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Quality Optimization of Hot Filled Pasteurized Fruit Purees: Container Characteristics and Filling Temperatures

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ABSTRACT

A mathematical model was developed to describe the pasteurization, by hot filling, of fruit purees. The model assumed that the puree reaches instantaneously a hot-fill temperature and, after introduced into the container, cooling by conduction takes place. The heat transfer was modelled by a finite differences method. Vitamin C and pectinesterase were used as quality and pasteurization criteria, respectively.

Specific filling temperatures combined with container dimensions are required to achieve a target pasteurization value. However, only some of the adequate conditions offer final products with maximum quality.

Several simulations were carried out to investigate the effect of filling temperature, container shape, type of cooling medium and pasteurization value on final quality retention expressed as vitamin C retention. Using statistical factorial analysis the most important parameters affecting quality were filling temperature and pasteurization value, followed by cooling medium. Shape was not considered significant (p > 0.05). Best quality was achieved with higher hot filling temperatures and small pasteurization values. © *1997 Elsevier Science Limited.*

NOTATION

C	Level of the quality attribute at time t
(C/C_o)	Quality retention
D	Decimal reduction time (min)
Gr	Grashof number (dimensionless)

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h	Surface heat transfer coefficient ($W/(m^2\ K)$)
K	Fruit puree thermal conductivity ($W/(m\ K)$)
k	Container thermal conductivity ($W/(m\ K)$)
l	Container half height (m)
P	Integrated lethality in a container point: pasteurization value (min)
Pr	Prandtl number (dimensionless)
r	Container radius (m)
S	Container shape, l/r ratio (dimensionless)
t	Time (min)
T	Temperature (°C)
U	Overall surface heat transfer coefficient ($W/(m^2\ K)$)
V	Container volume (m^3)
x	Container thickness (m)
y	Container characteristic dimension (m)
z	z-value: number of degrees Celsius required to reduce the D-value by a factor of 10 (°C)
α	Fruit puree thermal diffusivity (m^2/s)
ε	Emissivity of the container (dimensionless)
ρ	Fruit puree density (kg/m^3)
σ	Boltzmann constant ($5.73 \times 10^{-8}\ W/(m^2\ K^4)$)

Subscripts

0	Initial time or time zero
air	Air
ave	Volume average
c	Natural convection
e	Enzyme
F	Refers to hot filling temperature
q	Quality
r	Radiative
refe	Enzyme reference temperature
refq	Quality parameter reference temperature
s	Container surface
T	Total
water	Water
∞	Cooling medium

INTRODUCTION

Fruit purees, besides being consumed directly as desserts or as a complement of cooked meats, such as apple puree, are used as ingredients in various food products: e.g. juices, nectars, jams, ice creams, baby foods, pastry. Several chemical-free processes can be used for its preservation: cooling, freezing, pasteurization, sterilization or combined processes such as pasteurization followed by low temperature storage. Pasteurization is a mild heat treatment where only the vegetative microbial cells

(bacteria, yeasts and moulds) and enzymes are inactivated. The treatment must target the microbial and enzyme inactivation, while maintaining the original organoleptic and nutritive fruit characteristics (Fellows, 1988). The severity of the heat treatment and the resulting shelf-life are determined mostly by the fruit pH (Fellows, 1988). Most parts of the fruits have low pH (<4.6) and therefore existing spores will not grow and will not be a main concern. In these cases, a pasteurization process should be enough for fruit preservation at ambient temperature. Sometimes natural fruit enzymes are more heat resistant than vegetative cells. In these cases the pasteurization process criterion is based upon enzyme inactivation. For instance, the thermal resistance of gram-positive non-spore-forming bacteria and yeast was found to be very low as compared with peroxidase and pectinesterase (Aung & Ross, 1965; Peralta *et al.*, 1973).

