless parameters: the initial time when separation appears and the maximum temperature difference between both centres. Also, influences of product thermal properties (heat capacity and thermal conductivity) and convection due surface heat transfer coefficient are studied. Copyright © 1996 Elsevier Science Limited

INTRODUCTION

Because of continuous improvement in freezing and frozen food storage technologies in the last years, today's consumers find at their disposal a huge diversity of seasonal and nonseasonal foods at any time.

Nevertheless, as chemical and biochemical reactions occurring in the product strongly depend on time–temperature history, and as frozen foods are invariably and unavoidably exposed to fluctuating storage temperatures, quality factors determining food stability like colour, flavour, nutrition and microbial status may change during storage. Consequently, precise knowledge of frozen food storage temperatures is needed to maintain quality within satisfactory ranges.

Many authors have studied experimentally as well as via predicting models how room temperature variations influence quality defining factors. Among the earliest studies is the one by Hicks (1944) who proposed a mathematical model to predict the extent of reaction with temperature varying regularly in sinusoidal and square wave patterns. Based on this study Powers *et al.* (1965) derived fluctuation coefficients for temperature amplitudes ranking from 2 to 160°C and reaction ratios of Q_{10} from 1 to 30 and evaluated kinetic variations. Later, Labuza (1979) extended the model by including equations for first order degradation cases. Singh (1978), from his works on quality degradation in the storage of frozen foods, developed a simulation model which predicted the quality index value with either constant or sinusoidal variable storage temperature. Recently Nunes & Swartzel (1990) improved Hicks' model by presenting a predictive model for an accurate shelf-life which used an approximated Arrhenius model including the order of reaction for sinusoidal fluctuation of temperature and covering the range of frozen and unfrozen foods. Scott & Heldman (1990) coupled temperature history to quality loss estimation in both one dimensional and two dimensional finite differences numerical models, and predicted degradation of frozen foods subject to step changes in storage temperatures assuming a limiting single quality deterioration process. Rosset *et al.* (1988) studied the microbiological and organoleptic characteristics in 5 lots of a quick-frozen cooked dish with different storage temperature vs. time variations. Poovarodon *et al.* (1993) considered the influence of frozen food packaging and simulated storage temperature fluctuations with different residence times on product quality through chemical, organoleptic, microbiological and weight-loss analyses. Also, Spieß (1994), by consideration of 'residence time' and 'temperature of exposure' parameters, proposed a method for estimation of quick frozen foods quality variation throughout the cold chain. Quality differences in frozen fish packed in lidded/unlidded carton boxes were detected by Magnussen & Hardarson (1993) for diverse storage temperatures.

In order to predict temperature variations in stored frozen foods when boundary conditions are time dependent, Zuritz & Sastry (1986) simulated a sine wave in a 1-D problem and analysed thermal conductivity, overall heat transfer coefficient and sample thickness effects on product temperature distribution. Besides, Zuritz & Singh (1985) developed a 2-D axisymmetrical finite element based model and applied it to predict the effect of temperature dependent physical properties on temperature predictions.

The aim of this work is to study the time varying temperature field in frozen foods with different physical properties, being stored in an environment whose temperature is subjected to different variations and having different surface heat transfer coefficients. In other words, it is intended to characterise the behaviour of thermal history through the evolution of two dimensionless variables in a homogeneous rectangular parallelepiped (a most-used geometrical shape in stored frozen foods) of different thermal conductivities and heat capacities under diverse boundary conditions.

MATHEMATICAL MODEL

The thermal process that takes place in the storage of frozen foods is that of a transient heat transfer phenomenon governed by the partial differential equation

$$\frac{\partial T}{\partial \tau} = \alpha \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right] \tag{1}$$

expressed in a three rectangular coordinate system, and where thermal diffusivity α is assumed to be temperature independent since values of thermal conductivity and heat capacity within the considered range scarcely vary.

The approach of considering initially all the product at the same temperature T_i is shown in the condition

$$T = T_i \quad \text{for } \tau = 0 \tag{2}$$

Moreover, adopting boundary conditions of the third kind so product surface heat transfer is assumed to be entirely by convection as a basis,

$$k\nabla T = h(T_a - T) \tag{3}$$

expression known as Newton's law of cooling where k stands for the product's thermal conductivity, h represents the surface heat transfer coefficient and the storage temperature T_a is supposed to undergo variations following previously established patterns.