The hot fill technique is a simple pasteurization process and can be easily implemented for acid fruit purees. The fruit puree is considered to reach a given hot filling temperature instantaneously and, after filling into the container, cooling by conduction takes place (Sandoval *et al.*, 1994). Given a filling temperature, specific container dimensions are required in order to achieve a target volume average pasteurization value for the most thermal resistant microorganism or spoilage enzyme (Sandoval *et al.*, 1994). Some research work concerning the use of pasteurization by hot filling for fruit purees or pastes has been reported in the literature. Nanjundaswamy *et al.* (1973) determined thermal process conditions for canned mango products. The authors concluded that filling temperature was very important in minimizing process time and ensuring adequate mango isolated yeast and peroxidase thermal inactivation. For 0.57 l 401×411 cans, filling temperatures between 76 and 80°C were required to achieve product stabilization. After filling, during the cooling phase, the cans were sealed and kept inverted for 2-3 minutes for lid 'sterilization'. This procedure was enough to ensure adequate commercial 'sterility'. Although there was no microbial inoculation before the thermal process, the process was industrially validated by analysing final enzyme and microbiological levels. Nath & Ranganna (1983a) determined process requirements and heat transfer characteristics for hot filled guava pulp. For hot fill cool procedures of fruits with a pH value lower than 4.0, the National Canners Association recommends the following process: a filling temperature higher than 85°C, followed by can sealing and 2 min immersion in steam or water at 88°C before cooling. However, the above procedure failed in small Indian canneries, because there was a holding time of 10–30 min between sealing and processing. In this work the authors studied and validated the existing thermal process. Can sizes of 401×411 were used for heat penetration tests. The effect of two different holding times (10 and 30 min), filling temperatures (72–88°C) and corresponding process time on the final pasteurization value (*P*-value) was evaluated. Inoculated pack studies were also carried out to test for commercial sterility. Using Fourier's law analytical solutions to model the heat transfer process, Sandoval *et al.* (1994) predicted the time–temperature relationships during air cooling following the hot fill process for tomato paste in glass jars. Three jar sizes and five filling temperatures were investigated. Hot filling temperatures of at least 94, 92 and 90°C for jar sizes of 0.2, 0.5 and 4 l, respectively, were suggested. These filling temperature–container size combinations ensure product microbial safety. The target microorganism employed was *Bacillus coagulans* and the pasteurization value at 90°C ($P_{90°C}$), for an initial microbial population of 10^5 per jar, was 24.5 min.

No optimization of the hot filling thermal processes, in terms of maximizing final quality retention, was investigated in the previous mentioned works. All the authors focused their attention on the process requirements in order to achieve a required *P*-value for adequate commercial pasteurization. Several pasteurization conditions (filling temperature, container radius and half-height, heating medium conditions, etc.) can achieve the same pasteurization value required for a specific fruit puree preservation. However, only one set of thermal treatment conditions gives maximum quality retention of the fruit pulp. The idea of minimizing quality losses during thermal processing of foods is not new and several quality optimization studies are available in the literature in the field of sterilization of prepackaged foods (Holdsworth, 1985; Silva *et al.*, 1994). The optimization is possible because the thermal degradation kinetics of quality factors such as colour, flavour, texture or nutrients is much less temperature sensitive than the destruction of microorganisms or enzymes (Teixeira *et al.*, 1969; Lund, 1977; Holdsworth, 1985). Nevertheless, few food-applied quality optimization studies were previously reported, except for a sterilization study with white beans in brine (Van Loey *et al.*, 1993) and another with canned tuna (Banga *et al.*, 1993). Furthermore, no quality optimization study with fruit puree/juice was found in the literature. The same happens with optimization of a hot filling process in general.

The objectives of this work were as follows:

(1) The development of a mathematical model to describe the pasteurization of a food product during the cooling phase of a hot fill process; experimental validation of predicted time–temperature profiles during the cooling phase.
(2) To study the effect of filling temperature, cooling medium (overall heat transfer coefficient), *P*-value and container shape on the container size required and corresponding achieved final quality retention.

MODELLING AND SIMULATION

In this section the mathematical model developed and used in all the simulations is described. Only the cooling phase of the hot fill pasteurization was modelled. The pasteurization achieved during cooling was assumed to be much larger than the pasteurization obtained during the puree heating and filling processes. The error committed with this assumption will never be dangerous in terms of product pasteurization and consumer safety. The product would probably be slightly overprocessed and never the contrary. Holding time was considered zero in all the simulations, and therefore, a specific pasteurization value was achieved based on adequate hot filling temperature–container size combination, instead of temperature–holding time. Heat transfer by conduction was predicted by a finite differences mathematical method. The constituents used for pasteurization criterion and quality evaluation were pectinesterase and vitamin C, respectively. All the simulations were carried out using the thermal characteristics of cupuaçu fruit (*Theobroma grandiflorum*), an Amazon high valuable crop (Table 4). This fruit has an average pH of 3.4, 10.5–10.8 °Brix and vitamin C content ranges from 14.43 to 28.32 mg/100 g (Barbosa *et al.*, 1978; Chaar, 1980; Oliveira, 1981; IBGE, 1981; Miranda, 1989).

A factorial design analysis was done to evaluate the main effects of different processing variables on quality retention and required container volume. The processing variables studied were: filling temperature (T_F); type of cooling medium

(water vs. air), i.e., overall heat transfer coefficient (U); volume average pasteurization value (P_{ave}) and container shape (S).

Heat transfer model

A PASCAL computer program was developed to model the pasteurization by an hot fill process. A finite cylindrical geometry was assumed as well as constant thermophysical properties (food thermal conductivity, thermal diffusivity and density). Heat transfer by conduction during the cooling by air or water was described by a finite differences method using non-capacitance surface nodes (Chau & Snyder, 1988; Chau & Gaffney, 1990; Silva, 1993). The overall surface heat transfer coefficient, U, which was determined using empirical equations (Holman, 1990), includes the resistances of the container wall, x/k, external radiation, h_r, and external natural convection, h_c (eqns 1, 2, and 3, 4, 5 in Table 1):

$$U = \frac{1}{\dfrac{1}{h_c + h_r} + \dfrac{x}{k}} \tag{1}$$

where x and k are the container thickness and thermal conductivity, respectively, and

$$h_r = \varepsilon \times \sigma \times \frac{T_s^4 - T_\infty^4}{T_s - T_\infty} \tag{2}$$

where ε is the container emissivity, σ the Boltzmann constant (5.73×10^{-8} W/(m^2 K^4)), and T_s and T_∞ the container surface and cooling medium temperatures, respectively. The radiation and container wall resistances are much smaller than the external natural convection resistance. The external natural convection coefficient

TABLE 1
Empirical Equations for Prediction of Natural Convection Surface Heat Transfer Coefficients in Vertical Cylindrical Walls (Holman, 1990)

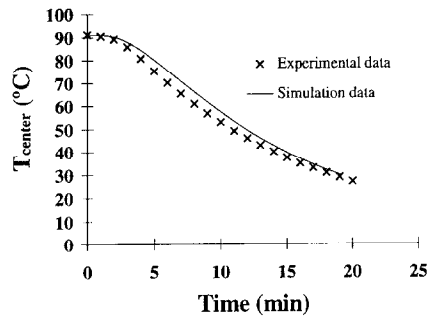| Cooling medium	Flow	$Gr \times Pr$	h_c (W/(m^2.K))	
Air	Laminar	$10^4 - 10^9$	$1.42 \times \left(\dfrac{T_s - T_\infty}{y} \right)^{\frac{1}{4}}$	(3)
Water	Laminar	$10^4 - 10^9$	$203 \times \left(\dfrac{T_s - T_\infty}{y} \right)^{\frac{1}{4}}$	(4)
Water	Turbulent	$> 10^9$	$315 \times (y)^{\frac{1}{3}} \times (T_s - T_\infty)^{\frac{2}{3}}$	(5)