For the purpose of predicting temperature evolution in a homogeneous and isotropic parallelepipedic body, it becomes necessary to solve the initial-boundary value problem expressed by the set of equations (1)–(3).

As analytical solutions are not applicable because of the variation of outside temperature, approximate methods were used. A numerical technique based on finite difference approximation methods has been adopted with an alternating direction implicit (ADI) scheme proposed by Douglas & Gunn (1964) which overcomes the stability limitations of explicit schemes as well as diminishes the large computation times of implicit ones.

Let $\mathscr{D}$ be the domain limited by the parallelepiped object of study. The origin of the coordinate system (0,0,0) is placed coincidentally with the geometric centre and therefore by symmetry only 1/8 of the total volume is to be taken into account.

Discretizing the space and time into increments Δx, Δy, Δz and $\Delta\tau$ respectively, the solution to eqn (1) is obtained by solving the linear system of equations in each time step

$$T^* - T = \frac{Fo_x}{2}\,\delta_x^2(T^* + T) + Fo_y\delta_y^2(T) + \frac{Fo_z}{2}\,\delta_z^2(T) \tag{4a}$$

$$T^* - T^{**} = \frac{Fo_y}{2}\,\delta_y^2(T - T^{**}) \tag{4b}$$

$$T^{**} - T^{***} = \frac{Fo_z}{2}\,\delta_z^2(T - T^{***}) \tag{4c}$$

where Fo is the Fourier number (e.g. $Fo_x = \alpha.\Delta\tau/\Delta x^2$) and δ means a derivative operator to be applied in finite differences form. So, from the knowledge of temperature T distribution in time τ, and through intermediate values T^* and T^{**} of no physical meaning, temperatures T^{***} in time $\tau + \Delta\tau$ can be evaluated.

Besides, boundary conditions expressing null flux along x, y and z directions in all the points on planes $x = 0$, $y = 0$ and $z = 0$ respectively, are to be incorporated into eqn (4), i.e.

$$T_{-1,y,z} = T_{1,y,z} \tag{5a}$$

$$T_{x,-1,z} = T_{x,1,z} \tag{5b}$$

$$T_{x,y,-1} = T_{x,y,1} \tag{5c}$$

in every $(x,y,z) \in \mathscr{D}$.

Condition (3) affecting all the points on external planes $x = L$, $y = M$ and $z = N$, after being approximated in finite differences respectively becomes

$$k\,\frac{T_{L+1} - T_{L-1}}{2\Delta x} = h(T_a - T_L) \tag{6a}$$

$$k\,\frac{T_{M+1} - T_{M-1}}{2\Delta y} = h(T_a - T_M) \tag{6b}$$

$$k\,\frac{T_{N+1} - T_{N-1}}{2\Delta z} = h(T_a - T_N) \tag{6c}$$

for every $(L,y,z) \cup (x,M,z) \cup (x,y,N) \in \mathscr{D}$.

In brief, the heat transfer problem is reduced to solving the system of eqn (4) along with initial condition (2) and boundary conditions (5) and (6).

RESULTS AND DISCUSSION

Previous to the numerical resolution of the problem, it was considered interesting to check precision and computing time of the ADI method against two well differentiated methods: one that applies Z transfer functions (ZTRF) proposed by Salvadori *et al.* (1994) and the other the known analytical solution (EXACT) given by Carslaw & Jaeger (1959) or Luikov (1968) for the case of a parallelepiped with radiation at the surface into a medium. As the latter applies when no variation of ambient temperature occurs, the case studied for this purpose referred to a parallelepiped ($0{\cdot}1 \times 0{\cdot}05 \times 0{\cdot}025$ m) initially at -18°C which was introduced to a constant temperature medium at -8°C. The thermal conductivity value was 1·65 w/m.K, heat capacity of $2{\cdot}59 \times 10^6$ J/m^3.K and surface heat transfer coefficient of 3 w/m^2.K. As ADI method characteristic parameters values of $\Delta x = \Delta y = \Delta z = 3{\cdot}125 \times 10^{-3}$ m and $\Delta\tau = 240$ s were chosen while the first 16 terms of the series were considered in the analytical solution.

Figure 1 shows application of the three methods to yield temperature values in the first hours, computed in node (0,0,0) the product's geometric centre and in (L,M,N), the farthest point from centre.

A full agreement was observed between EXACT and ADI methods.

Computing time valuation of the three methods, i.e. consumed time in each step of calculating temperature in all the domain points with a 386 processor equipped computer, is presented in Fig. 2.

The inferiority of EXACT regarding the other two methods is clear when computing time is assesed. Furthermore, the same computing routine in a 286 processor meant 2–3 times more time while with a 486 processor the time was shortened by a factor of about $4{\cdot}5 \times 10^4$. Therefore it can be concluded that ADI is a fair choice for modelling the phenomenon.

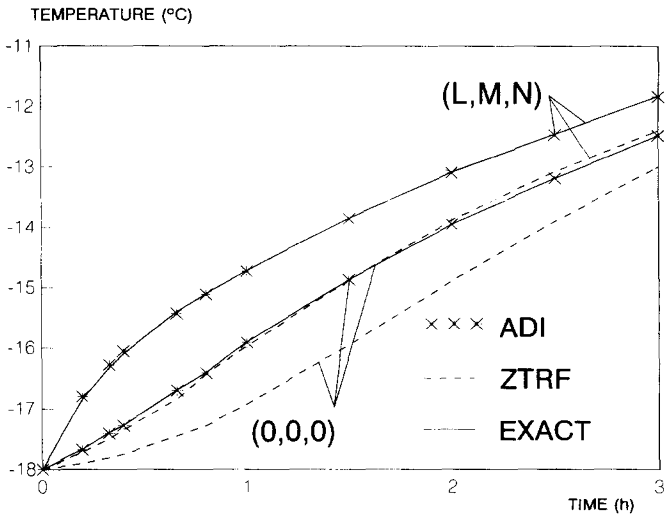

Fig. 1. Performance of the three methods.

When a stored frozen food at a homogeneous temperature undergoes a heating/cooling variation in the storage temperature, the geometric centre and the thermal centre (the product's coldest/warmest point) are coincident. Nevertheless, if after a while the trend is inverted and room temperature begins to decrease/increase, sooner or later a separation between both points occurs and the geometric centre is

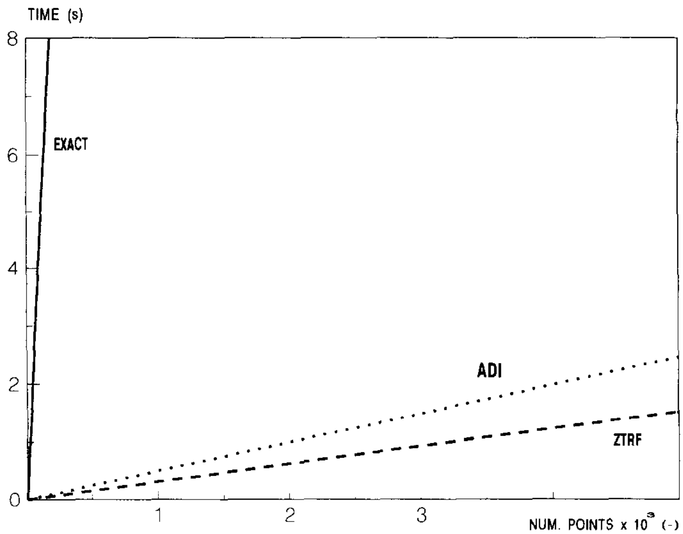

Fig. 2. Computing time of methods.