Fig. 1. Temperature at the container geometric centre as a function of time during the water cooling of cupuaçu in tin plate cans ($T_0 = 91°C$, $T_{water} = 11°C$, $r = 3.6$ cm, $l = 1.75$ cm).

varies with the type of cooling medium, type of flow, cylinder characteristic dimension (height or diameter), y, and temperature difference between the container surface and environmental temperature (eqns 3, 4 and 5 in Table 1). During the cooling process, temperature gradient, $T_s - T_\infty$, decreases because the container surface temperature decreases; therefore, h_c also decreases and so does the overall surface heat transfer coefficient, U.

The conduction heat transfer equations and their solution using a finite differences method have been described in other previously published works (Chau & Snyder, 1988; Chau & Gaffney, 1990; Silva, 1993).

Cupuaçu (*Theobroma grandiflorum*), a tropical fruit from the Amazon, was used for the experimental validation of the predicted time–temperature history. Two experiments involving water and air cooling were carried out (Figs 1 and 2). Each experimental data curve was obtained using a thermocouple inserted at the container geometric centre coupled to a data acquisition system.
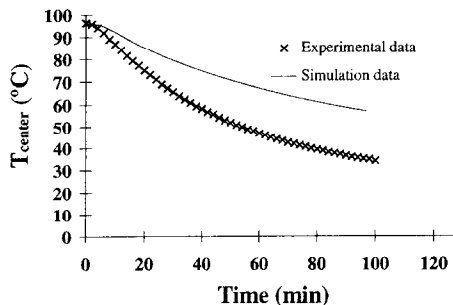

Fig. 2. Temperature at the container geometric centre as a function of time during the air cooling of cupuaçu in tin plate cans ($T_0 = 96°C$, $T_{air} = 21°C$, $r = 3.6$ cm, $l = 1.75$ cm).

TABLE 2
Fruit Characteristics and Pectinesterase (PE) Inactivation Kinetic Data

Fruit	Medium	pH	Soluble solids (°Brix)	$D_{85°C}$ (min)	z_e (°C)	T range (°C)	Reference
Papaya	Puree	3.5	7–9	4.8	14.8	75–85	Argáiz (1994)
		3.8		5.7	14.7		
		4.0		7.2	14.2		
Papaya	Acidified pulp	4.0	10–12	3.9	15.0	82–102	Nath & Ranganna (1981)
Papaya	Nectar	3.8	14	5.0	15.1	75–85	Argáiz (1994)
Mandarin orange	Juice	3.6	12	2.2	11.4	82–94	Nath & Ranganna (1977)
		4.0	12	3.6	10.1		

Pasteurization target and quality parameter: kinetics used for the simulations

Most parts of the fruits are acid (pH < 4.6), and therefore microbial spores do not grow. Due to this fact, thermal processes are designed based on the inactivation of the most thermal resistant enzyme. Examples of these enzymes are peroxidase and pectinesterase (Dastur *et al.*, 1968; Nanjundaswamy *et al.*, 1973; Nath & Ranganna, 1977, 1980, 1981, 1983a, 1983b). If not inactivated, these enzymes have deterioration effects on the fruit quality. Pectinesterase (PE) is an enzyme often present in several tropical fruits – guava, papaya, mango, grapefruit, orange, mandarin (Table 2) – and can be used as pasteurization criterion. Several studies have already been done to determine PE thermal degradation kinetics in different fruits. All the authors used first-order inactivation kinetic models (Table 2).

In all the simulations carried out in this study, the PE kinetic data of Argáiz (1994) in papaya puree at pH 3.5 was used once the pH and soluble solids of this fruit are similar to those of cupuaçu fruit puree. All the simulations were done using cupuaçu thermal properties (Table 4).