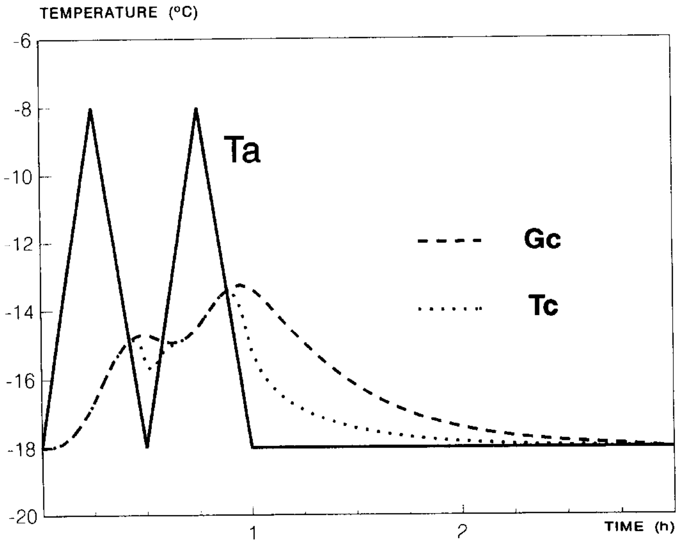

Fig. 3. Example of separation of geometric (Gc) and thermal (Tc) centres.

no longer the coldest/warmest point. Once more, switching to heating/cooling conditions or maintaining unchanged the storage temperature and after a certain time, both points will again tend to come together and so on. A typical example of this occurrence is shown on Fig. 3.

Parameters characterising that eventual separation will have to show two main items: the 'when' and the 'how', that is the initial time the detachment is reported to appear and the maximum value of the temperature difference between the geometric and thermal centres. In that way, a dimensionless time τ^* is defined as the quotient of the first time τ_{ini} when a separation between both points is detected (absolute value of $T_{geom} - T_{ther}$ being $\geq 10^{-4}$), divided by the time τ_{swi} when perturbation in ambient temperature switches for the first time from heating/cooling to cooling/heating

$$\tau^* = \tau_{ini}/\tau_{swi} \tag{7}$$

τ^*, obviously always >1 evaluates the promptness of reaction to an outer inversion: the bigger τ^* is, the later the separation occurs. Also a dimensionless temperature difference δ^* is considered, defined as the quotient between the maximum value δ_{max} of the temperature difference between centres and the span ΔTa_{span} in storage temperature

$$\delta^* = \delta_{max}/\Delta Ta_{span} \tag{8}$$

The above parameters will depend on diverse factors among which the storage temperature variation in time, the surface heat transfer coefficient and the material thermal properties will be hereafter taken into account.

The phenomenon was traced considering the following variations in storage temperature:

S24: sine of 24 h period and 10°C amplitude
S6: sine of 6 h period and 10°C amplitude
S1: sine of 1 h period and 10°C amplitude
T1: step of 1 h and 10°C amplitude
T2: step of 2 h and 10°C amplitude
TTP: double step: 1st h of 10°C and 2nd h of 5°C ampl.
RR: triangular ramp of 2 h and 10°C amplitude
EX: exponential sine of 2 h and 10°C amplitude
sS: semi-sine of 2 h and 10°C amplitude

and always room temperature remaining below the fusion point of the product to avoid phenomena of melting.

In order to avoid confusion in the interpretation of the results, the variations of the storage temperature were grouped (Fig. 4) into three sets attending to pattern similitudes: Set 1 comprising **S24**, **S6** and **S1** curves, Set 2 composed of **T1**, **T2** and **TTP** and Set 3 including **RR**, **EX** and **sS** variations.

The product was considered to be brick shaped ($0{\cdot}1 \times 0{\cdot}05 \times 0{\cdot}025$ m) and being initially uniformly at -18°C.

The values taken into account for the surface heat transfer coefficient ran from 3 to 1500 w/m^2K. Heat capacity values of the material were supposed to be those of a food simile (Tylose), ranking from $1{\cdot}45 \times 10^6$ to $3{\cdot}72 \times 10^6$ J/m^3K which correspond to temperatures of -28°C and -8°C respectively as stated by Sanz *et al.* (1988), and