During cooling, the pasteurization value (*P*-value) at a single point of the container was computed using eqn (6):

$$P = \int_0^{t_T} 10^{\frac{T - T_{refe}}{z_e}} \, \partial t \qquad (6)$$

To use this equation, enzyme inactivation kinetic parameters are necessary: T_{refe}, reference temperature for the enzyme; and z_e-value for the enzyme. Temperatures lower than 55°C were considered to have negligible lethality and were not included for pasteurization value calculations.

The quality indicator used for process optimization was vitamin C. This very heat-labile vitamin is an important nutritional component present in several fruits. Table

TABLE 3
Fruit Characteristics and Vitamin C Inactivation Kinetic Data

Fruit	Medium	pH	Soluble solids (°Brix)	$D_{85°C}$ (min)	z_q (°C)	T range (°C)	Reference
Grapefruit	Juice	3.1	11.8	296	124	61–96	Saguy et al. (1978)
Mandarin (Sierra)	Juice	–	11.1	406	47	20–92	Alvarado & Viteri (1989)
Mandarin (Costa)	Juice	–	13.4	542	58	20–92	Alvarado & Viteri (1989)
Grapefruit	Juice	–	11.2	829	44	20–92	Alvarado & Viteri (1989)
Lemon (Sierra)	Juice	–	7.6	1147	72	20–92	Alvarado & Viteri (1989)
Lime	Juice	–	6.3	741	44	20–92	Alvarado & Viteri (1989)

3 shows inactivation kinetic studies of vitamin C in several fruits. First-order kinetics modelled adequately the inactivation kinetics of vitamin C in all the reported work.

During the pasteurization process, quality retention (C/C_o) at a single point in the container can be calculated using eqn (7):

$$\frac{C}{C_0} = 10^{\left(\frac{-1}{D_{\text{refq}}} \int_0^{t_T} 10^{\frac{T - T_{\text{refq}}}{z_q}} \partial t\right)} \qquad (7)$$

where Trefq is the reference temperature for vitamin C thermal inactivation, and z_q and Drefq are the z-value and decimal reduction time at the reference temperature for the quality parameter (vitamin C), respectively. In this work the kinetic quality parameters chosen refer to vitamin C kinetics in mandarin juice with 11.1°Brix.

Simulation data

Table 4 presents the cupuaçu fruit properties and kinetic data used in all computer simulations. The cupuaçu thermal diffusivity was determined experimentally using the Dickerson (1965) method. The pasteurization value, (P), and vitamin C retention, (C/C_0), can be determined at the container centre, surface or in terms of volume average. Usually the container's coldest point is the point used for P-value calculation. In this work the cooling phase is being modelled and therefore under-processing would occur when the container surface is chosen, whereas overprocessing would occur if the centre is chosen. This is the reason why a target volume average pasteurization value was chosen (eqn 8) (Sandoval et al., 1994). Once vitamin C is established as a nutritional quality indicator, the overall quality retention (Silva et al., 1992) can also be calculated (eqn 9):

TABLE 4
Input Data for Simulations

Cupuaçu properties/kinetic data		Source
K	0.539 W/(m.°C)	Empirical equations (Sweat, 1986)
ρ	1031 (± 0.003) kg/m^3	Experimentally determined, picnometer
α	1.671 (± 0.124) $\times 10^{-7}$m^2/s	Experimentally determined (Dickerson, 1965)
T_{refc}	85°C	Pectinesterase inactivation in papaya puree, pH = 3.5
D_{refc}	4.8 min	(Argáiz, 1994)
z_c	14.8°C	
T_{refq}	85°C	Vitamin C deterioration in mandarin juice, 11.10°Brix
D_{refq}	406 min	(Alvarado & Viteri, 1989)
z_q	47°C	

$$P_{ave} = \frac{1}{V_T} \int_0^{V_T} P\, \partial V \tag{8}$$

$$\left(\frac{C}{C_0}\right)_{ave} = \frac{1}{V_T} \int_0^{V_T} \frac{C}{C_0}\, \partial V \tag{9}$$

where V is the container volume.