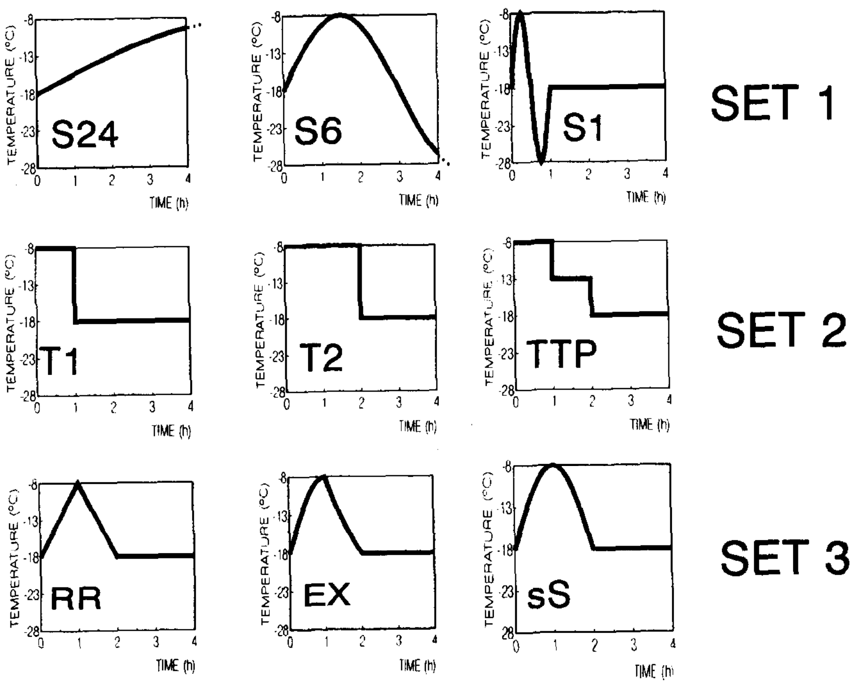

Fig. 4. Storage temperature variations.

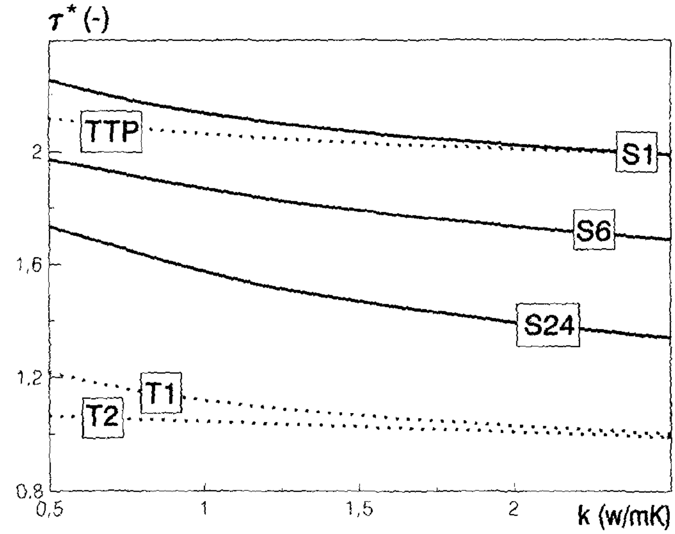

Fig. 5. Thermal conductivity vs. τ^*.

as for thermal conductivity values from 0·5 to 2·5 w/mK were chosen intending to have a widespread scope of frozen foods.

When the influence of thermal conductivity on τ^* is examined, all of the boundary variations considered have a similar behaviour: when k is augmented there is a diminishment in τ^* trending towards a constant value, as it can be seen in Fig. 5. Sine waves show increasing τ^* values with frequencies, i.e. the effect of thermal centre separating from geometric centre is delayed. Curves of Set 3, not shown, behave as **S6** does and those of Set 2 have small incidence on τ^* when k is varied, but if steps **T1** and **T2** are combined into a double step **TTP** the latter brings out much higher values of τ^* than the former. As for the k vs. δ^* relationship appearing in Fig. 6 only one curve from Set 2 (**T2**) and one from Set 3 (**RR**) are shown as set representatives since the remainder behave similarly, the separation δ^* being always bigger in Set 2 than in Set 3. Concerning Set 1 curves, it is worthwhile to emphasize the opposite behaviour attending to their frequency: for increasing values of k, **S24** presents diminishing δ^* values while **S1** shows increasing ones. **S6** performing like **S1** appears to have a maximum value of δ^* at $k \simeq 1{\cdot}6$ W/mK, probably meaning that a compromise has been reached between perturbation lasting time and heat conduction ability.

The variation of heat capacity scarcely influences τ^* values, as indicated by Fig. 7, where only the two curves provoking the highest (**S1**) and the lowest (**T2**) values of dimensionless time of detachment appear. Nevertheless, the influence of C on δ^* shown in Fig. 8 is important and strongly depends on the variation in room temperature. Again, as observed in the k vs. δ^* relationship, sine curves behave in an opposite manner depending on their frequency but now for greater C; lower frequencies imply bigger values of δ^*. Also a maximum value for δ^* is suggested in **S6**. Besides, it is noted that Sets 2 and 3 are very alike and therefore only the extremes of the interval are presented, namely **T2** and **RR**.

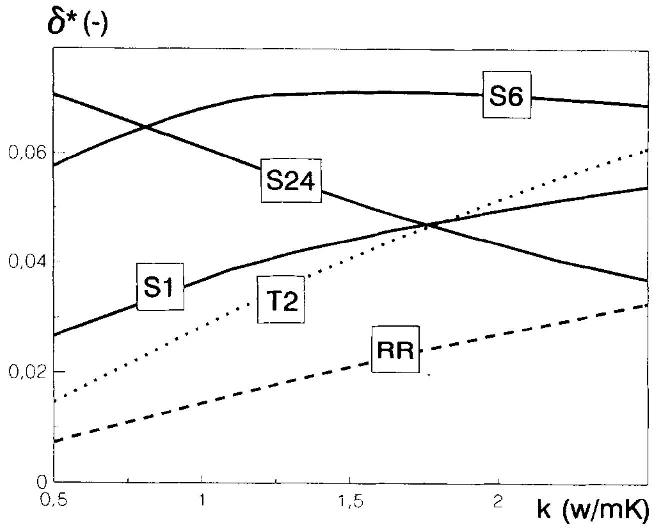

Fig. 6. Thermal conductivity vs. δ^*.

Regarding the influence of diverse surface heat transfer coefficients on detachment time τ^*, it is noted in Fig. 9 that for very small h values, i.e. when convection is not a significant heat transfer mechanism, very important τ^* variations are detected for different boundary condition curves, those of Sets 2 and 3 being especially important. As h is enlarged, and because of the instantaneousness of the phenomenon, the variation becomes unimportant and τ^* gradually trends towards

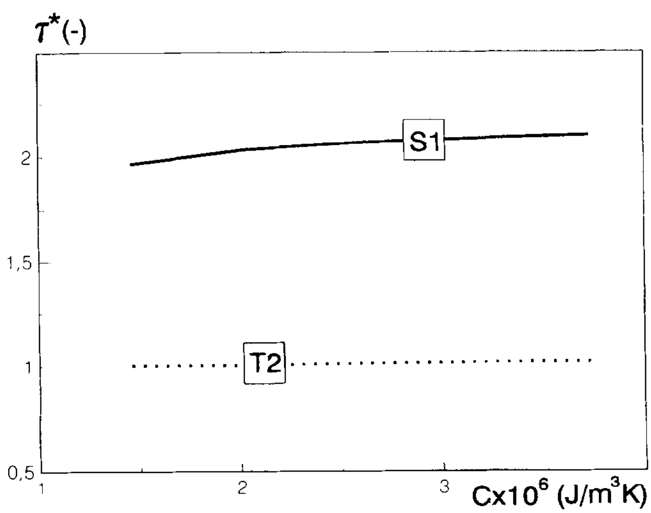

Fig. 7. Heat capacity vs. τ^*.