Heat transfer characteristics of tin plate cans with cupuaçu puree were used in all the computer simulations. Overall surface heat transfer coefficients were recalculated during the simulated cooling process (eqns 1 and 2, and 3, 4, 5 in Table 1) and ranged between 3 and 50 W/(m^2 K) for air cooling and 92 and 1000 W/(m^2 K) for water cooling, both at 20°C.

Factorial simulation design

In order to study effectively linear and quadratic effects of four different processing variables on the final volume average quality retention of the product as well as the container volume required, a modified factorial design and analysis were performed (Box & Behnken, 1960; Box *et al.*, 1978). Statistical software, Statgraphics (Version 5), was used for analysis. Three-level factor design was carried out for filling temperature (T_F = 70, 90, 110°C), P-value (P_{ave} = 5, 10, 15 min) and container shape ($S = l/r = 0.2$, 1.0, 2.0). The water cooling versus air cooling variable, which corresponds to different U values, was studied at two levels. Values of 26 and 546 W/(m^2 K)) were the average of U for air and water free convection cooling, respectively. The values for filling temperature and container shape were chosen from within the practical range. In commercial canning of fruit products a P-value between two decimal reductions, 2D, and 3D is recommended (Nath & Ranganna, 1977, 1980, 1981, 1983b). Consequently, P-values of 10 and 15 min, which correspond approximately to 2D and 3D respectively, for PE inactivation were tested in

the computer simulations. A total of 54 computer simulations were conducted: 27 for water cooling and the other 27 for air cooling. For every simulation, a certain container volume is required, for a specific filling temperature, in order to achieve a given volume average P-value. Each set of pasteurization conditions results in a specific product quality. Container volume and product quality retention responses are directly related and cannot be studied separately.

RESULTS AND DISCUSSION

Experimental validation of the predicted time–temperature history

Two experiments involving water and air cooling were carried out for the experimental validation of the predicted time–temperature history in the can centre. Cupuaçu pulp was canned using tin plate cans with 3.6 cm radius and 1.75 cm half-height. The experiment of cooling with water at 11°C is shown in Fig. 1. The hot-filling temperature was 91°C and the container geometric centre reached 30°C after approximately 20 min. For cooling with air at 21°C (Fig. 2) approximately 120 min were necessary to reach 30°C at the container centre. The computer program temperature predictions were successfully validated for water cooling. On the other hand, average differences, between experimental and predicted temperatures, of approximately 15°C were observed for air cooling. Hence, it was concluded that the empirical equations used for surface heat transfer coefficient prediction, during air cooling, were not very accurate.

Simulation results

A total of 54 simulations were conducted to evaluate the effect of four different processing variables on product (cupuaçu) final quality. Vitamin C retention was the quality factor predicted by the computer simulations. Specific pasteurization conditions (T_F, P_{ave}, U, S) were tested in each computer simulation case study and a certain container volume (V) is required to achieve the target volume average P-value. For each case, volume average quality retention was computed. When using the same set of conditions (T_F, P_{ave}, S), the $(C/C_0)_{ave}$ is slightly lower for air cooling than water cooling. Table 5 shows the range of container volumes and quality

TABLE 5
Range of Volume and Quality Retention Values Obtained with the Simulations