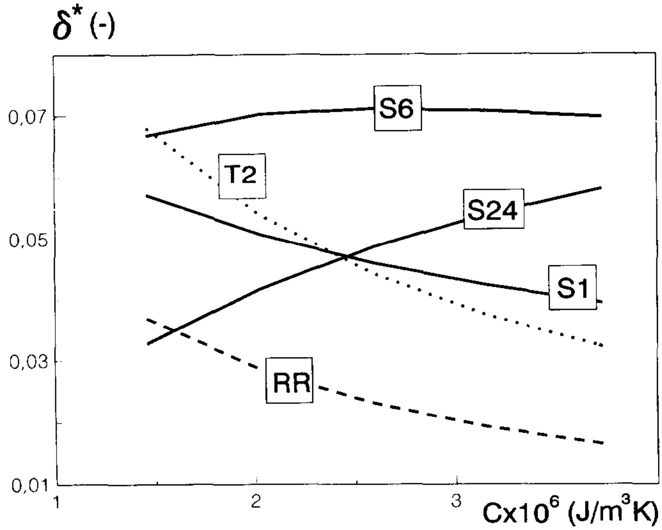

Fig. 8. Heat capacity vs. δ^*.

constant values. Figure 10 features the effect of different storage temperature functions upon the dimensionless maximum temperature difference δ^* between centres. As long as h is maintained approximately below 100 W/m^{2}K, Sets 1 and 3 present fast growing values of δ^*, have a maximum (the biggest in **S1**) and

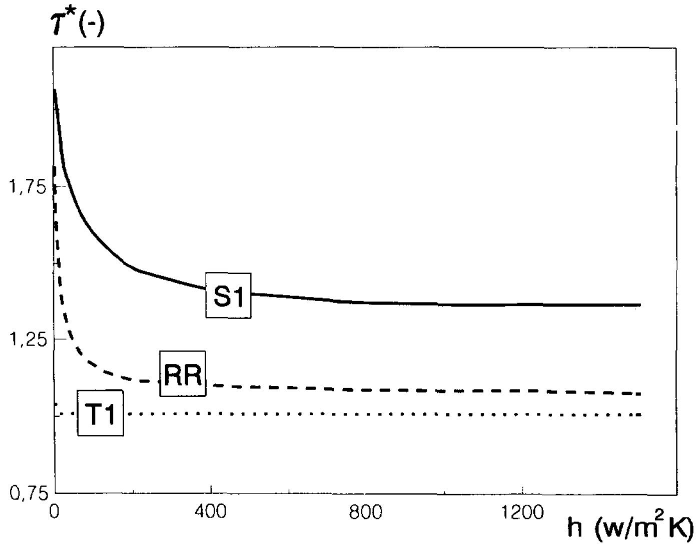

Fig. 9. Surface coefficient vs. τ^*.

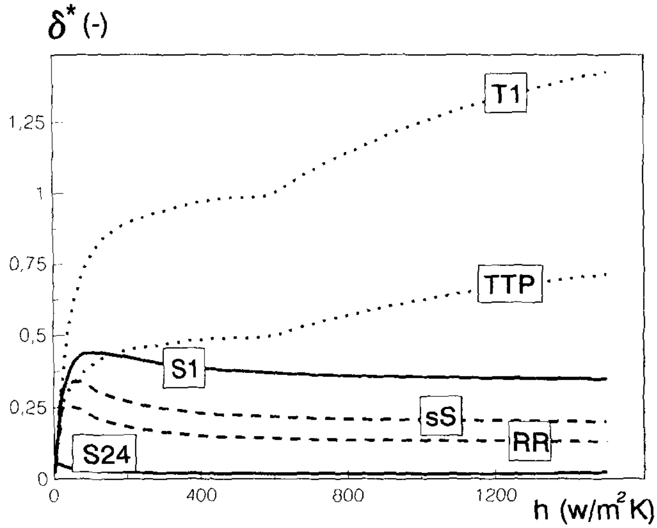

Fig. 10. Surface coefficient vs. δ^*.

afterwards slightly decrease approaching a constant value for very high transfer coefficients. Set 2 in turn makes δ^* to be much more sensitive to h variation; there is no maximum, but an exponential type growth up to around $h = 600$ W/m^{2}K where curvature changes meaning a faster increase in δ^*. This fact is particularly important in **T1** (and in **T2**) when a remarkable surface convection is added to a significant jump in temperature between product and air from the very start of the operation.

CONCLUSIONS

A computer simulation procedure has been developed to deal with the separation occurring between thermal and geometric centres of a brick shaped frozen food, initially at a homogeneous temperature, when storage temperature is submitted to different fluctuations.

Two parameters in association to the causative agent are proposed to characterise the detachment: the time of appearance and the maximum temperature difference reached between both centres.

Several functional forms for room temperature variation have been considered. Also, incidence of thermal properties of the product such as heat capacity and thermal conductivity on the detaching behaviour as well as different surface heat transfer conditions have been analysed.

The procedure herein proposed may be useful in predicting the presence and amount of undesirable temperature gradients in a frozen food while in storage, and inversely in approximating the thermal characterisation of a heterogeneous product behaving as if it were homogeneous.

Further studies on these topics should include the composition of various functional forms for room temperature variation in order to approximate more realistic situations. Besides, redefinition of characterising parameters and/or extension to new ones will have to follow.

REFERENCES

Carslaw, H. S. & Jaeger, J. C. (1959). *Conduction of Heat in Solids*. Clarendon Press, Oxford.

Douglas, J. & Gunn, J.E. (1964). A general formulation of alternating direction methods. Part I. Parabolic and Hyperbolic problems. *Num. Mathematik*, **6**, 428–53.

Hicks, E.W. (1944). Note on the estimation of the effect of diurnal temperature fluctuations on reaction rates in stored foodstuffs and other materials. *J. Counc. Sci. Ind. Res.*, **17**, 111.

Labuza, T.P. (1979). A theoretical comparison of losses in foods under fluctuating temperature sequences. *J. Food Sci.*, **44**, 1162–8.

Luikov, A. V. (1968). *Analytical Heat Diffusion Theory*. Academic Press, New York.

Magnussen, O. M. & Hardarson, V. (1993). Freezing of Mackerel in carton boxes. Heat flow and freezing time. I.I.F.-I.I.R. Commissions B1, B2, D1, D2/3-Palmerston North (New Zealand), pp. 242–8.

Nunes, R. V. & Swartzel, K. R. (1990). Modelling chemical and biochemical changes under sinusoidal temperature fluctuations. *J. Food Eng.*, **11**, 119–32.

Poovarodon, N., Letang, G., Bouvier, J. & Billiard, F. (1993). Influencia del embalaje y fluctuaciones de la temperatura de conservación sobre la calidad de las mercancías alimenticias congeladas, Frío Calor y Aire Acondicionado, **235**, 6–15.

Powers, J. J., Lukaszewicz, W., Wheeler, R. & Dornseifer, T. P. (1965). Chemical and microbial activity rates under square-wave and sinusoidal temperature fluctuations. *J. Food Sci.*, **30**, 520–30.

Rosset, R. Albisu, M. Poumeyrol, G. & Giulani, L. (1988). L'influence des variations de température au cours du stockage. Les qualités microbiologiques et organoleptiques d'un plat cuisiné surgelé. Rev. Gen. Froid. Oct., pp. 513–16.

Salvadori, V. O., Sanz, P. D., Dominguez, M. & Mascheroni, R.H. (1994). Application of z transfer functions to heat or mass transfer problems: their calculation by numerical methods. *J. Food Eng.*, **23**, 293–307.

Sanz, P. D., Domínguez, M. & Mascheroni, R. H. (1988). Predicción de las variaciones de la temperatura en los alimentos congelados sometidos a diferentes condiciones de conservación, mediante la analogía eléctrica con ordenador. In Desarrollo de la Cadena del Frío en Latinoamérica. Tomo I. Buenos Aires, pp. 227–32.

Scott, E. P. & Heldman, D. R. (1990). Simulation of temperature dependent quality deterioration in frozen foods. *J. Food Eng.*, **11**, 43–65.

Singh, R. P. (1978). Prediction of food quality during frozen food storage. *Int. J. Refrig.*, **1** (2) 108–12.

Spieß, W. E. L. (1994). Modificaciones cualitativas de los productos ultracongelados en la cadena del frío. *Frío Calor y Aire Acondicionado*, **247**, 27–39.

Zuritz, C. A. & Singh, R. P. (1985). Modelling temperature fluctuations in stored frozen foods. *Int. J. Refrig.*, **8**, 289–93.

Zuritz, C. A. & Sastry, S. S. (1986). Effect of packaging materials on temperature fluctuations in frozen foods: mathematical model and experimental studies. *J. Food Sci.*, **51** (4), 1050–6.