Cooling medium at 20°C		Air		Water	
Simulation conditions (input)	T_F (°C)	110	70	110	70
	P_{ave} (min)	5	15	5	15
	S	0.2	0.2	1.0	0.2
Predicted/calculated Results (output)	V (l)	6.9×10^{-5}	68.4	3.85×10^{-3}	755
	$(C/C_0)_{ave}$	0.992	0.198	0.995	0.268

retention obtained in all different simulations. Volumes can go up to 755 l if water cooling is used. Handschuh (1995) reports that transportation of juices, purees or concentrates from South America to Europe can be done in soft/rigid tanks with volumes up to 1000 l. Larger filling temperatures (110°C) and smaller P-values (5 min) require very small container sizes ($\leq$ 15.3 ml) and give the product best final quality (> 0.99). For air cooling, filling temperatures of 110°C require container volumes smaller than 0.535 ml. Those volumes are not commercially feasible. There-fore for cupuaçu fruit and using the kinetics mentioned before, filling temperatures closer to 110°C should not be used, to avoid overprocessing.

In Fig. 3, the Pareto chart shows the standardized effects of different parameters on product volume average quality retention, $(C/C_0)_{ave}$. An effect that exceeds the vertical line (critical t-value, $\alpha = 0.05$) may be considered significant. The most important factors in decreasing order are T_F and P_{ave}, followed by U. Quality retention is not a linear function of T_F and P_{ave} because $(T_F)^2$ and $(P_{ave})^2$ also have a significant effect on $(C/C_0)_{ave}$. The interaction effect of T_F and P_{ave}, given by $T_F \times P_{ave}$, arises from a difference in $(C/C_0)_{ave}$ sensitivity to P_{ave} changes for dif-ferent filling temperatures. Container shape, S, was not significant for the final quality within the ranges of variable values simulated. Figure 4 shows the predicted response (cupuaçu volume average vitamin C retention) surface as a function of the main variables (filling temperature and pasteurization value), for water cooling at 20°C. A total of 27 simulation results were used for the surface prediction. This figure reinforces the conclusions taken from the Pareto chart (Fig. 3). Final quality is greatly improved when using higher filling temperatures. Minimum pasteurization values also give better quality, although temperature is the major variable for maximum quality retention. The quadratic effect of temperature $(T_F)^2$ within the
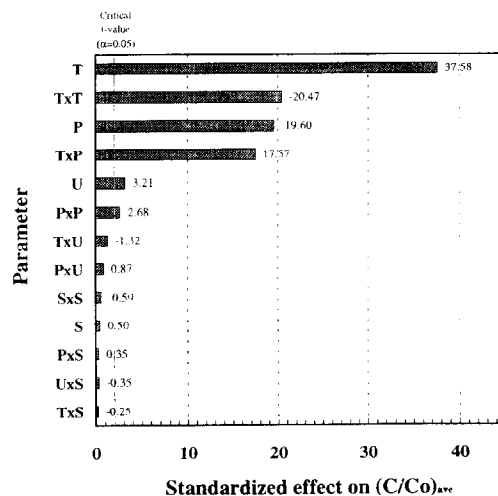

Fig. 3. Pareto chart for the evaluation of several parameter standardized effects on product volume average quality retention ($T = T_F$, $P = P_{ave}$).
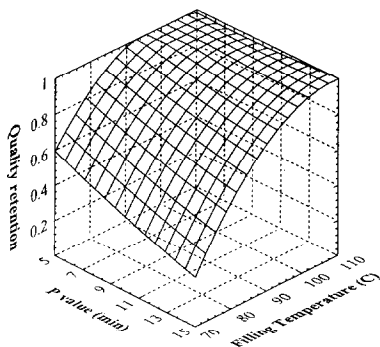
Fig. 4. Effect of filling temperature and pasteurization value on the predicted response surface $(C/C_0)_{ave}$, for water cooling at 20°C.

P_{ave} range is apparent from the surface shape shown in Fig. 4. The interaction effect of temperature and pasteurization value $(T_F \times P_{ave})$ is also clear because at 70°C quality is much more sensitive to P_{ave} than at 110°C.

Since no real kinetic data for vitamin C or PE inactivation in cupuaçu is available, an experimental validation of the conclusions drawn from this theoretical study would be very important. This subject will be object of further work in this research area.

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